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线性代数

主编 / 刘木伙

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内 容 简 介

本书共 6 章，前三章以求线性方程组的解为脉络，第 1 章主要介绍行列式；第 2 章通过线性方程组的同解变换引入矩阵定义，并从矩阵方程的求解出发引出逆矩阵；第 3 章从一般线性方程组的求解出发引入向量线性关系；第 4 章从生物繁衍实例出发引入矩阵的对角化问题和对角化方法；第 5 章介绍特殊矩阵即实对称矩阵的对角化问题，引入二次型知识的介绍；第 6 章主要介绍线性代数中常用的数学软件处理方法，包括矩阵、行列式和方程组求解等的 MATLAB 软件命令.

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（五）正文：

1. 面上项目、地区科学基金项目：如果《批准通知》所附“项目评审意见及修改意见表”中“修改意见”栏目没有修改要求的，只需选择“研究内容和研究目标按照申请书执行”即可；如果《批准通知》中上述栏目明确要求调整研究期限或研究内容等的，须选择“根据研究方案修改意见更改”并填报相关修改内容。

2. 重点项目、重点国际（地区）合作研究项目、重大项目、国家重大科研仪器研制项目、原创探索计划项目：须选择“根据研究方案修改意见更改”，根据《批准通知》的要求填写研究（研制）内容，不得自行降低、更改研究目标（或仪器研制的技术性能与主要技术指标、验收技术指标等）或缩减研究（研制）内容。此外，还要突出以下几点：

（1）研究的难点和在实施过程中可能遇到的问题（或仪器研制风险），拟采用的研究（研制）方案和技术路线；

（2）项目主要参与者分工，合作研究单位（如有）之间的关系与分工，重大项目还需说明课题之间的关联；

（3）详细的年度研究（研制）计划。

3. 创新研究群体项目：须选择“根据研究方案修改意见更改”，按下列提纲撰写：

（1）研究方向；

（2）结合国内外研究现状，说明研究工作的学术思想和科学意义（限两个页面）；

（3）研究内容、研究方案及预期目标（限两个页面）；

（4）年度研究计划；

（5）研究队伍的组成情况。

4. 基础科学中心项目：须选择“根据研究方案修改意见更改”，根据《批准通知》的要求和现场考察专家组的意见和建议，进一步完善并细化研究计划，按下列提纲撰写：

（1）五年拟开展的研究工作（包括主要研究方向、关键科学问题与研究内容）；

（2）研究方案（包括骨干成员之间的分工及合作方式、学科交叉融合研究计划等）；

（3）年度研究计划；

（4）五年预期目标和可能取得的重大突破等；

（5）研究队伍的组成情况。

5. 对于其他类型项目，参照面上项目的方式进行选择和填写。

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项目摘要

中文摘要：

图谱理论是组合数学与代数图论的一个重要课题，本课题拟综合运用组合工具、结构分析与矩阵理论方法，主要围绕以下两类问题展开研究:(1)图结构的谱刻画；(2)依图谱对图进行分类。这两类问题都与图的结构有密切联系，受到广泛的关注与研究。本课题研究的重点和目标如下：在图坚韧度的谱刻画方面，课题组将尝试解决与哈密顿圈谱刻画相关的Krivelevich-Sudakov猜想和Gu猜想，并改进与图坚韧度谱刻画相关的Haemers猜想的已有研究结果；在图的划分及其谱刻画方面，课题组将尝试引入图谱为工具来研究图的划分问题，并改进与高连通图结构相关的Thomassen猜想的已有研究结果；在Hoffman问题的研究中，课题组将尝试确定所有第二大邻接特征值不大于1的无爪图或正则图，并改进该领域的一些经典结论。本课题的开展将为图谱理论和图的划分的研究提供更有成效的方法和工具，并进一步揭示图谱与图的结构之间的内部联系。

Abstract：

Graph Spectrum is an important topic of Combinatorics and Algebraic Graph Theory. In this project,we shall apply combinatorial tools,structural analysis and Matrix theory to investigate the following two types of problems:(1)the spectral characterization of graph structure;(2)classifying graphs according to their spectra.These two types of problems are closely related with graph structure,and have attracted much attentions and interests.This project aims on the following targets:In the study of spectral characterization of graph toughness,the research group will try to solve the Krivelevich-Sudakov Conjecture and Gu Conjecture,which both confirm the existence of a Hamilton cycle.And try to improve the known results on the Haemers Conjecture,which is related with spectral characterization of graph toughness;In the research of graph partition and its spectral characterization,we shall try to employ graph spectrum to study graph partition, and hope to improve related results on the Thomassen Conjecture of highly connected graphs;On the Hoffman Problem,the research group will try to improve some classic conclusions by determining all these claw-free graphs or regular graphs,whose second adjacency eigenvalues do not exceed 1.The progress of this project will provide more effective methods and tools to the research of graph spectrum theory and graph partition,and reveal the close relationship between the spectra and structures of graphs.

关键词(用分号分开)：图谱；图的划分；图谱的确定性；图的谱半径；特征值

Keywords(用分号分开)： Graph spectrum; Graph partition; Determined by graph spectrum; Spectral radius of graph; Eigenvalues

项目组主要成员

编号	姓名	出生年月	性别	职称	学位	单位名称	电话	证件号码	项目分工	每年工作时间（月）
1	刘木伙	1981.03	男	副教授	博士	华南农业大学	020-85285393	440106198103044017	项目负责人	8
2	单海英	1973.05	男	教授	博士	同济大学	13564007288	310110197305103653	哈密顿圈的谱刻画	4
3	魏福义	1964.01	男	教授	硕士	华南农业大学	13022065535	140103196401286314	高连通图的结构	4
4	林文水	1979.10	男	讲师	博士	厦门大学	13606012000	350524197910202032	图坚韧度的谱刻画	3
5	李倩	1978.08	女	讲师	硕士	华南农业大学	13533065316	370631197808300528	图的划分的谱刻画	6
6	李凤	1980.08	女	讲师	硕士	华南农业大学	13450205625	510129198008253526	第二大特征值问题	6
7	朱艳丽	1979.12	女	讲师	硕士	华南农业大学	13560479406	440106197912134026	第二大特征值问题	6

总人数	高级	中级	初级	博士后	博士生	硕士生
13	3	4	0	0	2	4

国家自然科学基金预算制项目预算表

项目批准号：12271182　　项目负责人：刘木伙　　金额单位：万元

序号	科目名称	金额
1	一、基金资助项目直接费用合计	46.0000
2	1、 设备费	0.0000
3	其中：设备购置费	0.0000
4	2、 业务费	31.0000
5	3、 劳务费	15.0000
6	二、 其他来源资金	0.0000
7	三、 合计	46.0000

注：请按照项目研究实际需要合理填写各科目预算金额。

预算说明书

（请按《国家自然科学基金项目资金预算表编制说明》中的要求，对各项支出的主要用途和测算理由及合作研究外拨资金、单价≥10万元的设备费等内容进行详细说明，可根据需要另加附页。）

本课题下达的科研直接经费 46 万，将外拨合作单位同济大学和厦门大学**各 12 万**，主要支出计划如下：

1. **设备费：** 无

   其中：设备购置费 无

2. **业务费 31 万，支出计划如下：**

(1) **国内学术会议费 12 万：**

课题组成员计划四年内参加国内学术会议共 24 人次，每人每次会议(按 4 天计算)的路费 0.27 万、会议注册费 0.08 万、住宿费 0.15 万等共 0.5 万，四年共 12 万；

(2) **市内学术交流费 2.5 万：**

用于课题组成员与市内同行进行学术交流。预计上海课题组成员每月 0.025 万市内交通费，广州课题组成员每月约 0.0375 万市内交通费，每个月共约 0.0625 万市内交通费，每年按 10 个月计算约 0.625 万，四年共 2.5 万；

(3) **国内学术交流费 5.5 万：**

用于到国内高校进行学术访问的费用，预计四年内共学术访问 11 人次，每人每次学术访问(按 4 天计算)的路费 0.3 万、住宿费和伙食费 0.05*4=0.2 万等共 0.5 万，四年共 5.5 万；

(4) **国际学术交流费 5 万:**

申请人计划到意大利那不勒斯费德里克二世大学和塞尔维亚贝尔格莱德大学进行学术交流各一次，每次(按 4 天计算)路费 1.2 万、住宿费和伙食费 0.1*4=0.4 万、公杂费和签证费 0.4 万等共 2 万，两次共 4 万；

此外，申请人计划邀请美国西弗吉尼亚大学的赖虹建教授来华南农业大学进行学术交流与科研指导一次，预计路费和住宿费等共 1 万元；

(5) **论文版面费和审稿费 3.2 万：**每年约 0.8 万，四年共 3.2 万；

(6) **图书资料费 2.4 万：**每年约 0.6 万，四年共 2.4 万；

(7) **科技查新和论文检索费 0.4 万：**每年约 0.1 万，四年共 0.4 万。

3. 劳务费 15 万，支出计划如下：

(1) **研究生劳务费 10.8 万：**

主要用于支付在校研究生处理文件、收集整理资料、校对论文等劳务费用，按平均每年 6 人计算，每人每月 0.05 万，每人每年工作 9 个月，每年共需 0.05*9*6=2.7 万研究生劳务费，四年共 10.8 万；

(2) **专家咨询费 4.2 万：**

计划四年内邀请 21 名专家学者来学校进行学术交流与科研指导，每人的专家咨询费约 0.2 万，四年共 0.2*21=4.2 万。

外拨合作单位同济大学 12 万科研经费，支出计划如下：

1. 业务费 7.6 万，支出计划如下：

(1) **国内学术会议费 3 万：**

四年内参加国内学术会议 6 人次，每人每次会议预算约 0.5 万，四年共 3 万；

(2) **市内学术交流费 1 万：**

用于市内学术交流的交通费用，每年约需 0.25 万，四年共 1 万；

(3) **国内学术交流费 1.5 万：**

用于国内学术访问的费用，预计四年内共学术访问 3 次，每次学术访问预算约 0.5 万，3 次共 1.5 万；

(4) **论文版面费和审稿费 0.4 万：**每年约 0.1 万，四年共 0.4 万；

(5) **图书资料费 1.5 万：**每年约 0.375 万，四年共 1.5 万；

(6) **科技查新和论文检索费 0.2 万：**每年约 0.05 万，四年共 0.2 万。

2. 劳务费 4.4 万，支出计划如下：

(1) **研究生劳务费 3.6 万：**

主要用于支付在校研究生处理文件、收集整理资料、校对论文等劳务费用，按平均每年 2 人计算，每人每月 0.05 万，每人每年工作 9 个月，每年共需 0.05*9*2=0.9 万研究生劳务费，四年共 3.6 万；

(2) **专家咨询费 0.8 万：**

计划四年内邀请 4 名专家学者来学校进行学术交流与科研指导，每人的专家咨询费约 0.2 万，四年共 0.2*4=0.8 万。

外拨合作单位厦门大学 12 万科研经费，支出计划如下：

1. 业务费 6.8 万，支出计划如下：

(1) **国内学术会议费 4 万：**

四年内参加国内学术会议 8 人次，每人每次会议预算约 0.5 万，四年共 4 万；

(2) **国内学术交流费 2 万：**

用于国内学术访问的费用，预计四年内共学术访问 4 次，每次学术访问预算约 0.5 万，4 次共 2 万；

(3) **论文版面费和审稿费 0.8 万：**每年约 0.2 万，四年共 0.8 万；

2. 劳务费 5.2 万，支出计划如下：

(1) **研究生劳务费 3.6 万：**

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(2) **专家咨询费 1.6 万：**

计划四年内邀请 8 名专家学者来学校进行学术交流与科研指导，每人的专家咨询费约 0.2 万，四年共 0.2*8=1.6 万。

报告正文

研究内容和研究目标按照申请书执行。

国家自然科学基金项目负责人、依托单位承诺书

国家自然科学基金项目负责人承诺书

本人郑重承诺：我接受国家自然科学基金的资助，严格遵守中共中央办公厅、国务院办公厅《关于进一步加强科研诚信建设的若干意见》《关于进一步弘扬科学家精神加强作风和学风建设的意见》《关于加强科技伦理治理的意见》等规定，及国家自然科学基金委员会关于资助项目管理、项目资金管理等各项规章，在《计划书》填写及项目执行过程中：

（一）按照《批准通知》《国家自然科学基金资助项目计划书填报说明》的要求填写《计划书》，未自行降低、更改目标任务或约定要求，或缩减研究（研制）内容；

（二）树立“红线”意识，严格履行科研合同义务，按照《计划书》负责实施本项目（批准号：12271182），切实保证研究工作时间，按时报送有关材料，及时报告重大情况变动，不违规将科研任务转包、分包他人，不以项目实施周期外或不相关成果充抵交差；

（三）遵守科研诚信、科技伦理规范和学术道德，认真开展研究工作，对资助项目发表的论著和取得的研究成果按规定进行标注，不在非本项目资助的成果或其他无关成果上标注本项目批准号，反对无实质学术贡献者“挂名”，不在成果署名、知识产权归属等方面侵占他人合法权益，并如实报告本人及项目组成员发生的违背科研诚信要求的任何行为；

（四）尊重科研规律，弘扬科学家精神，严谨求实，追求卓越，反对浮夸浮躁、投机取巧，不人为夸大学术或技术价值，不传播未经科学验证的现象和观点；

（五）将项目资金全部用于与本项目研究工作相关的支出，并结合科研活动需要，科学合理安排项目资金支出进度；

（六）做好项目组成员的教育和管理，确保遵守以上相关要求。

如违背上述承诺，本人愿接受国家自然科学基金委员会和相关部门做出的各项处理决定。

项目负责人（签字）：刘木依

2022年 9 月 29 日

依托单位科研管理部门：	依托单位财务管理部门：
负责人（签章） 2022年 9 月 30 日	负责人（签章）： 2022年 9 月 30 日

国家自然科学基金项目依托单位承诺书

我单位同意承担上述国家自然科学基金项目，将保证项目负责人及其研究队伍的稳定和研究项目实施所需的条件，严格遵守国家自然科学基金委员会有关资助项目管理、项目资金管理、科研诚信管理和科技伦理管理等各项规定，并督促实施。

依托单位（公章）

2022年 9 月 30 日

国家自然科学基金资助项目签批审核表

本栏目由自然科学基金委填写

科学处审查意见：

同意按计划执行

负责人（签章）：赵萍桂

2022年 11月 1日

科学部审查意见：

同意按计划执行

负责人（签章）：孟国庆

2022年 11月 1日

受理编号：c22140500002165

项目编号：2022A1515011786

文件编号：粤基金字〔2022〕3号

广东省基础与应用基础研究基金项目

任务书

项目名称：图谱确定性的研究

项目类别：广东省自然科学基金-面上项目

项目起止时间：2022-01-01 至 2024-12-31

管理单位（甲方）：广东省基础与应用基础研究基金委员会

依托单位（乙方）：华南农业大学

通讯地址：广东省广州市天河区五山路483号

邮政编码：510642 单位电话：020-85283435

项目负责人：刘木伙 联系电话：13560018860

（广东科技微信公众号） （查看任务书信息） （受理纸质材料二维码）

广东省基础与应用基础研究
基金委员会
二〇二〇年制

填写说明

一、项目任务书内容原则上要求与申报书相关内容保持一致，不得无故修改。

二、项目承担单位通过广东省科技业务管理阳光政务平台下载项目任务书，按要求完成签名盖章后提交至省科技厅受理窗口。

三、签名盖章说明。请分别在单位工作分工及经费分配情况页、人员信息页、签约各方页等地方按要求签字或盖章，签章不合规或错漏将不予受理。其中，人员信息页要求所有参与人员本人亲笔签名，代签或印章无效，漏签将不予受理。

四、本任务书自签字并加盖公章之日起生效，各方均应负本任务书的法律责任，不应受机构、人事变动影响。

一、主要研究内容和要达到的目标

本项目将围绕图谱确定性、第二大特征值不大于1的图类确定性和图结构的谱确定性等问题展开研究，研究内容和预期目标如下：

第一、图谱确定性与图的同构问题密切联系，也在化学理论中有重要应用，因此成为图谱理论的研究热点之一。图谱确定性研究的一般技巧都是先证明同谱则同度序列，然后证明同度序列且同谱则同构。于是，申请人与合作者提出了度序列的图谱确定性问题。此外，近年来W. H. Haemers等人开始探索大图类的图谱确定问题。本项目中，课题团队希望能找到更多被图谱确定的度序列或找到新的度序列被图谱确定的充分或必要条件，同时还希望能找到有效的方法来处理大图类的谱确定性。

第二、1982年，著名的数学家A. J. Hoffman提出了第二大(邻接)特征值不大于1的图类确定性问题。在此领域中，M. Petrovic等人确定了所有的第二大特征值不大于1的线图和二部图，Z. Stanic确定了所有第二大特征值不大于1的门阀图，黄琼湘等人确定了所有第二大特征值不大于1的广义θ图，洪渊、徐光辉、郭曙光和李书超等人分别确定了所有第二大特征值不大于1的树、单圈图、双圈图和三圈图。最近，J. H. Koolen等人确定了所有第二大特征值不大于1且刚好有三个不同特征值的图类，而申请人与合作者把线图的结果推广到了不包含五个顶点的完全图去掉一条边且不包含四个顶点的星图为导出子图的图类。在本项目中课题团队将继续对该问题进行深入研究，希望能把我们的已有结果推广到不包含五个顶点的完全图去掉一条边或不包含四个顶点的星图之一为导出子图的图类。此外，我们还将探索以第二大(无符号)拉普拉斯特征值为上下界的图类确定性等问题。

第三、近年来一些图谱专家考虑如何以图谱为工具对图的结构进行研究，尝试以图谱为工具得到更理想的结果。在此方向上，赖虹建等人研究了图的边不交的支撑树的谱确定性，S. M. Cioaba与合作者研究了图的边连通度和匹配数的谱确定性，冯立华等人研究了图的点连通度的谱确定性，V. Nikiforov和翟明清等人则研究了特殊圈和特殊路的谱确定性，宁博、周波和王力工等人还研究了图的哈密顿路、哈密顿圈和哈密顿连通等的谱确定性问题。最近，申请人与合作者以图谱为工具改进了著名数学家P. Erdos等人关于极小点覆盖图的一个经典上界。本项目中，课题团队将重点考虑图的划分问题的谱确定性结果，希望能得到一些有意义的新结论。

二、项目预期获得的研究成果及形式

<table>
<tr><td rowspan="3">论文及专著情况</td><td colspan="2">国家统计源刊物以上刊物发表论文（篇）</td><td colspan="2">8</td><td colspan="2">科技报告（篇）</td><td colspan="2">1</td></tr>
<tr><td colspan="2">其中被SCI/EI/ISTP收录论文数（篇）</td><td colspan="2">8</td><td colspan="2">培养人才（人）</td><td colspan="2">2</td></tr>
<tr><td colspan="2">专著（册）</td><td colspan="2">0</td><td colspan="2">引进人才（人）</td><td colspan="2">0</td></tr>
<tr><td rowspan="3">专利情况(项)</td><td colspan="2">发明专利</td><td colspan="2">实用新型专利</td><td colspan="2">外观设计专利</td><td colspan="2">国外专利</td></tr>
<tr><td>申请</td><td>授权</td><td>申请</td><td>授权</td><td>申请</td><td>授权</td><td>申请</td><td>授权</td></tr>
<tr><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td></tr>
</table>

三、项目进度和阶段目标

（一）项目起止时间： 2022-01-01 至 2024-12-31

（二）项目实施进度及阶段主要目标：

开始日期	结束日期	主要工作内容
2022-01-01	2022-12-31	主要研究图谱确定性问题，将探索新的被图谱确定的度序列或新的度序列被图谱确定的充分或必要条件，寻找新的被图谱确定的大图类，并研究如何从旧的被图谱确定的图类出发构造新的被图谱确定的图类的方法和技巧。本年度预期发表高水平的SCI论文2-3篇。
2023-01-01	2023-12-31	主要研究第二大特征值不大于1的图类确定性问题，包括第二大特征值不大于1的图类确定性、以第二大特征值为上下界的一些新的图类性质等问题。本年度预期发表高水平的SCI论文2-3篇。
2024-01-01	2024-12-31	主要对图结构的谱确定性问题进行研究，将重点研究图的划分问题的谱确定性结果，希望能得到一些有意义的新结论。本年度预期发表高水平的SCI论文2-3篇。

四、项目总经费及省基金委经费预算

1. 省基金委经费下达总额： （大写）壹拾万圆整；（小写 ）10万元；

2. 省基金委经费年度下达计划：

年度	2022 年	年	年	年	年
经费(万元)	10.00				

3. 总经费及省基金委经费开支预算计划：

经费筹集情况： （单位：万元）

省基金委经费	自筹资金				合计
	自有资金	贷款	地方政府投入	其它	
10.00	0.00	0.00	0.00	0.00	10.00

政府部门、境外资金及其他资金投入情况说明：	

与本项目相关的其他经费来源	（单位：万元）
其他计划资助经费：	0.00
单位配套经费：	0.00
其他经费资助：	0.00
其他经费来源合计：	

五、人员信息

项目负责人								
姓名	证件号码	年龄	性别	职称	学历	在项目中承担的任务	所在单位	签名
刘木伙	440106198103044017	41	男	副教授	博士研究生	项目负责人	华南农业大学	刘木伙

项目组主要成员								
姓名	证件号码	年龄	性别	职称	学历	在项目中承担的任务	所在单位	签名
魏福义	140103196401286314	58	男	教授	硕士研究生	图结构的谱确定性	华南农业大学	魏福义
李倩	370631197808300528	44	女	讲师	硕士研究生	第二大特征值不大于1的图类确定性	华南农业大学	李倩
李凤	510129198008253526	42	女	讲师	硕士研究生	图谱的确定性	华南农业大学	李凤
朱艳丽	440106197912134026	43	女	讲师	硕士研究生	图谱的确定性	华南农业大学	朱艳丽
陈超辉	441283199708043977	25	男	未取得	本科	收集整理资料	华南农业大学	陈超辉
杨晓婷	441323199709122529	25	女	未取得	本科	收集整理资料	华南农业大学	杨晓婷

六、工作分工及经费分配

承担/参与单位名称（盖章）	工作分工	总经费分摊（万元）	省基金委经费分配（万元）
华南农业大学	课题团队由魏福义教授、刘木伙副教授、李倩、李凤、朱艳丽以及研究生陈超辉和杨晓婷同学组成，主要分工如下：申请人刘木伙副教授负责组织课题的顺利开展和课题的主要理论分析，魏福义教授负责图结构的谱确定性的研究，李凤和朱艳丽负责图谱的确定性研究，李倩负责第二大特征值不大于1的图类确定性的研究，而陈超辉和杨晓婷同学则负责资料的收集和整理等工作。	10.00	10.00
	合计	10.00	10.00

2022A1515011786

七、任务书条款

第一条 甲方与乙方根据《中华人民共和国民法典》及国家有关法规和规定，按照《广东省科学技术厅关于广东省基础与应用基础研究基金（省自然科学基金、联合基金等）项目管理的实施细则（试行）》《广东省省级科技计划项目验收结题工作规程（试行）》等规定，为顺利完成（2022）年图谱确定性的研究专项项目（文件编号：粤基金字〔2022〕3号 ）经协商一致，特订立本任务书，作为甲乙双方在项目实施管理过程中共同遵守的依据。

第二条 甲方的权利义务：

1. 按任务书规定进行经费核拨的有关工作协调。

2. 根据甲方需要，在不影响乙方工作的前提下，定期或不定期对乙方项目的实施情况和经费使用情况进行检查或抽查。

3. 根据《广东省科研诚信管理办法(试行)》等规定对乙方进行科技计划信用管理。

第三条 乙方的权利义务：

1. 确保落实自筹经费及有关保障条件。

2. 按任务书规定，对甲方核拨的经费实行专款专用，单独列账，并随时配合甲方进行监督检查。

3. 经费使用按照广东省级财政科研项目经费使用等有关规定进行管理。

4. 项目依托单位应制定经费使用“负面清单+包干制”内部管理制度并报甲方备案。

5. 使用财政资金采购设备、原材料等，按照《广东省实施〈中华人民共和国招标投标法〉办法》有关规定，符合招标条件的须进行招标。

6. 项目任务书任务完成后，或任务书规定的任务、指标及经费投入等提前完成的，乙方可提出验收结题申请，并按甲方要求做好项目验收结题工作。

7. 若项目发生需要终止结题的情况，乙方须提出终止结题申请，并按甲方要求做好项目终止结题工作。

8. 在每年规定时间内向甲方如实提交上年度工作情况报告，报告内容包含上年度项目进展情况、经费决算和取得的成果等。

9. 按照国家和省有关规定，提交科技报告及其他材料。

10. 利用甲方的经费获得的研究成果，项目负责人和参与者应当注明获得“广东省基础与应用基础研究基金（英文：Guangdong Basic and Applied Basic Research Foundation）（项目编号）”资助或作有关说明。

11. 乙方要恪守科学道德准则，遵守科研活动规范，践行科研诚信要求，不得抄袭、剽窃他人科研成果或者伪造、篡改研究数据、研究结论；不得购买、代写、代投论文，虚构同行评议专家及评议意见；不得违反论文署名规范，擅自标注或虚假标注获得科技计划（专项、基金等）等资助；不得弄虚作假，骗取科技计划（专项、基金等）项目、科研经费以及奖励、荣誉等；不得有其他违背科研诚信要求的行为。

12. 确保本项目开展的研究工作符合我国科技伦理管理相关规定。

第四条 在履行本任务书的过程中，如出现广东省相关政策法规重大改变等不可抗力情况，甲方有权对所核拨经费的数量和时间进行相应调整。

第五条 在履行本任务书的过程中，当事人一方发现可能导致项目整体或部分失败的情形时，应及时通知另一方，并采取适当措施减少损失，没有及时通知并采取适当措施，致使损失扩大的，应当就扩大的损失承担责任。

第六条 本项目技术成果的归属、转让和实施技术成果所产生的经济利益的分享，除双方另有约定外，按国家和广东省有关法规执行。

第七条 根据项目具体情况，经双方另行协商订立的附加条款，作为本任务书正式内容的一部分，与本任务书具有同等效力。

第八条 本任务书一式三份，各份具有同等效力。甲、乙方及项目负责人各执一份，三方签字、盖章后即生效，有效期至项目结题后一年内。各方均应负任务书的法律责任，不应受机构、人事变动的影响。

第九条 乙方必须接受甲方聘请的本项目任务书监理单位的监督和管理。监理单位按照甲方赋予的权利对本项目任务书的履行进行审核、进度调查，对项目任务书变更、经费使用情况进行监督管理及组织项目验收。

说明：1.本任务书中，凡是当事人约定无需填写的内容，应在空白处划（/）。

2.委托代理人签订本任务书的，应出具合法、有效的委托书。

八、本任务书签约各方

管理单位（甲方）：　　广东省基础与应用基础研究基金委员会　（盖章）

法定代表人（或法人代理）：　曾路　（签章）

2022 年　04 月　21 日

依托单位（乙方）：　华南农业大学　（盖章）

法定代表人（或法人代理）：　刘雅红　（签章）

联系人（项目主管）姓名：　倪慧群　（签章）

Email：　kjcgxk@scau.edu.cn

电话：　020-85283435　/　15920301530

开户单位名称：　华南农业大学

开户银行名称：　广东广州工行五山支行

开户银行帐号：　3602002609000310520

2022 年 4 月 23 日

联系人（项目负责人）姓名：　刘木伙　（签名）刘木伙

Email：　liumuhuo@163.com

电话：　13560018860

2022 年 4 月 23 日

受理编号：c24140500003144

项目编号：2024A1515011899

文件编号：粤基金字〔2024〕7号

广东省基础与应用基础研究基金项目

任务书

项目名称：基于最大和次大邻接特征值的一些图谱问题的研究

项目类别：广东省自然科学基金-面上项目

项目起止时间：2024-01-01 至 2026-12-31

管理单位（甲方）：广东省基础与应用基础研究基金委员会

依托单位（乙方）：华南农业大学

通讯地址：广东省广州市天河区五山路483号

邮政编码：510642 单位电话：020-85283435

项目负责人：刘木伙 联系电话：13560018860

（广东科技微信公众号） （查看任务书信息） （受理纸质材料二维码）

广东省基础与应用基础研究
基金委员会
二〇二〇年制

填写说明

一、项目任务书内容原则上要求与申报书相关内容保持一致，不得无故修改。

二、项目承担单位通过广东省科技业务管理阳光政务平台下载项目任务书，按要求完成签名盖章后扫描上传到广东省科技业务管理阳光政务平台。

三、签名盖章说明。请分别在单位工作分工及经费分配情况页、人员信息页、签约各方页等地方按要求签字或盖章，签章不合规或错漏将不予受理。其中，人员信息页要求所有参与人员本人亲笔签名，代签或印章无效，漏签将不予受理。

四、本任务书自签字并加盖公章之日起生效，各方均应负本任务书的法律责任，不应受机构、人事变动影响。

五、根据《广东省科学技术厅广东省财政厅关于深入推进省基础与应用基础研究基金项目经费使用“负面清单+包干制”改革试点工作的通知》（粤科规范字〔2022〕2号），2022年度及以后立项资助的全部省基金项目(包括省自然科学基金、省市联合基金、省企联合基金项目等)均适用“负面清单+包干制”，项目提交申请书和任务书时无需编制费用明细科目预算。

2024A1515011620

一、主要研究内容和要达到的目标

图的最大和次大邻接特征值也分别称为图的谱半径和第二大邻接特征值，本项目将主要围绕图谱的优超理论、Hoffman问题和赵宇飞问题展开研究，研究内容和预期目标如下：

第一、2008年J.Leydold和张晓东等人分别发现了优超理论是研究图谱极值理论的十分有效的工具，后来王力工以及尤利华等人还发现优超理论可以解决张量的极值排序问题。最近，林辉球、宁博和宝音都仍通过图谱的优超方法解决了著名的Bollobas-Nikiforov猜想的特殊情形，翟明清和林辉球还借助于图谱的优超工具解决了图谱专家M.Tait的一个谱极值猜想。本项目将致力于寻找新的图谱的优超定理，并探索优超理论在图谱的极值理论研究的新应用。

第二、1982年著名的数学家A.J.Hoffman提出了第二大邻接特征值不大于1的图类确定性问题，Hoffman问题的研究非常困难。经过四十多年的探索，只有第二大邻接特征值不大于1的线图、二部图、门阀图、广义θ图、树、单圈图、双圈图、三圈图、恰有三个不同特征值的图类和外平面图被完全确定。为此，学者们提出了通过第二大邻接特征值不大于某给定常数的图类确定性的研究来寻找Hoffman问题的解决办法。1993年，曹大松和洪渊确定了所有第二大邻接特征值小于1/3的图类，并提出了确定所有第二个邻接特征值大于1/3而小于黄金分割点的图类的问题。最近，申请人与合作者把第二大邻接特征值不大于1的线图结果进行了推广。本项目将重点关注曹大松-洪渊问题的研究，还将尝试对第二大邻接特征值不大于1的正则图的已有研究结果进行改进。

第三、利用一个第二大邻接特征值重数的新上界为工具，赵宇飞等人解决了等角线上的一个古老的几何难题。同时，他们提出了最大度不超过D的n阶连通图中第二大邻接特征值重数的最优上界是多少的问题。最近，陈冠涛等人得到了平面图和外平面图的第二大邻接特征值重数的紧的上界。本项目将关注于第二大邻接特征值的重数与图的结构之间的内部联系，希望能在赵宇飞问题的研究中得到一些有意义的研究结果。连通非正则图的谱半径严格小于最大度，因此最大度和谱半径的差异成为衡量图的正则性的重要参数，该参数引起了柳柏濂、冯荣权、张晓东、史灵生、D.Stevanovic、S.M.Cioaba和V.Nikiforov等人的关注与研究。本项目还将对给定最大度的连通非正则图类中谱半径的上界等问题展开深入研究，希望能在相关研究中取得一些新的突破。

二、项目预期获得的研究成果及形式

<table>
<tr><td rowspan="3">论文及专著情况</td><td colspan="2">国家统计源刊物以上刊物发表论文（篇）</td><td colspan="2">10</td><td colspan="2">科技报告（篇）</td><td colspan="2">0</td></tr>
<tr><td colspan="2">其中被SCI/EI/ISTP收录论文数（篇）</td><td colspan="2">10</td><td colspan="2">培养人才（人）</td><td colspan="2">4</td></tr>
<tr><td colspan="2">专著（册）</td><td colspan="2">0</td><td colspan="2">引进人才（人）</td><td colspan="2">0</td></tr>
<tr><td rowspan="3">专利情况(项)</td><td colspan="2">发明专利</td><td colspan="2">实用新型专利</td><td colspan="2">外观设计专利</td><td colspan="2">国外专利</td></tr>
<tr><td>申请</td><td>授权</td><td>申请</td><td>授权</td><td>申请</td><td>授权</td><td>申请</td><td>授权</td></tr>
<tr><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td></tr>
</table>

2024A1515011899

三、项目进度和阶段目标

（一）项目起止时间： 2024-01-01 至 2026-12-31		
（二）项目实施进度及阶段主要目标：		
开始日期	结束日期	主要工作内容
2024-01-01	2024-12-31	主要对图谱的优超理论展开研究，希望能得到新的图谱领域的优超定理，并能发现优超理论在图谱的极值理论研究的新应用。本年度预期发表高水平的SCI论文3-4篇。
2025-01-01	2025-12-31	主要关注Hoffman问题的研究，尝试把已有的第二大邻接特征值不大于1的图类确定性结果进行推广，更希望能确定第二大邻接特征值不大于黄金分割点的所有图类。本年度预期发表高水平的SCI论文3-4篇。
2026-01-01	2026-12-31	主要对赵宇飞问题进行研究，包括对第二大邻接特征值的重数与图的结构的内部联系、第二大邻接特征值重数不大于最小度的图类的结构特点以及给定最大度的连通非正则图类中谱半径的上界等问题展开深入研究。本年度预期发表高水平的SCI论文3-4篇。

2024A1515011599

四、项目总经费及省基金委经费预算

1.省基金委经费下达总额：　（大写）壹拾伍万圆整；（小写 ）15万元；					
2.省基金委经费年度下达计划：					
年度	2024 年	年	年	年	年
经费(万元)	15.00				

2024A1515011899

五、人员信息

项目负责人								
姓名	证件号码	年龄	性别	职称	学历	在项目中承担的任务	所在单位	签名
刘木伙	440106198103044017	43	男	副教授	博士研究生	项目负责人	华南农业大学	刘木伙

项目组主要成员								
姓名	证件号码	年龄	性别	职称	学历	在项目中承担的任务	所在单位	签名
魏福义	140103196401286314	60	男	教授	硕士研究生	图谱的优超理论	华南农业大学	魏福义
魏佳	412826199111056688	33	女	讲师	博士研究生	赵宇飞问题	华南农业大学	魏佳
李倩	370631197808300528	46	女	讲师	硕士研究生	赵宇飞问题	华南农业大学	李倩
李凤	510129198008253526	44	女	讲师	硕士研究生	Hoffman问题	华南农业大学	李凤
朱艳丽	440106197912134026	45	女	讲师	硕士研究生	Hoffman问题	华南农业大学	朱艳丽
蓝玉玲	360782199811052O2X	26	女	未取得	本科	收集整理资料	华南农业大学	蓝玉玲
卫培超	410422200004291013	24	男	未取得	本科	收集整理资料	华南农业大学	卫培超
郑瑞林	441522199710031717	27	男	未取得	本科	收集整理资料	华南农业大学	郑瑞林

六、工作分工及财政经费分配

承担/参与单位名称（盖章）	工作分工	省级财政科技资金分配（万元）
华南农业大学	课题团队由魏福义教授、刘木伙副教授、魏佳、李倩、李凤、朱艳丽四名讲师以及蓝玉玲、卫培超、郑瑞林三名研究生组成，主要分工如下：申请人刘木伙副教授负责组织课题按期开展和课题的理论分析，魏福义教授负责图谱的优超理论的研究，魏佳和李倩讲师负责赵宇飞问题的研究，李凤和朱艳丽讲师负责Hoffman问题的研究，而蓝玉玲、卫培超和郑瑞林同学则负责资料的收集和整理。	15.00
	合计	15.00

2024A1515011899

七、任务书条款

第一条 甲方与乙方根据《中华人民共和国民法典》及国家有关法规和规定，按照《广东省科学技术厅关于广东省基础与应用基础研究基金（省自然科学基金、联合基金等）项目管理的实施细则（试行）》《省级科技计划项目任务书管理细则》《广东省省级科技计划项目验收结题工作规程（试行）》等规定，为顺利完成（2024）年基于最大和次大邻接特征值的一些图谱问题的研究专项项目（项目编号：2024A1515011899）经协商一致，特订立本任务书，作为甲乙双方在项目实施管理过程中共同遵守的依据。

第二条 甲方的权利义务：

1. 按任务书规定进行经费核拨的有关工作协调。

2. 根据甲方需要，在不影响乙方工作的前提下，定期或不定期对乙方项目的实施情况和经费使用情况进行检查或抽查。

3. 根据《广东省科研诚信管理办法(试行)》等规定对乙方进行科技计划信用管理。

第三条 乙方的权利义务：

1. 确保落实自筹经费及有关保障条件。

2. 按任务书规定，对甲方核拨的经费实行专款专用，单独列账，并随时配合甲方进行监督检查。

3. 经费使用按照广东省级财政科研项目经费使用等有关规定进行管理。

4. 项目依托单位应制定经费使用“负面清单+包干制”内部管理制度并报甲方备案。

5. 使用财政资金采购设备、原材料等，按照《广东省实施〈中华人民共和国招标投标法〉办法》有关规定，符合招标条件的须进行招标。

6. 项目任务书任务完成后，或任务书规定的任务、指标及经费投入等提前完成的，乙方可提出验收结题申请，并按甲方要求做好项目验收结题工作。

7. 若项目发生需要终止结题的情况，乙方须提出终止结题申请，并按甲方要求做好项目终止结题工作。

8. 在每年规定时间内向甲方如实提交上年度工作情况报告，报告内容包含上年度项目进展情况、经费决算和取得的成果等。

9. 按照国家和省有关规定，提交科技报告及其他材料。

10. 利用甲方的经费获得的研究成果，项目负责人和参与者应当注明获得“广东省基础与应用基础研究基金（英文：Guangdong Basic and Applied Basic Research Foundation）（项目编号）”资助或作有关说明。

11. 乙方要恪守科学道德准则，遵守科研活动规范，践行科研诚信要求，不得抄袭、剽窃他人科研成果或者伪造、篡改研究数据、研究结论；不得购买、代写、代投论文，虚构同行评议专家及评议意见；不得违反论文署名规范，擅自标注或虚假标注获得科技计划（专项、基金等）等资助；不得弄虚作假，骗取科技计划（专项、基金等）项目、科研经费以及奖励、荣誉等；不得有其他违背科研诚信要求的行为。

12. 确保本项目开展的研究工作符合我国科技伦理管理相关规定。

第四条 在履行本任务书的过程中，如出现广东省相关政策法规重大改变等不可抗力情况，甲方有权对所核拨经费的数量和时间进行相应调整。

第五条 在履行本任务书的过程中，当事人一方发现可能导致项目整体或部分失败的情形时，应及时通知另一方，并采取适当措施减少损失，没有及时通知并采取适当措施，致使损失扩大的，应当就扩大的损失承担责任。

第六条 本项目技术成果的归属、转让和实施技术成果所产生的经济利益的分享，除双方另有约定外，按国家和广东省有关法规执行。

第七条 根据项目具体情况，经双方另行协商订立的附加条款，作为本任务书正式内容的一部分，与本任务书具有同等效力。

第八条 本任务书一式三份，各份具有同等效力。甲、乙方及项目负责人各执一份，三方签字、盖章后即生效，有效期至项目结题后一年内。各方均应负任务书的法律责任，不应受机构、人事变动的影响。

第九条 乙方必须接受甲方聘请的本项目任务书监理单位的监督和管理。监理单位按照甲方赋予的权利对本项目任务书的履行进行审核、进度调查，对项目任务书变更、经费使用情况进行监督管理及组织项目验收。

说明：1. 本任务书中，凡是当事人约定无需填写的内容，应在空白处划（/）。

2. 委托代理人签订本任务书的，应出具合法、有效的委托书。

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八、本任务书签约各方

管理单位（甲方）：　　广东省基础与应用基础研究基金委员会　（盖章）

法定代表人（或法人代理）：　曾路　（签章）

2024 年　05 月　22 日

依托单位（乙方）：　华南农业大学　（盖章）

法定代表人（或法人代理）：　薛红卫　（签章）

联系人（项目主管）姓名：　倪慧群　（签章）

Email：　kjcgxk@scau.edu.cn

电话：　020-85283435　/　15920301530

开户单位名称：　华南农业大学

开户银行名称：　广东广州工行五山支行

开户银行账号：　3602002609000310520

2024 年 5 月 31 日

联系人（项目负责人）姓名：　刘木伙　（签名）刘木伙

Email：　liumuhuo@163.com

电话：　13560018860

2024 年 5 月 22 日

2024151501189

项目编号: 2017KTSCX020

广东省教育厅2017年重点平台及科研项目（自然科学类）

合同书

签约各方共同遵守《关于印发“广东省高等教育‘创新强校工程’专项资金管理办法”的通知》（粤财教〔2014〕130号）和《广东省教育厅关于做好“创新强校工程”科研项目管理工作的通知》（粤科教函〔2017〕22号）。

为顺利完成广东省普通高校省级重大科研项目（特色创新类）“图谱的优超理论”遵守条款如下：

1．管理单位（甲方）为华南农业大学；承担单位（乙方）是指该项目具体实施的依托学院（单位）。

2．合同书中的主要研究内容、项目成员、经费预算、进度和阶段性目标及预期成果等参照申请书执行。

3．乙方必须按要求于次年年初向甲方报送上一年度项目进展报告。逾期不报，甲方有权暂停拨款。

4．合同执行过程中，乙方如需调整任务或修改合同中的部分条款，应按《管理办法》向甲方提出变更内容及其理由的申请报告，经甲方审定后实施。甲方提出变更合同，要与乙方达成书面协议。未经正式批准或达成协议前，双方须按原合同履行。

5．乙方因某种原因致使任务无法执行，而要求终止合同，应视不同情况，部分或全部退还所拨经费并追究相关人员责任；如乙方没有提出终止合同的要求，甲方有权根据实际情况提出终止合同的处理建议。

6．经费必须按《关于印发“广东省高等教育‘创新强校工程’专项资金管理办法”的通知》（粤财教〔2014〕130号）使用。

7．合同正式文本一式贰份，存甲方壹份，乙方壹份。

本合同签约各方

甲方：华南农业大学（公章）

代表人（签名）：

2018 年 5 月 11 日

乙方：所在学院（公章）

负责人（签名）：

年　　月　　日

同意按照合同规定执行.

项目负责人（签名）：

2018 年 5 月 8 日

SCAULIB202625131

检索证明

根据委托人提供的论文材料，委托人华南农业大学数学与信息学院 刘木伙(学科类型:自然科学) 2 篇论文收录情况如下表。

序号	论文名称	发表刊物及发表的年月卷期/页码等	作者排名	论文等级	作者文中单位	收录情况	影响因子	中科院大类分区
1	Graphs with Large Clique Number whose Second Largest Eigenvalue does not Exceed (√5-1)/2	ELECTRONIC JOURNAL OF COMBINATORICS 出版年：2025 出版日期：APR 25 卷期：32 2 页码：- 文献号：P213 文献类型：Article	第一作者	B 类	华南农业大学数学系	SCI	IF2-year=0.7 IF5-year=0.7 （2024）	数学 3 区 Top 期刊：否 OA 期刊：是 （2025）
2	Maximal Lanzhou index of trees and unicyclic graphs with prescribed diameter	APPLIED MATHEMATICS AND COMPUTATION 出版年：2025 出版日期：MAR 1 卷期：488 页码：- 文献号：129116 文献类型：Article	唯一通讯作者	A 类	华南农业大学数学系	SCI	IF2-year=3.4 IF5-year=3.2 （2024）	数学 2 区 Top 期刊：否 OA 期刊：否 （2025）

说明：论文等级和中科院大类分区按《华南农业大学学术论文评价方案（试行）》划分。

报告免责声明:如未盖章,报告无效

检索员：刘汉思

华南农业大学图书馆

南京农业大学图书馆
2026-03-02
检索专用章

SCAULIB202519396

检索证明

根据委托人提供的论文材料，委托人**华南农业大学数信学院 刘木伙** 2 篇论文收录情况如下表。

序号	论文名称	发表刊物及发表的年月卷期/页码等	作者排名	论文等级	作者文中单位	收录情况	影响因子	中科院大类分区
1	Spectral characterization of the complete graph removing a cycle	JOURNAL OF COMBINATORIAL THEORY SERIES A 出版年：2024 出版日期：JUL 卷期：205 页码：- 文献号：105868 文献类型：Article	第一	B 类	华南农业大学数学系	SCI	IF2-year=1.2 IF5-year=1.2 （2024）	数学 3 区 Top 期刊：否 （2025）
2	Connected (K₄ - e)-free graphs whose second largest eigenvalue does not exceed 1	EUROPEAN JOURNAL OF COMBINATORICS 出版年：2024 出版日期：JAN 卷期：115 页码：- 文献号：103775 文献类型：Article	第一	A 类	华南农业大学数学系	SCI	IF2-year=0.9 IF5-year=1.0 （2024）	数学 2 区 Top 期刊：否 （2025）

说明：论文等级和中科院大类分区按《华南农业大学学术论文评价方案（试行）》划分。

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检索员：尹银林

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2025-07-17
信息检索专用章

华南农业大学图书馆SCAULIB20251396

SCAULIB202405486

检索证明

根据委托人提供的论文材料，委托人**华南农业大学数学与信息学院数学系 刘木伙** 35 篇论文收录情况如下表。

序号	论文名称	发表刊物及发表的年月卷期/页码等	作者排名	论文等级	作者文中单位	收录情况	影响因子	中科院大类分区
1	The A_α-spectral radius of dense graphs	LINEAR & MULTILINEAR ALGEBRA 出版年：2023 卷期：71 6 页码：1044-1053 文献号： 文献类型：Article,Early Access	第一	B 类	华南农业大学	SCI	IF2-year=1.1 IF5-year=1.1 （2022）	数学 4 区 Top 期刊：否 （2023）
2	The k-apex trees with minimum augmented Zagreb index	DISCRETE MATHEMATICS 出版年：2023 卷期：346 7 页码：- 文献号：113390 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.8 IF5-year=0.9 （2022）	数学 3 区 Top 期刊：否 （2023）
3	On connected partition with degree constraints	DISCRETE MATHEMATICS 出版年：2022 卷期：345 2 页码：- 文献号：112680 文献类型：Article,Early Access	第一	B 类	华南农业大学	SCI	IF2-year=0.8 IF5-year=0.9 （2022）	数学 3 区 Top 期刊：否 （2022）
4	Spectral strengthening of a theorem on transversal critical	DISCRETE MATHEMATICS 出版年：2022 卷期：345 3 页码：-	第一	B 类	华南农业大学	SCI	IF2-year=0.8 IF5-year=0.9 （2022）	数学 3 区 Top 期刊：否 （2022）

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	graphs	文献号：112717 文献类型：Article, Early Access						
5	Minimum augmented Zagreb index of c-cyclic graphs	DISCRETE APPLIED MATHEMATICS 出版年：2021 卷期：295 页码：32-38 文献号： 文献类型：Article, Early Access	第一	B 类	华南农业大学	SCI	IF2-year=1.254 IF5-year=1.209 （2021）	数学 3 区 Top 期刊：否 （2021）
6	On a conjecture of Schweser and Stiebitz	DISCRETE APPLIED MATHEMATICS 出版年：2021 卷期：295 页码：25-31 文献号： 文献类型：Article, Early Access	第一	B 类	华南农业大学	SCI	IF2-year=1.254 IF5-year=1.209 （2021）	数学 3 区 Top 期刊：否 （2021）
7	Spectral characterization of the complete graph removing a path: Completing the proof of Camara-Haemers Conjecture	DISCRETE MATHEMATICS 出版年：2021 卷期：344 4 页码：- 文献号：112275 文献类型：Article, Early Access	第一	B 类	华南农业大学	SCI	IF2-year=0.961 IF5-year=0.97 （2021）	数学 3 区 Top 期刊：否 （2021）
8	Unified extremal results for k-apex unicyclic graphs (trees)	DISCRETE APPLIED MATHEMATICS 出版年：2021 卷期：288 页码：35-49	第一	B 类	华南农业大学	SCI	IF2-year=1.254 IF5-year=1.209 （2021）	数学 3 区 Top 期刊：否 （2021）

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华南农业大学图书馆 信息检索专用章

		文献号： 文献类型：Article						
9	On graphs whose second largest eigenvalue is at most 1	EUROPEAN JOURNAL OF COMBINATORICS 出版年：2021 卷期：97 页码：- 文献号：103385 文献类型：Article,Early Access	第一	A 类	华南农业大学	SCI	IF2-year=0.89 IF5-year=0.976 （2021）	数学 2 区 Top 期刊：否 （2021）
10	The Maximum Number of Spanning Trees of a Graph with Given Matching Number	BULLETIN OF THE MALAYSIAN MATHEMATICAL SCIENCES SOCIETY 出版年：2021 卷期：44 6 页码：3725-3732 文献号： 文献类型：Article,Early Access	第一	B 类	华南农业大学	SCI	IF2-year=1.397 IF5-year=1.193 （2021）	数学 3 区 Top 期刊：否 （2021）
11	Some notes on the extremal k-generalized quasi-unicyclic graphs with respect to Zagreb indices	DISCRETE APPLIED MATHEMATICS 出版年：2020 卷期：284 页码：616-621 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=1.139 IF5-year=1.179 （2020）	数学 3 区 Top 期刊：否 （2020）
12	Spectral characterization of the complete graph removing a path	DISCRETE APPLIED MATHEMATICS 出版年：2020 卷期：284 页码：499-512 文献号：	第一	B 类	华南农业大学	SCI	IF2-year=1.139 IF5-year=1.179 （2020）	数学 3 区 Top 期刊：否 （2020）

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信息检索专用章
华南农业大学图书馆SCAULIB20240405486

		文献类型：Article						
13	The Fan Graph is Determined by its Signless Laplacian Spectrum	CZECHOSLOVAK MATHEMATICAL JOURNAL 出版年：2020 卷期：70 1 页码：21-31 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.338 IF5-year=0.445 （2020）	数学 4 区 Top 期刊：否 （2020）
14	Extremal Results for Cacti	BULLETIN OF THE MALAYSIAN MATHEMATICAL SCIENCES SOCIETY 出版年：2020 卷期：43 3 页码：2783-2798 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=1.554 IF5-year=1.266 （2020）	数学 4 区 Top 期刊：否 （2020）
15	Some Properties of Algebraic Connectivity	NATIONAL ACADEMY SCIENCE LETTERS-INDIA 出版年：2020 卷期：43 6 页码：537-542 文献号： 文献类型：Article,Early Access	第一	B 类	华南农业大学	SCI	IF2-year=0.788 IF5-year=0.767 （2020）	综合性期刊 4 区 Top 期刊：否 （2020）
16	Unified Spectral Hamiltonian Results of Balanced Bipartite	GRAPHS AND COMBINATORICS 出版年：2020 卷期：36 5 页码：1363-1390	第一	B 类	华南农业大学	SCI	IF2-year=0.498 IF5-year=0.626 （2020）	数学 4 区 Top 期刊：否 （2020）

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17	Extremal graphs for vertex-degree-based invariants with given degree sequences	DISCRETE APPLIED MATHEMATICS 出版年：2019 卷期：255 页码：267-277 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=1.041 IF5-year=1.082 （2019）	数学 3 区 Top 期刊：否 （2019）
18	Spectral results on Hamiltonian problem	DISCRETE MATHEMATICS 出版年：2019 卷期：342 6 页码：1718-1730 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.77 IF5-year=0.794 （2019）	数学 3 区 Top 期刊：否 （2019）
19	On the ordering of distance-based invariants of graphs	APPLIED MATHEMATICS AND COMPUTATION 出版年：2018 卷期：324 页码：191-201 文献号： 文献类型：Article	第一	A 类	华南农业大学	SCI	IF2-year=3.092 IF5-year=2.429 （2018）	数学 2 区 Top 期刊：是 （2018）
20	Which cospectral graphs have same degree sequences	DISCRETE MATHEMATICS 出版年：2018 卷期：341 11 页码：2969-2976 文献号：	第一	B 类	华南农业大学	SCI	IF2-year=0.728 IF5-year=0.756 （2018）	数学 4 区 Top 期刊：否 （2018）

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21	The spectral characterization of butterfly-like graphs	LINEAR ALGEBRA AND ITS APPLICATIONS 出版年：2017 卷期：513 页码：55-68 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.972 IF5-year=1.043 （2017）	数学 3 区 Top 期刊：否 （2017）
22	The (signless) Laplacian spectral radii of c-cyclic graphs with n vertices, girth g and k pendant vertices	LINEAR & MULTILINEAR ALGEBRA 出版年：2017 卷期：65 5 页码：869-881 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.835 IF5-year=0.806 （2017）	数学 3 区 Top 期刊：否 （2017）
23	On partitions of graphs under degree constraints	DISCRETE APPLIED MATHEMATICS 出版年：2017 卷期：226 页码：87-93 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.932 IF5-year=1.008 （2017）	数学 3 区 Top 期刊：否 （2017）
24	图的 k 部划分的一个注记	数学学报(中文版) 出版年：2016 卷期：2016,59(02) 02 页码：247-	第一	A 类	华南农业大学 (A)	北大核心	无	无

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		252 文献号： 文献类型：期刊论文						
25	Ordering (signless) Laplacian spectral radii with maximum degrees of graphs	DISCRETE MATHEMATICS 出版年：2015 卷期：338 2 页码：159-163 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.6 IF5-year=0.629 （2015）	数学 4 区 Top 期刊：否 （2015）
26	Bipartition of graph under degree constraints	SCIENCE CHINA-MATHEMATICS 出版年：2015 卷期：58 4 页码：869-874 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.761 IF5-year=0.692 （2015）	数学 4 区 Top 期刊：否 （2015）
27	On the signless Laplacian spectra of bicyclic and tricyclic graphs	ARS COMBINATORIA 出版年：2015 卷期：120 页码：169-180 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.265 IF5-year=0.278 （2015）	数学 4 区 Top 期刊：否 （2015）
28	RECENT RESULTS ON THE MAJORIZATION THEORY OF GRAPH SPECTRUM AND TOPOLOGICAL INDEX THEORY - A SURVEY	ELECTRONIC JOURNAL OF LINEAR ALGEBRA 出版年：2015 卷期：30 页码：402-421 文献号：	第一	B 类	华南农业大学	SCI	IF2-year=0.463 IF5-year=0.518 （2015）	数学 4 区 Top 期刊：否 （2015）

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29	The strong pseudoachromatic number of a graph	UTILITAS MATHEMATICA 出版年：2015 卷期：98 页码：3-21 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.273 IF5-year=0.351 （2015）	数学 4 区 Top 期刊：否 （2015）
30	The nine smallest hyper-Wiener indices of trees and the eight smallest hyper-Wiener (Wiener) indices of unicyclic graphs	UTILITAS MATHEMATICA 出版年：2014 卷期：95 页码：129-139 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.354 IF5-year=0.341 （2014）	数学 4 区 Top 期刊：否 （2014）
31	The majorization theorem of extremal pseudographs	LINEAR ALGEBRA AND ITS APPLICATIONS 出版年：2014 卷期：459 页码：13-22 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.939 IF5-year=0.948 （2014）	数学 3 区 Top 期刊：否 （2014）
32	On the Laplacian spectral radii of tricyclic graphs	ARS COMBINATORIA 出版年：2014 卷期：114 页码：129-143	第一	B 类	华南农业大学	SCI	IF2-year=0.259 IF5-year=0.255 （2014）	数学 4 区 Top 期刊：否 （2014）

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33	The First to Ninth Greatest LEL-invariants of Connected Graphs	UTILITAS MATHEMATICA 出版年：2014 卷期：93 页码：153-160 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.354 IF5-year=0.341 （2014）	数学 4 区 Top 期刊：否 （2014）
34	The proof of a conjecture on the lewin number of primitive non-powerful signed digraphs	LINEAR ALGEBRA AND ITS APPLICATIONS 出版年：2013 卷期：438 5 页码：2366-2377 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=0.983 IF5-year=1.086 （2013）	数学 3 区 Top 期刊：否 （2013）
35	Ordering the Zagreb Coindices of Connected Graphs	MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY 出版年：2013 卷期：70 3 页码：939-948 文献号： 文献类型：Article	第一	B 类	华南农业大学	SCI	IF2-year=1.829 IF5-year=1.506 （2013）	化学 3 区 Top 期刊：否 （2013）

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1	Note on Sombor index of connected graphs with given degree sequence	DISCRETE APPLIED MATHEMATICS 出版年：2023 卷期：330 页码：51-55 文献号： 文献类型：Article	通讯作者	B 类	华南农业大学	SCI	IF2-year=1.1 IF5-year=1.1 （2022）	数学 3 区 Top 期刊：否 （2023）
2	Extremal augmented Zagreb index of trees with given numbers of vertices and leaves	DISCRETE MATHEMATICS 出版年：2022 卷期：345 4 页码：- 文献号：112753 文献类型：Article	通讯作者	B 类	华南农业大学	SCI	IF2-year=0.8 IF5-year=0.9 （2022）	数学 3 区 Top 期刊：否 （2022）
3	On general ABC-type index of connected graphs	DISCRETE APPLIED MATHEMATICS 出版年：2022 卷期：315 页码：27-35 文献号： 文献类型：Article	通讯作者	B 类	华南农业大学	SCI	IF2-year=1.1 IF5-year=1.1 （2022）	数学 3 区 Top 期刊：否 （2022）
4	The minimal augmented Zagreb index of k-apex trees for k $\in$ {1,2,3}	APPLIED MATHEMATICS AND COMPUTATION 出版年：2021	通讯作者	A 类	华南农业大学	SCI	IF2-year=4.397 IF5-year=3.767 （2021）	数学 2 区 Top 期刊：是 （2021）

		卷期：402 页码：- 文献号：126139 文献类型：Article,Early Access						
5	Extremal polygonal cacti for bond incident degree indices	DISCRETE APPLIED MATHEMATICS 出版年：2019 卷期：257 页码：289-298 文献号： 文献类型：Article	通讯作者	B 类	华南农业大学	SCI	IF2-year=1.041 IF5-year=1.082 （2019）	数学 3 区 Top 期刊：否 （2019）
6	Some Extremal Results for Vertex-Degree-Based Invariants	MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY 出版年：2019 卷期：81 2 页码：325-344 文献号： 文献类型：Article	通讯作者	A 类	华南农业大学	SCI	IF2-year=1.949 IF5-year=1.787 （2019）	化学 2 区 Top 期刊：否 （2019）
7	Unified Extremal Results for Vertex-Degree-Based Graph Invariants with Given Diameter	MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY 出版年：2019 卷期：82 3 页码：699-714 文献号： 文献类型：Article	通讯作者	A 类	华南农业大学	SCI	IF2-year=1.949 IF5-year=1.787 （2019）	化学 2 区 Top 期刊：否 （2019）

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8	Unified extremal results of topological indices and spectral invariants of graphs	DISCRETE APPLIED MATHEMATICS 出版年：2019 卷期：271 页码：218-232 文献号： 文献类型：Article	通讯作者	B类	华南农业大学	SCI	IF2-year=1.041 IF5-year=1.082 （2019）	数学 3区 Top期刊：否 （2019）

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Graphs with Large Clique Number whose Second Largest Eigenvalue does not Exceed $(\sqrt{5}-1)/2$

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Abstract

In 1993, Cao and Hong [J. Graph Theory, 17 (1993), 325–331] posed the problem of characterizing graphs whose second largest eigenvalue is less than the golden section bound. In further considerations, the problem is extended to 'less than or equal to the golden section'. Several results giving partial characterizations appeared in the proceeding years, and what have remained are the most complicated cases. These cases are treated very sporadically in the period of the next 25 years. In this paper, we give a positive resolution to the problem for graphs containing a large clique. Actually, we characterize graphs whose second largest eigenvalue does not exceed the golden section bound and whose clique number is at least 54. If a graph has a pendant vertex, the result is improved to clique number at least 8.

Mathematics Subject Classifications: 05C50, 05C22

1 Introduction

In this paper we deal with finite undirected graphs without loops or multiple edges. For such a graph G, we denote its vertex set by $V(G)$ and edge set by $E(G)$. The number of vertices is denoted by n and called the *order* of G. We use $H \subset G$ to designate that H is an induced subgraph of G. In particular, if H is a complete graph, then it is called a *clique* (of G). The *clique number* ω (or $\omega(G)$) is the order of a maximum clique of G.

A vertex of degree 1 is referred to as a *pendant vertex*. As usual, K_n, P_n and C_n denote the complete graph, the path and the cycle of order n, respectively. Also, $K_{s,t}$ denotes the complete bipartite graph with s vertices in one colour class and t vertices in the other

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colour class. We write $W_{s,t}$ for the graph obtained by taking the complete graph K_s with vertex set $\{u_1, u_2, \ldots, u_s\}$ and t ($t \leqslant s$) isolated vertices $v_1, v_2, \ldots, v_t$, and inserting the edges $u_1v_1, u_2v_2, \ldots, u_tv_t$. For a graph G, sG and $\overline{G}$ denote the disjoint union of s copies of G and the complementary graph of G, respectively. For G and H, $G \vee H$ denotes their *join*, i.e., the graph obtained by inserting an edge between every vertex of G and every vertex of H. If F is an induced subgraph of G, then $H \vee (F|G)$ is the graph obtained by inserting an edge between every vertex of H and every vertex of F (This operation reduces to the join when $F \cong G$.)

We write λ_2 to denote the second largest eigenvalue of G, that is the second largest eigenvalue of the standard $\{0,1\}$-adjacency matrix of G. Graphs whose second largest eigenvalue is comparatively small have received a great deal of attention in the last five decades. Many results obtained before 2015 are surveyed in [24], whereas for the recent progress we refer the reader to [5, 16, 17, 26]. In particular, graphs with $\lambda_2 \leqslant \frac{1}{3}$ are known for a long period, and graphs with $\lambda_2 \leqslant \frac{1}{2}$ have been determined in 2023 [26]. Since every rational eigenvalue is an integer, λ_2 never attains the previous bounds. Graphs with $\lambda_2 \leqslant 1$ are extensively studied, and some notable references are [7, 10, 20, 21]. According to [17], to conclude determination of these graphs it remains to identify those which contain an induced subgraph isomorphic to $K_4 - e$, that is the graph obtained by removing an edge from the complete graph of order 4.

Another upper bound for λ_2, located between the previous two, has been studied, again with the absence of a complete characterization of the corresponding graphs. This is the so-called *golden section* (also known as the *golden ratio*) $\frac{\sqrt{5}-1}{2} \approx 0.618$. This constant appears in the spectrum of many graphs, say it is the second largest eigenvalue of the 4-vertex path. In 1993, Cao and Hong formulated the following problem.

Problem 1. *[4]* Characterize graphs with $\frac{1}{3} < \lambda_2 < \frac{\sqrt{5}-1}{2}$.

Henceforth, we make the reading easier by denoting $\sigma = \frac{\sqrt{5}-1}{2}$ and abbreviating a connected graph with $\lambda_2 \leqslant \sigma$ to a *σ-graph*. This terminology is consistent with [2, 7, 9, 23]. Before this paper, it has been shown that every σ-graph is either complete multipartite, or an induced subgraph of the 5-vertex cycle, or contains a triangle and its diameter is at most 3 [8]. Further characterizations of those with a triangle are given in the same reference. Considering the existing results on σ-graphs, it is worth mentioning that Simić has proved in [23] that the set of minimal forbidden induced subgraphs for $\lambda_2 < \sigma$ is finite. A partial list of these subgraphs can be found in [9]. The same result is extended to σ-graphs by Cvetković and Simić in [8], again with the absence of the complete list of the corresponding forbidden subgraphs.

All former results concerning σ-graphs were noteworthy and, in contrast to them, a complete characterization of these graphs requires intensive technical considerations and a multiple case analysis. In the light of the aforementioned unresolved case for $\lambda_2 \leqslant 1$, a possible method to deal with the golden section bound is to determine σ-graphs that do not contain $K_4 - e$ as an induced subgraph (they are already identified among graphs with $\lambda_2 \leqslant 1$), and consider the remaining ones (with an induced subgraph isomorphic to $K_4 - e$). However, it occurs that the existence of such a subgraph is very common for

graphs with small λ_2, and this approach would be rather difficult. In this contribution, our attention is focused on σ-graphs with a comparatively large clique number. This is motivated by the following empirical observations. By considering connected graphs whose second largest eigenvalue is bounded by some of the aforementioned constants, one may deduce that they have smaller diameter (see [23]), and consequently more 'round' shape followed by higher clique number and girth (length of a shortest cycle). On the contrary, for large values of λ_2, the graphs have larger diameter, and consequently more 'path-like' shape followed by smaller clique number and girth. An explanation in the case of regular graphs is offered by Cvetković [6], and Alon and Chung [1]. The latter result is the famous Expander Mixing Lemma that can also be found in [24], and whose concept appeared in the work of Haemers [14]. By observing that σ-graphs do not deviate from the previous structural description, one may see that a restriction on the clique number arises in a natural way.

To formulate our main result, we set $D_{a,b} \cong K_1 \vee (K_a \cup K_b)$, for $b \geqslant a \geqslant 2$, and

$$\mathcal{D} = \{H_s \vee (K_s|W_{s,s}) : s \geqslant 1\}, \text{ where } \overline{H}_s = s\big((K_1 \vee C_5) \cup \overline{W}_{3,3} \cup D_{2,3} \cup W_{s,s}\big).$$

The result reads as follows.

Theorem 2. *Let G be a connected graph that satisfies either*

(i) $\omega(G) \geqslant 54$ or

(ii) $\omega(G) \geqslant 8$ and G has a pendant vertex.

Then $\lambda_2(G) \leqslant \frac{\sqrt{5}-1}{2}$ holds if and only if G is an induced subgraph of some graph of $\mathcal{D} \cup \{\overline{D}_{2,4} \vee K_{52}\}$.

Since $\omega(\overline{D}_{2,4} \vee K_{52}) = 54$, the previous theorem implies the following result.

Corollary 3. *For a connected graph G with $\omega(G) \geqslant 55$, $\lambda_2(G) \leqslant \frac{\sqrt{5}-1}{2}$ holds if and only if G is an induced subgraph of some graph of $\mathcal{D}$.*

The connectedness of G is not a significant obstacle, since a disconnected graph with $\lambda_2 \leqslant \sigma$ is the disjoint union of a connected one and a set of isolated vertices, provided by $\lambda_2(2K_2) > \sigma$. The proof of Theorem 2 is based on two statements, each belonging to a wider context. The first of them is the forthcoming Theorem 5 concerning the determinant of a particular complex matrix and an application giving the upper bound for its second largest eigenvalue under certain additional assumptions. The second one (Theorem 7) establishes all connected graphs with $\lambda_2 \leqslant \sigma$ under the caveat that their clique number is at least 8 and they do not contain particular induced subgraphs.

Regarding a comparison with recently obtained graphs satisfying $\lambda_2 < \frac{1}{2}$, it is worth mentioning that these graphs are classified into the 13 structured types and each of them contains graphs obtained by combining unions and joins of complete graphs, or complete bipartite graphs, or their complements. Of course, all of them with large clique are covered by Theorem 2. Concerning the difference, i.e., graphs characterized by the same

theorem but not belonging to any class with $\lambda_2 < \frac{1}{2}$, it occurs that such graphs are obtained easily. For instance, $\lambda_2(\overline{D}_{2,4} \vee K_t) > \frac{1}{2}$ holds whenever $t \geqslant 3$, and there is a similar conclusion for graphs of $\mathcal{D}$. The method applied in [26] is elegant and relies on facts that the complement of a non-trivial graph with $\lambda_2 > \frac{1}{2}$ must be disconnected with each component containing a dominating vertex. This approach is not applicable in our study, since in general neither of the previous restrictions holds for a complement of a σ-graph. However, we also deal with complementary graphs having some structural restrictions, where these restrictions refer to the discussion on the existence of prescribed components called special components (see Section 4). The limits on clique numbers given in Theorem 2 arise from the existence of these components, which can be seen from the proof of the necessity in this theorem. Another comparison with [26] is given in the last section of this paper.

Our contribution echoes the results of [23] since this reference classifies graphs with a relaxed restriction $\lambda_2 < \sigma$ into the nine structured types, and a simple analysis on them shows that the clique number of these graphs is $\leqslant 54$, unless they are complete multipartite. Accordingly, Theorem 2(i) starts with a boundary case $\omega = 54$ and continues with $\omega > 54$.

We proceed with other related results. A *cograph* is a graph which does not contain P_4 as an induced subgraph. There is no inclusion between the class of σ-graphs and the class of cographs; for example, a σ-graph of diameter 3 is not a cograph, whereas a cograph that contains $2K_2$ as an induced subgraph is not a σ-graph. However, there is an interplay between these classes, and in some investigations they are considered simultaneously. In particular, this occurs in the context of the polynomial reconstruction [2], spectral characterization [4, 11], control theory [13] or the rank of graphs [22].

There are results concerning relationships between the clique number and some other eigenvalues of a graph. We know from Nikiforov's [18, 19] that

$$\lambda_1 \leqslant \sqrt{\frac{\omega-1}{\omega}2m} < \frac{\omega-1}{\omega} \quad \text{and} \quad \lambda_n < -\frac{2^{\omega-1}m^{\omega}}{\omega n^{2\omega-1}},$$

where λ_1 is the largest eigenvalue, λ_n is the least eigenvalue, n is the order and m is the number of edges; the latter inequality for λ_1 is the classical Wilf's inequality [25]. Since the clique number of graphs of Theorem 2 can be computed explicitly (for $\mathcal{D}$, in terms of s), the previous inequalities give upper bounds on λ_1 and λ_n for the obtained σ-graphs. More relationships between λ_1 and ω are obtained by Bollobás and Nikiforov [3]. Another interplay between λ_1, λ_n and ω is obtained by Gregory et al. [12]. Each of the foregoing inequalities can also be found in [24].

The remaining sections are organized in the following way. Section 2 is preparatory. In Section 3, we prove the sufficiency in Theorem 2. The necessity, which is the main contribution of this paper, is proved in Section 4. Some concluding remarks and comparisons are given in Section 5.

2 Preliminaries

This is a short section collecting all what is needed. We use I, J, O, $\mathbf{j}$ and $\mathbf{0}$ to denote the identity matrix, the all-1 matrix, the all-0 matrix, the all-1 vector and the all-0 vector, respectively. The size may be given in the subscript.

We write $N(v)$ and $d(v)$ for the neighbourhood and the degree of a vertex v of a graph G. For any subset U of $V(G)$ and vertex $v \notin U$, we denote by $N_U(v) = N_G(v) \cap U$ and $N_U[v] = N_U(v) \cup \{v\}$ the open and the closed neighbourhood of v in U, respectively. To simplify, for an induced subgraph H of G, $N_{V(H)}(v)$ is abbreviated to $N_H(v)$. The graph induced by the vertex set U is denoted by $G[U]$, and $G\backslash U$ denotes the graph obtained by removing the vertices of U. A *component* of a graph is a maximal connected induced subgraph.

In the entire paper, we assume that the eigenvalues of a graph G are indexed non-increasingly as $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. The corresponding characteristic polynomial is denoted by $\Phi(G)$. To avoid an unnecessary quoting of the order n, we also use $\lambda_{\min}$ to denote the least eigenvalue. The same notation is used for every real symmetric matrix.

We will use the next lemma.

Lemma 4 ([15, p. 20])**.** *The following statements hold true:*

(i) Let

$$S = \begin{pmatrix} M & N \\ P & Q \end{pmatrix}$$

be a square block matrix, such that M is invertible. Then $\det(S) = \det(M)\det(Q - PM^{-1}N)$;

(ii) If A is an $n \times n$ matrix and $\mathbf{x}$ and $\mathbf{y}$ are $n \times 1$ vectors, then $\det(A + \mathbf{x}\mathbf{y}^\intercal) = \det(A) + \mathbf{y}^\intercal \operatorname{adj}(A)\mathbf{x}$, *where* $\operatorname{adj}(A)$ *stands for the adjugate matrix.*

Item (i) is known as the Schur's formula. The entire lemma holds for complex matrices and vectors.

3 Sufficiency

It follows from the Interlacing Theorem that the property $\lambda_2 \leqslant \sigma$ is hereditary in the sense that if it holds for a graph G then it holds for every induced subgraph of G. Therefore, to prove the sufficiency in Theorem 2, it is enough to prove that the graphs of $\mathcal{D}$ and $\overline{D}_{2,4} \vee K_{52}$ are σ-graphs.

Observe that Lemma 4(ii), implies

$$\det(A) = \det(A + \mathbf{x}\mathbf{y}^\intercal - \mathbf{x}\mathbf{y}^\intercal) = \det(A + \mathbf{x}\mathbf{y}^\intercal) - \mathbf{y}^\intercal \operatorname{adj}(A + \mathbf{x}\mathbf{y}^\intercal)\mathbf{x}, \tag{1}$$

where, of course, $\mathbf{x}, \mathbf{y}$ and A are of feasible size. We proceed with the following theorem.

Theorem 5. *Let*

$$A = \begin{pmatrix} A_1 & \alpha\beta^\intercal \\ \beta\alpha^\intercal & A_2 \end{pmatrix},$$

where α and β are real column vectors. Then

$$\begin{aligned}\det(\lambda I - A) =& \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2) + \det(\lambda I - A_1)\det(\lambda I - A_2 + \beta\beta^\intercal) \\ & - \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2 + \beta\beta^\intercal). \end{aligned} \tag{2}$$

Moreover, if A is real, non-negative and symmetric, τ is a real number and

$$\min\{\lambda_{\min}(\alpha\alpha^\intercal - I - A_1), \lambda_{\min}(\beta\beta^\intercal - I - A_2)\} \geqslant -1 - \tau,$$

then $\lambda_2(A) \leqslant \tau$, with equality when $\lambda_1(A) > \tau$ and $\lambda_{\min}(\alpha\alpha^\intercal - I - A_1) = \lambda_{\min}(\beta\beta^\intercal - I - A_2) = -1 - \tau$.

Proof. We set $\mathbf{r}^\intercal = (\alpha^\intercal, \beta^\intercal)$ and

$$B = \begin{pmatrix} \lambda I - A_1 + \alpha\alpha^\intercal & O \\ O & \lambda I - A_2 + \beta\beta^\intercal \end{pmatrix}.$$

If B is invertible, then by (1) and Lemma 4, we have

$$\begin{aligned}\det(\lambda I - A) =& \det(B - \mathbf{r}\mathbf{r}^\intercal) = \det(B) - \mathbf{r}^\intercal \operatorname{adj}(B)\mathbf{r} \\ =& \det(B) - \mathbf{r}^\intercal \det(B)\ B^{-1}\mathbf{r} \\ =& \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2 + \beta\beta^\intercal) \\ & - \alpha^\intercal \operatorname{adj}(\lambda I - A_1 + \alpha\alpha^\intercal)\alpha \det(\lambda I - A_2 + \beta\beta^\intercal) \\ & - \det(\lambda I - A_1 + \alpha\alpha^\intercal)\beta^\intercal \operatorname{adj}(\lambda I - A_2 + \beta\beta^\intercal)\beta \\ =& \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2 + \beta\beta^\intercal) \\ & - (\det(\lambda I - A_1 + \alpha\alpha^\intercal) - \det(\lambda I - A_1))\det(\lambda I - A_2 + \beta\beta^\intercal) \\ & - \det(\lambda I - A_1 + \alpha\alpha^\intercal)(\det(\lambda I - A_2 + \beta\beta^\intercal) - \det(\lambda I - A_2)) \\ =& \det(\lambda I - A_1)\det(\lambda I - A_2 + \beta\beta^\intercal) + \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2) \\ & - \det(\lambda I - A_1 + \alpha\alpha^\intercal)\det(\lambda I - A_2 + \beta\beta^\intercal). \end{aligned}$$

Note that there are infinite choices for λ such that B is invertible and both sides the last equality are univariate polynomials in λ. Thus, the formula (2) holds.

Now, set $\lambda = \tau + \epsilon$, with $\epsilon > 0$. Since $\min\{\lambda_{\min}(\alpha\alpha^\intercal - I - A_1), \lambda_{\min}(\beta\beta^\intercal - I - A_2)\} \geqslant -1-\tau$, it follows that B is positive definite. Therefore, there exists an invertible matrix P_1 such that $P_1 B P_1^\intercal = I$. Let $C = P_1\mathbf{r}\mathbf{r}^\intercal P_1^\intercal$. Since the rank of C is equal to the rank of $\mathbf{r}\mathbf{r}^\intercal$, it is not larger than one. This implies the existence of another orthogonal matrix P_2 such that $P_2 C P_2^\intercal = \operatorname{diag}(\mu, 0, \ldots, 0)$. Let $P = P_2 P_1$. Then

$$P(\lambda I - A)P^\intercal = PBP^\intercal - P\mathbf{r}\mathbf{r}^\intercal P^\intercal = P_2(P_1 B P_1^\intercal)P_2^\intercal - P_2 C P_2^\intercal = I - \operatorname{diag}(\mu, 0, \ldots, 0).$$

Since $\lambda I - A$ and $I - \operatorname{diag}(\mu, 0, \ldots, 0)$ are congruent, they have the same inertia indices. Hence, $\lambda_{n-1}(\lambda I - A) = \lambda - \lambda_2(A) = \tau + \epsilon - \lambda_2(A) > 0$, where n is the order of A. From $\epsilon > 0$, we have $\lambda_2(A) \leqslant \tau$.

It remains to consider the equality case. For $\lambda_{\min}(\alpha\alpha^{\intercal}-I-A_1)=\lambda_{\min}(\beta\beta^{\intercal}-I-A_2)=-1-\tau$, it holds $\det(\tau I-A_1+\alpha\alpha^{\intercal})=\det(\tau I-A_2+\beta\beta^{\intercal})=0$. From (2), we have $\det(\tau I-A)=0$ and $\lambda_2(A)=\tau$, since by the statement assumption there is $\lambda_1(A)>\tau$. □

We prove the following consequence.

Corollary 6 (**Sufficiency in Theorem 2**). *Every graph of* $\mathcal{D}\cup\{\overline{D}_{2,4}\vee K_{52}\}$ *is a* σ*-graph.*

Proof. First, the inequality $\lambda_2(\overline{D}_{2,4}\vee K_{52})\leqslant\sigma$ is confirmed by direct computation. Let $G\in\mathcal{D}$, i.e., $G\cong H_s\vee(K_s|W_{s,s})$, for $s\geqslant 1$.

Suppose that the order of H_s is k. By taking $\alpha=\mathbf{j}_k$ and $\beta^{\intercal}=(\mathbf{j}_s^{\intercal},\mathbf{0}_s^{\intercal})$, we arrive at

$$A(G)=\begin{pmatrix}A(H_s) & \alpha\beta^{\intercal}\\ \beta\alpha^{\intercal} & A(W_{s,s})\end{pmatrix}=\begin{pmatrix}A(H_s) & J_{k\times s} & O\\ J_{s\times k} & J_s-I_s & I_s\\ O & I_s & O\end{pmatrix}.$$

Since

$$\det\Big(\lambda I-\big(\beta\beta^{\intercal}-I-A(W_{s,s})\big)\Big)=\det\begin{pmatrix}\lambda I_s & -I_s\\ -I_s & (\lambda+1)I_s\end{pmatrix}=(\lambda^2+\lambda-1)^s,$$

by employing Lemma 4(i), we obtain $\lambda_{\min}(\beta\beta^{\intercal}-I-A(W_{s,s}))=-1-\sigma$.

Note that $\Phi(K_1\vee C_5)=(\lambda^2+\lambda-1)^2(\lambda^2-2\lambda-5)$, $\Phi(\overline{W}_{3,3})=(\lambda^2+\lambda-1)^2(\lambda^2-2\lambda-4)$, $\Phi(D_{2,3})=(\lambda+1)^3(\lambda^3-3\lambda^2-3\lambda+7)$ and

$$\begin{aligned}\Phi(W_{s,s})&=\det\begin{pmatrix}(\lambda+1)I_s-J_s & -I_s\\ -I_s & \lambda I_s\end{pmatrix}\\ &=\det(\lambda I_s)\det\left[(\lambda+1)I_s-J_s-\lambda^{-1}I_s\right]=(\lambda^2+\lambda-1)^{s-1}\left(\lambda^2-(s-1)\lambda-1\right),\end{aligned}$$

where the last equality holds since the eigenvalues of J_s are s and $s-1$ copies of 0. Since the least root of these four polynomials is not less than $-1-\sigma$ and $\overline{H}_s=s\big((K_1\vee C_5)\cup\overline{W}_{3,3}\cup D_{2,3}\cup W_{s,s}\big)$, we deduce $\lambda_{\min}(A(\overline{H}_s))\geqslant-1-\sigma$. Combining $\lambda_{\min}(\beta\beta^{\intercal}-I-A(W_{s,s}))=-1-\sigma$ with

$$\lambda_{\min}(\alpha\alpha^{\intercal}-I-A(H_s))=\lambda_{\min}(A(\overline{H}_s))\geqslant-1-\sigma,$$

we obtain $\lambda_2(G)\leqslant\sigma$ by Theorem 5. □

4 Necessity

Let $R_1,R_2,\ldots,R_7$ be the graphs illustrated in Figure 1. One can easily check that none of them is a σ-graph. In other words, these graphs do not appear as induced subgraphs of σ-graphs, or they are forbidden induced subgraphs for σ-graphs.

One more term is needed. If $D_{a,b}$, with either $3=a\leqslant b\leqslant 5$ or $a=2<4\leqslant b\leqslant 18$, is a component of $\overline{G}$, then we say that $D_{a,b}$ is a *special component* of $\overline{G}$.

The following theorem features as another meaningful result of this paper. It plays a crucial role in the proof of Theorem 2.

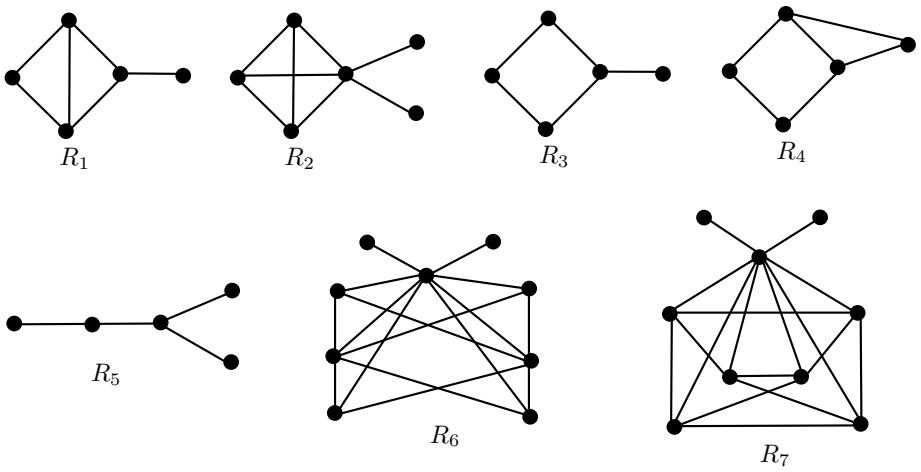


Figure 1: Forbidden induced subgraphs for σ-graphs.

Theorem 7. *Let G be a connected graph. If $\overline{G}$ contains no special component and $\omega(G) \geqslant 8$, then $\lambda_2(G) \leqslant \sigma$ if and only if either*

(i) G is an induced subgraph of $\mathcal{D}$, or

(ii) $\overline{G}$ is an induced subgraph of some graph of $\{D_{2,27} \cup 6K_1, D_{2,21} \cup W_{6,6}, D_{2,21} \cup \overline{W}_{3,3} \cup 3K_1, D_{2,21} \cup C_5 \cup 4K_1, D_{2,19} \cup K_4 \cup 5K_1\}$, or

(iii) $\overline{G} \subset D_{4,4} \cup H$, for $H \in \{\overline{W}_{3,3} \cup 3K_1, C_5 \cup 4K_1, W_{6,6}, K_4 \cup 5K_1\}$, or

(iv) $\overline{G} \subset D_{3,6} \cup H$, for $H \in \{\overline{W}_{3,3} \cup 3K_1, C_5 \cup 4K_1, W_{6,6}\}$.

The proof is based on a sequence of facts and lemmas. In what follows, G denotes a graph of the previous theorem. We always suppose that $\omega(G) = q$ and K_q is a fixed maximum clique of G, with $V(K_q) = \{w_1, w_2, \ldots, w_q\}$. We also denote by V_1 (resp. V_2) the set of vertices of $V(G) \setminus V(K_q)$, such that each of them is adjacent to exactly one (more than one) vertex of K_q. In the first four facts, we do not need the assumption $q \geqslant 8$ (as formulated in the previous theorem); this assumption will be imposed after Lemma 13.

The first fact tells us that $V(G) = V(K_q) \cup V_1 \cup V_2$, for $q \geqslant 3$.

Fact 8. *If $q \geqslant 3$, then for every $x \in V(G) \setminus V(K_q)$, x is adjacent to at least one vertex of K_q.*

Proof. For a contradiction, assume that G contains some vertex, which is not a neighbour of any vertex of K_q. Since G is connected, we can choose a vertex x of G such that x is not adjacent to any vertex of K_q, $xy \in E(G)$ for $y \in V(G) \setminus V(K_q)$, and y is adjacent to some vertices of K_q. Since $2K_2 \subset G$ when $|N_{K_q}(y)| = 1$ and $R_1 \subset G$ when $|N_{K_q}(y)| \geqslant 2$, we have $\lambda_2(G) > \sigma$, which is a contradiction. □

We proceed with the following, more or less simple, facts. They lead to the forthcoming Lemma 13.

Fact 9. *Let $k = |N_{K_q}(x)|$, for $x \in V_2$. We have $1 \leqslant q - k \leqslant 3$, where $q = k + 3$ implies $q \in \{5, 6\}$. In other words, if $q \geqslant 7$, then $q - 2 \leqslant k \leqslant q - 1$.*

Proof. Since $\omega(G) = q$, it follows that $k \leqslant q - 1$. Let $H = K_1 \vee (K_k | K_q)$. Since $H \subset G$ and $x \in V_2$, we have $\lambda_2(H) \geqslant \lambda_2(K_1 \vee (K_2 | K_6)) > \sigma$, whenever $2 \leqslant k \leqslant q - 4$. Therefore, $q \leqslant k + 3$. If $q = k + 3 \geqslant 7$, again $\lambda_2(H) \geqslant \lambda_2(K_1 \vee (K_4 | K_7)) > \sigma$ leads to the impossible scenario. Hence, $q \in \{5, 6\}$, as $k = 1$ is eliminated by definition of V_2. □

Fact 10. *Let $x_1, x_2 \in V(G) \setminus V(K_q)$ where x_i is adjacent to exactly k_i vertices of K_q, for $1 \leqslant i \leqslant 2$. If $q \geqslant 2 + k_1 + k_2$, then x_1 is not adjacent to x_2.*

Proof. If $x_1 x_2 \in E(G)$, then $2K_2 \subset G$ (as $q \geqslant 2 + k_1 + k_2$), which is not in line with $\lambda_2(G) \leqslant \sigma$. □

We recall the reader that the independent set is a vertex subset that do not contain adjacent vertices. In other words, it is the complement of a clique.

Fact 11. *If $q \geqslant 4$, then each vertex of K_q is adjacent to at most one vertex of V_1, and V_1 is an independent set of G.*

Proof. Assume for a contradiction that there exists a vertex $x \in V(K_q)$ adjacent to at least two vertices of V_1. In this case, either $2K_2 \subset G$ or $R_2 \subset G$, which contradicts $\lambda_2(G) \leqslant \sigma$. Combining this with Fact 10, we arrive at the desired result. □

Fact 12. *If $q \geqslant 8$ and $y \in V_1$ with $N_{K_q}(y) = \{z\}$, then z is adjacent to every vertex of V_2 and y is a pendant vertex of G.*

Proof. Suppose that $x \in V_2$. By Fact 9, we have $q - 2 \leqslant |N_{K_q}(x)| \leqslant q - 1$.

If $z \notin N_{K_q}(x)$, then $xy \in E(G)$, as $R_1 \not\subset G$. Thus, we have $\overline{K_2 \cup K_{1,7}} \subset G$ for $|N_{K_q}(x)| = q - 1 \geqslant 7$ or $R_4 \subset G$ for $|N_{K_q}(x)| = q - 2$, contradicting $\lambda_2(G) \leqslant \sigma$. Therefore, $z \in N_{K_q}(x)$, which implies that z is adjacent to every vertex of V_2.

Since $R_1 \not\subset G$ and $q - |N_{K_q}(x)| \geqslant 1$ with $q \geqslant 8$, we have $xy \notin E(G)$. Now, Facts 8 and 11 imply that y is a pendant vertex of G. □

At this point we single out one possibility for V_2.

Lemma 13. *If $|V_2| \leqslant 1$ and $q \geqslant 8$, then G is an induced subgraph of $W_{q,q}$ or $(K_1 \cup K_2) \vee (K_{q-1} | W_{q-1,q-1})$. Consequently, G is an induced subgraph of some graph of $\mathcal{D}$.*

Proof. If $|V_2| = 0$, then $G \subset W_{q,q}$ by Fact 11. Let $V_2 = \{x\}$. By Fact 9, we have $q - 2 \leqslant |N_{K_q}(x)| \leqslant q - 1$. By Fact 12, G is an induced subgraph of $(K_1 \cup K_2) \vee (K_{q-1} | W_{q-1,q-1}) \subset (\overline{K_1 \vee C_5}) \vee (K_{q-1} | W_{q-1,q-1})$.

In any case, G is an induced subgraph of some graph of $\mathcal{D}$, as follows by definition of the latter class. □

Henceforth, we always suppose that V_2 contains at least two vertices and that $q \geqslant 8$ holds. Further, by Fact 9, we have $q-2 \leqslant |N_{K_q}(x)| \leqslant q-1$, for every $x \in V_2$. Accordingly, we set

$$S_j = \big\{x : x \in V_2, |N_{K_q}(x)| = j\big\}, \text{ for } j \in \{q-2, q-1\}.$$

For fixed vertices w_1, w_2 of $V(K_q)$, we define

$$X_{w_1,w_2} = \{x : x \in S_{q-2}, w_1 \notin N_{K_q}(x) \text{ and } w_2 \notin N_{K_q}(x)\}$$

and

$$Y_w = \{x : x \in S_{q-1}, w \notin N_{K_q}(x)\}.$$

Observe that Y_w is an independent set of G, for every $w \in V(K_q)$, as $q = \omega(G)$.

We establish some structural characterizations of G. Facts 14–18 deal with $X_{w,w'}$ and Y_w.

Fact 14. *If w_1, w_2 are distinct vertices of $V(K_q)$ with $z_1 \in Y_{w_1}$ and $z_2 \in Y_{w_2}$, then $N_{X_{w_1,w_2}}(z_1) = N_{X_{w_1,w_2}}(z_2)$. Moreover, if $z_1z_2 \in E(G)$, then $N_{X_{w_1,w_2}}(z_1) = N_{X_{w_1,w_2}}(z_2) = \emptyset$.*

Proof. By the symmetry, we may suppose that $u \in X_{w_1,w_2}$ with $z_1u \in E(G)$ and $z_2u \notin E(G)$. Then either $G[u, z_1, z_2, w_1] \cong 2K_2 \subset G$ for $z_1z_2 \notin E(G)$ or $G[u, z_1, z_2, w_1, w_2] \cong R_3 \subset G$ for $z_1z_2 \in E(G)$. Thus, $N_{X_{w_1,w_2}}(z_1) = N_{X_{w_1,w_2}}(z_2)$.

Next, if $z_1z_2 \in E(G)$ and $u \in N_{X_{w_1,w_2}}(z_1) = N_{X_{w_1,w_2}}(z_2) \neq \emptyset$, then $G[u, z_1, z_2, w_1, w_2] \cong R_4$. Hence, $N_{X_{w_1,w_2}}(z_1) = N_{X_{w_1,w_2}}(z_2) = \emptyset$. □

Fact 15. *If w_1, w_2 are distinct vertices of $V(K_q)$ with $\max\{|Y_{w_1}|, |Y_{w_2}|\} \geqslant 2$, then every vertex of Y_{w_1} is adjacent to every vertex of Y_{w_2}, and there is no edge between T and X_{w_1,w_2}, where $T = Y_{w_1} \cup Y_{w_2}$.*

Proof. We may suppose that $|Y_{w_1}| \geqslant |Y_{w_2}| \geqslant 0$ with $z_1, z_2 \in Y_{w_1}$. Recall that Y_{w_1} and Y_{w_2} are independent sets of G. If $z_3 \in Y_{w_2}$ and either $z_1z_3 \notin E(G)$ or $z_2z_3 \notin E(G)$, then $G[w_1, w_2, z_1, z_2, z_3] \in \{R_3, R_5\}$. Hence, every vertex of Y_{w_1} is adjacent to every vertex of Y_{w_2}.

Suppose that $u \in X_{w_1,w_2}$. If $\{z_1u, z_2u\} \cap E(G) \neq \emptyset$, then $G[w_1, w_2, z_1, z_2, u] \in \{R_3, R_5\}$. If $z_3 \in Y_{w_2} \neq \emptyset$ and $z_3u \in E(G)$, then $G[w_1, w_2, z_1, z_3, u] \cong R_3$. Hence, there is no edge between T and X_{w_1,w_2}. □

Fact 16. *For any pair of vertices w_1, $w_2 \in V(K_q)$, X_{w_1,w_2} is an independent set of G and $|X_{w_1,w_2}| \leqslant 2$. Moreover, if $|X_{w_1,w_2}| = 2$ and $z \in Y_{w_1} \cup Y_{w_2}$, then $|N(z) \cap X_{w_1,w_2}| = 1$.*

Proof. Since $2K_2 \not\subset G$, X_{w_1,w_2} is an independent set of G. Since $q \geqslant 8$ and $K_3 \vee (3K_1 \cup K_2) \not\subset G$, we have $|X_{w_1,w_2}| \leqslant 2$. Next, suppose that $|X_{w_1,w_2}| = 2$. Since $K_3 \vee (2K_1 \cup W_{2,1}) \not\subset G$, we also have $|N(z) \cap X_{w_1,w_2}| \geqslant 1$. On the other hand, we have $|N(z) \cap X_{w_1,w_2}| \leqslant 1$ as $R_5 \not\subset G$. Thus, $|N(z) \cap X_{w_1,w_2}| = 1$. □

From Facts 15 and 16, we immediately obtain the following one.

Fact 17. *If w_1, w_2 are distinct vertices of $V(K_q)$ with $\max\{|Y_{w_1}|, |Y_{w_2}|\} \geqslant 2$, then we have $|X_{w_1,w_2}| \leqslant 1$.*

Fact 18. *Let w_1, w_2, w_3 be distinct vertices of $V(K_q)$ and $z_j \in Y_{w_j}$ for $j \in \{1,2,3\}$. If $z_1z_2 \in E(G)$, then $|N(z_3) \cap \{z_1, z_2\}| \geqslant 1$.*

Proof. If $|N(z_3) \cap \{z_1, z_2\}| = 0$, then $G[z_1, z_2, z_3, w_2, w_3] \cong R_1$. Therefore, we have $|N(z_3) \cap \{z_1, z_2\}| \geqslant 1$. □

Now, we include sets S_j (defined above).

Fact 19. *If $x, y \in S_{q-2}$, then $q-4 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-2$, along with $xy \notin E(G)$ for $q-3 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-2$ and $xy \in E(G)$ for $|N_{K_q}(x) \cap N_{K_q}(y)| = q-4$.*

Proof. Under the given assumptions, we have $q-4 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-2$.

If $|N_{K_q}(x) \cap N_{K_q}(y)| = q-2$, then $xy \notin E(G)$, as $2K_2 \not\subset G$. If $|N_{K_q}(x) \cap N_{K_q}(y)| = q-3$, then $xy \notin E(G)$, as $R_4 \not\subset G$. If $|N_{K_q}(x) \cap N_{K_q}(y)| = q-4$, then $xy \in E(G)$, as $R_1 \not\subset G$. □

Fact 20. *If $x \in S_{q-2}$ and $y \in S_{q-1}$, then $q-3 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-2$, where $|N_{K_q}(x) \cap N_{K_q}(y)| = q-3$ implies $xy \in E(G)$.*

Proof. Since $x \in S_{q-2}$ and $y \in S_{q-1}$, we have $q-3 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-2$. If $|N_{K_q}(x) \cap N_{K_q}(y)| = q-3$, then $xy \in E(G)$, as $R_1 \not\subset G$. □

Fact 21. *If $x, y \in S_{q-1}$, then $q-2 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-1$, where $|N_{K_q}(x) \cap N_{K_q}(y)| = q-1$ implies $xy \notin E(G)$.*

Proof. We have $q-2 \leqslant |N_{K_q}(x) \cap N_{K_q}(y)| \leqslant q-1$. If $|N_{K_q}(x) \cap N_{K_q}(y)| = q-1$, then $xy \notin E(G)$, as $q = \omega(G)$. □

In Facts 22–24, we fix some vertices of K_q and consider the interplay between X_{w_1,w_2}s and Y_{w_1}s.

Fact 22. *Let w_1, w_2, w_3 be distinct vertices of K_q. Then:*

(i) $|X_{w_1,w_2} \cup X_{w_2,w_3}| \leqslant 2$;

(ii) If $\min\{|Y_{w_1}|, |X_{w_2,w_3}|\} \geqslant 1$, then $X_{w_1,w_2} = \emptyset$ and every vertex of Y_{w_1} is adjacent to every vertex of Y_{w_2};

(iii) if $x \in X_{w_1,w_2}$, $y \in X_{w_2,w_3}$ and $z \in Y_{w_2}$, then $|N(z) \cap \{x, y\}| \in \{0, 2\}$.

Proof. (i): By Facts 16 and 19, we have that $X_{w_1,w_2} \cup X_{w_2,w_3}$ is an independent set of G, along with $\max\{|X_{w_1,w_2}|, |X_{w_2,w_3}|\} \leqslant 2$. If z_1, z_2, z_3 are distinct vertices of $X_{w_1,w_2} \cup X_{w_2,w_3}$, then $G[z_1, z_2, z_3, w_1, w_3]$ is R_5. Hence, $|X_{w_1,w_2} \cup X_{w_2,w_3}| \leqslant 2$.

(ii): Let $x \in Y_{w_1}$ and $y \in X_{w_2,w_3}$. Assume that $z \in X_{w_1,w_2}$. By Facts 19 and 20, we have $xy \in E(G)$ and $yz \notin E(G)$. This implies $G[x, y, z, w_1, w_3] \cong R_3$ for $xz \notin E(G)$ and $G[x, y, z, w_1, w_3] \cong R_4$ for $xz \in E(G)$. Hence, $X_{w_1,w_2} = \emptyset$. Next, suppose that $z \in Y_{w_2}$. If $xz \notin E(G)$, we obtain $G[x, y, z, w_1, w_2] \cong R_3$ for $yz \notin E(G)$ and $G[x, y, z, w_1, w_2] \cong R_4$ for $yz \in E(G)$. Hence, $xz \in E(G)$.

(iii): From $x \in X_{w_1,w_2}$ and $y \in X_{w_2,w_3}$, we have $xy \notin E(G)$ by Fact 19. If $|N(z) \cap \{x, y\}| = 1$, then $G[x, y, z, w_1, w_3] \cong R_1$. Hence, $|N(z) \cap \{x, y\}| \in \{0, 2\}$. □

Fact 23. $\min\{|X_{w_1,w_2}|, |X_{w_3,w_4}|, |X_{w_1,w_3}|\} = 0$ *holds for distinct vertices* w_1, w_2, w_3, w_4 *of* K_q.

Proof. Assume that $x_1 \in Y_{w_1,w_2}$, $y_1 \in X_{w_3,w_4}$ and $y_2 \in X_{w_1,w_3}$. By Fact 19, we have $x_1y_1 \in E(G)$ and $y_2 \notin N_G(x_1) \cup N_G(y_1)$. This implies $G[w_2, w_3, x_1, y_1, y_2] \cong R_3$, and we are done. □

Fact 24. *If* $\min\{|Y_{w_1}|, |Y_{w_2}|\} \geqslant 1$ *with* $|Y_{w_1}| + |Y_{w_2}| \geqslant 4$ *and* $|X_{w_1,w_2}| \geqslant 1$, *then* $V_1 = \emptyset$.

Proof. By Fact 15, every vertex of Y_{w_1} is adjacent to every vertex of Y_{w_2}, and every vertex of X_{w_1,w_2} is not adjacent to any vertex of $Y_{w_1} \cup Y_{w_2}$. Assume that $z \in V_1$ with $N_{K_q}(z) = \{w_3\}$. By employing Fact 12, we deduce that $w_3 \notin \{w_1, w_2\}$ and R_6 or R_7 is an induced subgraph of $G[U]$ with $U = \{w_1, w_2, w_3, z\} \cup Y_{w_1} \cup Y_{w_2} \cup X_{w_1,w_2}$. This contradiction leads to $V_1 = \emptyset$. □

We recall from Section 2 that $N_Y[x]$ denotes the closed neighbourhood of x in Y. Let

$$N_Y(X) = \{y : y \in Y \text{ and } |N_X(y)| > 0\} \quad \text{and} \quad N_Y[X] = N_Y(X) \cup X.$$

We also set $\widetilde{N}_Y(X) = \{y : y \in Y \text{ and } N_X(y) \neq X\}$.

By Facts 11 and 12, every vertex of $V(G) \setminus N_{K_q}[V_1]$ is adjacent to every vertex of $N_{K_q}(V_1)$, which implies that $G \cong G_0 \vee (K_h | W_{h,h})$, where $G_0 = G \setminus N_{K_q}[V_1]$ and $|V_1| = h$. In the remainder of this section, G_0 is always as in the previous sentence. The next fact gives the structure of components of $\overline{G}_0$.

Fact 25. *If* H *is a component of* $\overline{G}_0$, *then either* $H \cong W_{t,j}$ *with* $0 \leqslant j \leqslant t$ *and* $t \geqslant 1$, *or* $H \cong D_{a,b}$ *with* $b \geqslant a \geqslant 2$, *or* $H \in \{K_1 \vee P_3, K_1 \vee P_4, K_1 \vee C_5, C_5, \overline{W}_{3,3}\}$. *Moreover, if* $H \cong D_{a,b}$ *with* $a + b \geqslant 6$, *then* $V_1 = \emptyset$ *with* $G \cong G_0$.

Proof. To avoid ambiguity, when we say that two vertices are adjacent, we always mean they are adjacent in G_0. When $V(H) \cap V_2 = \emptyset$, we have $V(H) \subseteq V(K_q)$. Thus $H \cong K_1 \cong W_{1,0}$. Next, we may suppose that $V(H) \cap V_2 \neq \emptyset$. Since $V_2 = S_{q-1} \cup S_{q-2}$ by Fact 9, we need to consider the following three cases:

*C*ase 1: $V(H) \cap S_{q-2} = \emptyset$.
This implies that $V(H) \cap S_{q-1} \neq \emptyset$. Let $x_1 \in V(H) \cap S_{q-1}$. Then there exists a unique vertex $w_{k_1} \in V(K_q)$, such that $x_1 w_{k_1} \in E(H)$. Since $Y_{w_{k_1}}$ is an independent set of G, we have $Y_{w_{k_1}} \cup \{w_{k_1}\} \subseteq V(H)$.

If $V(H) = Y_{w_{k_1}} \cup \{w_{k_1}\}$, then $H \cong K_t \cong W_{t,0}$, where $t = |Y_{w_{k_1}}| + 1 \geqslant 2$. Next, we suppose that $V(H) \neq Y_{w_{k_1}} \cup \{w_{k_1}\}$.

If $|Y_{w_{k_1}}| \geqslant 2$, then every vertex of the independent set $Y_{w_{k_1}}$ is adjacent to every vertex of $S_{q-1} \setminus Y_{w_{k_1}}$ by Fact 15. This implies $V(H) = Y_{w_{k_1}} \cup \{w_{k_1}\}$, which is a contradiction. Hence, $Y_{w_{k_1}} = \{x_1\}$.

Since $V(H) \neq Y_{w_{k_1}} \cup \{w_{k_1}\}$, x_1 is not adjacent to some vertex $y_1 \in Y_{w_h}$, where $h \neq k_1$. By Fact 15, we have $|Y_{w_h}| = 1$. Let S be a maximum independent set of $G_0[S_{q-1}]$ containing x_1. Then, $|S| \geqslant 2$. By the maximality of $|S|$ and Fact 18, we conclude that every vertex of $S' = S_{q-1} \setminus S$ (if not empty) is adjacent to every vertex

of S. Since $|Y_{w_{k_1}}| = 1$ holds for every $w_1 \in \widetilde{N}_{K_q}(S)$ by Fact 15, we have $Y_{w_{k_1}} \subset S$. Therefore, every vertex of $S' = S_{q-1} \setminus S$ is adjacent to every vertex of $\widetilde{N}_{K_q}(S)$. This implies $V(H) = S \cup \widetilde{N}_{K_q}(S)$, and so $H \cong W_{t,t}$, where $t = |S| \geqslant 2$.

Case 2: $V(H) \cap S_{q-1} = \emptyset$.

Let $x_1 \in V(H) \cap S_{q-2}$. Then there exists a unique pair $\{w_{k_1}, w_{l_1}\} \subset V(K_q)$ such that $x_1 \in X_{w_{k_1},w_{l_1}}$, that is, $x_1w_{k_1}, x_1w_{l_1} \in E(H)$. If $V(H) = X_{w_{k_1},w_{l_1}} \cup \{w_{k_1}, w_{l_1}\}$, then H is isomorphic to $W_{2,1}$ or $K_1 \vee P_3$, as $X_{w_{k_1},w_{l_1}}$ is an independent set and $|X_{w_{k_1},w_{l_1}}| \leqslant 2$ by Fact 16. Next, suppose that $V(H) \neq X_{w_{k_1},w_{l_1}} \cup \{w_{k_1}, w_{l_1}\}$. Since $V(H) \cap S_{q-1} = \emptyset$, there must exist $y_1 \in X_{w_{k_2},w_{l_2}}$ with $\{k_2, l_2\} \neq \{k_1, l_1\}$ such that y_1 is not adjacent to some vertex of $\{w_{k_1}, w_{l_1}\} \cup X_{w_{k_1},w_{l_1}}$.

By Fact 19, we have $|\{k_2, l_2\} \cap \{k_1, l_1\}| = 1$, and thus we may suppose that $k_1 = k_2$ and $l_2 \neq l_1$. Now, since $|\{k_2, l_2\} \cap \{k_1, l_1\}| = 1$, we have $X_{w_{k_1},w_{l_1}} = \{x_1\}$, $X_{w_{k_1},w_{l_2}} = \{y_1\}$ and $x_1y_1 \notin E(G)$ by Facts 19 and 22(i). If $V(H) = \{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$, then $H \cong W_{3,2}$.

Next, suppose that $V(H) \neq \{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. Then there must exist $z_1 \in X_{w_{k_3},w_{l_3}}$ such that $z_1 \notin \{x_1, y_1\}$ and z_1 is not adjacent to some vertex of $\{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. We claim that

$$|\{k_1, l_1\} \cap \{k_3, l_3\}| = 1 = |\{k_1, l_2\} \cap \{k_3, l_3\}|. \tag{3}$$

Indeed, by assuming that $|\{k_1, l_1\} \cap \{k_3, l_3\}| = 0$, on the basis of $\min\{|X_{w_{k_1},w_{l_1}}|, |X_{w_{k_3},w_{l_3}}|, |X_{w_{k_1},w_{l_2}}|\} \geqslant 1$ and Fact 23, we deduce $l_2 \notin \{k_3, l_3\}$, and thus $|\{k_1, l_2\} \cap \{k_3, l_3\}| = 0$. Now, from Fact 19, z_1 is adjacent to every vertex belonging to $\{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$, which is impossible, and this confirms (3).

We first suppose that $k_1 \notin \{k_3, l_3\}$. By (3), we have $\{k_3, l_3\} = \{l_1, l_2\}$ and thus $X_{w_{l_1},w_{l_2}} = \{z_1\}$ by Fact 22(i). We claim that $V(H) = \{x_1, y_1, z_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. Otherwise, there exists $z_2 \in X_{w_{k_4},w_{l_4}}$ such that $z_2 \notin \{x_1, y_1, z_1\}$ and z_2 is not adjacent to some vertex of $\{x_1, y_1, z_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. If z_2 is adjacent to every vertex of $\{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$, then $\{k_4, l_4\} \cap \{k_1, l_1, l_2\} = \emptyset$ by Fact 19, and thus $z_1z_2 \in E(G)$ holds by the same fact, which contradicts the choice of z_2. Thus, z_2 is not adjacent to some vertex of $\{x_1, y_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. By the symmetry of z_1 and z_2, we have $k_1 \in \{k_4, l_4\}$ by (3) (replacing $\{k_3, l_3\}$ with $\{k_4, l_4\}$) and $\{k_4, l_4\} \cap \{l_1, l_2\} = \emptyset$, as $X_{w_{l_1},w_{l_2}} = \{z_1\}$ and $z_2 \notin \{x_1, y_1, z_1\}$. Suppose that $k_4 = k_1$. Then $\min\{|X_{w_{k_1},w_{l_4}}|, |X_{w_{l_1},w_{l_2}}|, |X_{w_{k_1},w_{l_1}}|\} \geqslant 1$, contradicting Fact 23. This confirms our claim that $V(H) = \{x_1, y_1, z_1, w_{k_1}, w_{l_1}, w_{l_2}\}$. By Fact 19, $\{x_1, y_1, z_1\}$ is an independent set of G and thus $H \cong \overline{W}_{3,3}$.

Secondly, we suppose that $k_1 \in \{k_3, l_3\}$. By (3), we have $k_3 = k_1$ and $l_3 \notin \{l_1, l_2\}$. By Facts 19 and 22 (i), we have $X_{w_{k_1},w_{l_3}} = \{z_1\}$ with $x_1, y_1 \notin N_G(z_1)$. Since $\{x_1, y_1, z_1, w_{k_1}, w_{l_1}, w_{l_2}, w_{l_3}\} \subseteq V(H)$, there exists $c \geqslant 3$, such that c is as large as possible and $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\} \subseteq V(H)$, where $X_{w_{k_1},w_{s_i}} = \{x_{s_i}\}$ for $1 \leqslant i \leqslant c$.

Next, we show that

$$V(H) = \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\}. \tag{4}$$

Otherwise, there exists $z_2 \in X_{w_f,w_g}$ such that $z_2 \notin \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$ and z_2 is not adjacent to some vertex of $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\}$. By Fact 19, we have $|\{f, g\} \cap$

$\{k_1, s_1, s_2, \ldots, s_c\}| \geqslant 1$. By the choice of c and $z_2 \notin \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$, we have $k_1 \notin \{f, g\}$. Suppose that $f = s_1$ and $g \neq s_2$, as $c \geqslant 3$. Thus $\min\{|X_{w_{k_1},w_{s_2}}|, |X_{w_{s_1},w_g}|, |X_{w_{k_1},w_{s_1}}|\} \geqslant 1$, which contradicts Fact 23. Hence, (4) holds.

By Fact 19, $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$ is an independent set of G, and thus $H \cong W_{t,t-1}$ with $t = c + 1 \geqslant 4$.

Case 3: $V(H) \cap S_{q-2} \neq \emptyset$ and $V(H) \cap S_{q-1} \neq \emptyset$.

We show that H contains a pair of vertices x_1, y_1, such that $x_1 \in Y_{w_{k_1}}$ and $y_1 \in X_{w_{l_1},w_{r_1}}$ with $k_1 \in \{l_1, r_1\}$. Suppose that $k_1 \notin \{l_1, r_1\}$ holds for every pair of vertices $x_1 \in Y_{w_{k_1}}$ and $y_1 \in X_{w_{l_1},w_{r_1}}$. Take $V_{2,1} = S_{q-1} \cup \widetilde{N}_{K_q}(S_{q-1})$ and $V_{2,2} = S_{q-2} \cup \widetilde{N}_{K_q}(S_{q-2})$. By Fact 20, every vertex of $V_{2,1}$ is adjacent to every vertex of $V_{2,2}$. Thus, $\overline{G_0[V_{2,1} \cup V_{2,2}]}$ is disconnected, but this contradicts $V(H) \cap S_{q-2} \neq \emptyset$ and $V(H) \cap S_{q-1} \neq \emptyset$. By symmetry, we may suppose that $k_1 = r_1$, that is, $x_1 \in Y_{w_{k_1}}$ and $y_1 \in X_{w_{k_1},w_{l_1}}$. Let $U = \{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup X_{w_{k_1},w_{l_1}}$.

We first suppose that $U = V(H)$. If $Y_{w_{k_1}} \cup X_{w_{k_1},w_{l_1}}$ is an independent set of G, then $|X_{w_{k_1},w_{l_1}}| = 1$ by Fact 16, and thus $H \cong W_{t,1}$ with $t = |Y_{w_{k_1}}| + 2 \geqslant 3$. If $Y_{w_{k_1}} \cup X_{w_{k_1},w_{l_1}}$ is not an independent set of G, we may suppose that $x_1y_1 \in E(G)$, as $Y_{w_{k_1}}$ and $X_{w_{k_1},w_{l_1}}$ are both independent sets, and so $|Y_{w_{k_1}}| = 1$ by Fact 15. If $|X_{w_{k_1},w_{l_1}}| = 1$, then $H \cong P_4 \cong W_{2,2}$ (as $x_1y_1 \in E(G)$). If $|X_{w_{k_1},w_{l_1}}| = 2$, then x_1 is adjacent to exactly one vertex of $X_{w_{k_1},w_{l_1}}$ by Fact 16. This implies $H \cong K_1 \vee P_4$.

Now, we suppose that $U \neq V(H)$. There exists $z_1 \in V(H) \cap V_2$ such that $z_1 \notin U$ and z_1 is not adjacent to some vertex of U. We claim that

$$\text{either } z_1 \in X_{w_{k_1},w_{l_2}} \text{ with } l_2 \neq l_1, \text{ or } z_1 \in Y_{w_{l_1}}. \tag{5}$$

Since $z_1 \in V_2 = S_{q-1} \cup S_{q-2}$, we have either $z_1 \in X_{w_{k_2},w_{l_2}}$ or $z_1 \in Y_{w_{l_2}}$, for some vertices $w_{k_2}, w_{l_2} \in V(K_q)$.

If $z_1 \in X_{w_{k_2},w_{l_2}}$, we first show that $|\{k_1, l_1\} \cap \{k_2, l_2\}| = 1$. By way of contradiction and $z_1 \notin X_{w_{k_1},w_{l_1}}$, assume that $|\{k_1, l_1\} \cap \{k_2, l_2\}| = 0$. From Facts 19 and 20, z_1 is adjacent to every vertex of $\{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup X_{w_{k_1},w_{l_1}}$, which is impossible. Thus, $|\{k_1, l_1\} \cap \{k_2, l_2\}| = 1$. By Facts 19 and 22(i), we have $X_{w_{k_1},w_{l_1}} = \{y_1\}$, $X_{w_{k_2},w_{l_2}} = \{z_1\}$ and $y_1z_1 \notin E(G)$. Further, from $x_1 \in Y_{w_{k_1}}$ and Fact 22(ii), we get $\{k_1, l_1\} \cap \{k_2, l_2\} = \{k_1\}$.

If $z_1 \in Y_{w_{l_2}}$, then we show that $l_2 = l_1$. As before, assume that $l_2 \neq l_1$. Since $z_1 \notin Y_{w_{k_1}}$, it holds $l_2 \notin \{k_1, l_1\}$. By Fact 20, z_1 is adjacent to every vertex of $\{w_{k_1}, w_{l_1}\} \cup X_{w_{k_1},w_{l_1}}$, and thus we may suppose that $x_1z_1 \notin E(G)$ by the choice of z_1. But this contradicts Fact 22(ii), and so $l_2 = l_1$. By the former arguments, we have either $z_1 \in X_{w_{k_1},w_{l_2}}$ with $l_2 \neq l_1$ or $z_1 \in Y_{w_{l_1}}$ and (5) holds. Accordingly, we distinguish the following subcases.

Subcase 3.1: $z_1 \in X_{w_{k_1},w_{l_2}}$.

Here we have $X_{w_{k_1},w_{l_1}} = \{y_1\}$, $X_{w_{k_1},w_{l_2}} = \{z_1\}$ and $y_1z_1 \notin E(G)$, by Facts 19 and 22(i).

Since $\{y_1, z_1, w_{k_1}, w_{l_1}, w_{l_2}\} \cup Y_{w_{k_1}} \subseteq V(H)$, there exists $c \geqslant 2$ such that c is as large as possible and $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\} \cup Y_{w_{k_1}} \subseteq V(H)$, where $X_{w_{k_1},w_{s_i}} = \{x_{s_i}\}$ for $1 \leqslant i \leqslant c$. Next, we show that

$$V(H) = \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\} \cup Y_{w_{k_1}}. \tag{6}$$

Otherwise, there exists a vertex $z_2 \in V(H) \cap V_2$ not belonging to $z_2 \notin \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\} \cup Y_{w_{k_1}}$ and non-adjacent to any vertex of $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}, w_{k_1}, w_{s_1}, w_{s_2}, \ldots, w_{s_c}\} \cup Y_{w_{k_1}}$. Without loss of generality, we may suppose that z_2 is not adjacent to some vertex of $\{x_{s_1}, w_{k_1}, w_{s_1}\} \cup Y_{w_{k_1}}$. By (5) and the symmetry of z_1 and z_2, either $z_2 \in X_{w_{k_1},w_h}$ with $h \neq s_1$ or $z_2 \in Y_{w_{s_1}}$ holds.

If $z_2 \in Y_{w_{s_1}}$, then $\min\{|Y_{w_{s_1}}|, |X_{w_{k_1},w_{s_2}}|, |X_{w_{k_1},w_{s_1}}|\} \geqslant 1$, contradicting Fact 22(ii). Thus, we have $z_2 \in X_{w_{k_1},w_h}$ with $h \neq s_1$. Since $z_2 \notin \{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$, we have $h \notin \{s_1, s_2, \ldots, s_c\}$, contrary to the choice of c. Hence, (6) holds.

From Facts 19 and 21, it holds that $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$ and $Y_{w_{k_1}}$ are two independent sets of G, respectively. If $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\} \cup Y_{w_{k_1}}$ is also an independent set of G, then $H \cong W_{t,c}$, for $t = 1 + |Y_{w_{k_1}}| + c \geqslant 4$. Otherwise, by Facts 15 and 22(iii), we have $Y_{w_{k_1}} = \{x_1\}$ and x_1 is adjacent to every vertex of $\{x_{s_1}, x_{s_2}, \ldots, x_{s_c}\}$. This implies $H \cong W_{t,t}$, where $t = c + 1 \geqslant 3$.

*S*ubcase 3.2: $z_1 \in Y_{w_{l_1}}$.
We claim that

$$V(H) = \{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup Y_{w_{l_1}} \cup X_{w_{k_1},w_{l_1}}. \tag{7}$$

Otherwise, assume that there is a vertex z_2 satisfying $z_2 \in V(H) \cap V_2$ and $z_2 \notin \{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup Y_{w_{l_1}} \cup X_{w_{k_1},w_{l_1}}$, such that z_2 is not adjacent to some vertex of $\{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup Y_{w_{l_1}} \cup X_{w_{k_1},w_{l_1}}$. By the symmetry of k_1 and l_1, we may suppose that z_2 is not adjacent to some vertex of $\{w_{k_1}, w_{l_1}\} \cup Y_{w_{k_1}} \cup X_{w_{k_1},w_{l_1}}$. From (5) and the symmetry of z_1 and z_2, we have either $z_2 \in X_{w_{k_1},w_h}$ with $h \neq l_1$, or $z_2 \in Y_{w_{l_1}}$. Moreover, by the choice of z_2, we have $z_2 \in X_{w_{k_1},w_h}$, with $h \neq l_1$. Then $\min\{|Y_{w_{l_1}}|, |X_{w_{k_1},w_h}|, |X_{w_{k_1},w_{l_1}}|\} \geqslant 1$, but this contradicts Fact 22(ii). Hence, (7) is confirmed.

By symmetry, suppose that $1 \leqslant |Y_{w_{k_1}}| \leqslant |Y_{w_{l_1}}|$. Recall that $x_1 \in Y_{w_{k_1}}$, $z_1 \in Y_{w_{l_1}}$ and $y_1 \in X_{w_{k_1},w_{l_1}}$.

We first suppose that $|Y_{w_{l_1}}| = 1$, that is, $Y_{w_{k_1}} = \{x_1\}$ and $Y_{w_{l_1}} = \{z_1\}$. If $x_1z_1 \in E(G)$, then y_1 is not adjacent to any vertex of $\{x_1, z_1\}$ by Fact 14. By Fact 16, we have $X_{w_{k_1},w_{l_1}} = \{y_1\}$ and thus $H \cong D_{2,2}$. Otherwise, $x_1z_1 \notin E(G)$, and then, by Fact 14, $|N_G(y_1) \cap \{x_1, z_1\}| \in \{0, 2\}$ holds. Fact 16 ensures that every vertex of $\{x_1, z_1\}$ is adjacent to the same one vertex of $X_{w_{k_1},w_{l_1}}$ for the case $|X_{w_{k_1},w_{l_1}}| = 2$. Since $|X_{w_{k_1},w_{l_1}}| \leqslant 2$ and $X_{w_{k_1},w_{l_1}}$ is an independent set of G, by employing Fact 16, we arrive at $H \in \{K_1 \vee C_5, K_1 \vee P_4, C_5\}$.

Next, we suppose that $|Y_{w_{l_1}}| \geqslant 2$. By Facts 15 and 17, $Y_{w_{l_1}}$ is an independent set of G, and its every vertex is adjacent to every vertex of $Y_{w_{k_1}}$. In addition, $X_{w_{k_1},w_{l_1}} = \{y_1\}$ and y_1 is not adjacent to any vertex of $Y_{w_{l_1}} \cup Y_{w_{k_1}}$. This implies $H \cong D_{a,b}$, where $b = |Y_{w_{l_1}}| + 1 \geqslant 3$ and $a = |Y_{w_{k_1}}| + 1 \geqslant 2$.

Gathering the obtained conclusions, we obtain that H is as in the statement formulation.

Moreover, if $H \cong D_{a,b}$ with $b \geqslant a \geqslant 2$ and $a + b \geqslant 6$, by the former arguments, we deduce that $|Y_{w_{k_1}}| + |Y_{w_{l_1}}| = a + b - 2 \geqslant 4$ and $|X_{w_{k_1},w_{l_1}}| = 1 \leqslant \min\{|Y_{w_{k_1}}|, |Y_{w_{l_1}}|\}$. By Fact 24, we have $V_1 = \emptyset$, which yields $G \cong G_0$. □

In the next result, we consider one possibility for a component of $\overline{G}_0$; in fact, it is a further characterization of G_0.

Fact 26. *If H is a non-complete component of $\overline{G}_0$ with independence number p, then $P_3 \cup (p-2)K_1 \subset H$.*

Proof. Due to Fact 25, we immediately have that the diameter of H is at most 3 and $K_{1,3} \not\subset H$. Suppose that $U = \{v_1, v_2, \ldots, v_p\}$ is a maximum independent set of H. Since H is non-complete we have $p \geqslant 2$ and $P_3 \subset H$. Hence, the desired conclusion holds for $p = 2$. Suppose that $p \geqslant 3$. If the distance between v_1 and v_2 is equal to 2, then let $P : v_1uv_2$ be an induced path of H. Since $K_{1,3} \not\subset H$, by taking into account that the diameter of H does not exceed 3, we deduce that $N_H(v_i) \cap V(P) = \emptyset$ holds for $3 \leqslant i \leqslant p$, which implies $P_3 \cup (p-2)K_1 \subset H$.

We next suppose that the distance between v_1 and v_2 is at least 3. Taking into account the diameter of H, we conclude that this distance is exactly 3. Let $P : v_1u_1u_2v_2$ be an induced path of H. If $N_H(v_i) \cap V(P) = \emptyset$ holds for $3 \leqslant i \leqslant p$, then we have what we need: $P_3 \cup (p-2)K_1 \subset H$. By the symmetry, we next assume that $N_H(v_3) \cap V(P) \neq \emptyset$. Then $N_H(v_3) \cap V(P) = \{u_1, u_2\}$ holds, as $K_{1,3} \not\subset H$ and U is an independent set. In other words, $V(P) \cup \{v_3\}$ induces $W_{3,2}$. Since $P_3 \cup K_1 \subset W_{3,2} \subset H$, we further suppose that $p \geqslant 4$. If there exists a vertex of $\{v_4, v_5, \ldots, v_p\}$, say v_4, such that $N_H(v_4) \cap V(P) \neq \emptyset$, then $N_H(v_4) \cap V(P) = \{u_1, u_2\}$, as before. But this implies that $\{v_1, u_1, v_3, v_4\}$ induces $K_{1,3}$, which is eliminated at the beginning of this proof. Hence, $N_H(v_i) \cap V(P) = \emptyset$ holds for $4 \leqslant i \leqslant p$, which implies $W_{3,2} \cup (p-3)K_1 \subset H$. The desired result follows from $P_3 \cup (p-2)K_1 \subset W_{3,2} \cup (p-3)K_1$. □

We proceed to consider the existence of $D_{a,b}$ in the collection of components of $\overline{G}_0$. First, we limit the parameters a and b as follows.

Fact 27. *Let $D_{a,b}$ be a component of $\overline{G}_0$. If $b \geqslant a \geqslant 4$ or $b \geqslant 6$ and $a = 3$, then either $\overline{G} \subset D_{4,4} \cup H$ for $H \in \{3K_1 \cup \overline{W}_{3,3}, 4K_1 \cup C_5, W_{6,6}, 5K_1 \cup K_4\}$ or $\overline{G} \subset D_{3,6} \cup H$ for $H \in \{3K_1 \cup \overline{W}_{3,3}, 4K_1 \cup C_5, W_{6,6}\}$.*

Proof. By Fact 25, we have $G_0 \cong G$ for $a + b \geqslant 6$. Since $6K_1 \cup D_{4,5}$ and $6K_1 \cup D_{3,7}$ are not σ-graphs, we have $6K_1 \cup D_{4,5} \not\subset \overline{G}$ and $6K_1 \cup D_{3,7} \not\subset \overline{G}$. As $\omega(G) \geqslant 8$, for $b \geqslant a \geqslant 4$ or $b \geqslant 6$ and $a = 3$, we have either $a = b = 4$ or $b = 6$ and $a = 3$. Let $F \in \{D_{4,4}, D_{3,6}\}$ be a component of $\overline{G}$. We shall distinguish these possibilities for F in the end of the proof; at this moment it is sufficient to take that F is one of these graphs. Since $7K_1 \cup F \not\subset \overline{G}$ and $|V(F) \cap V(K_q)| = 2$, we have $q = 8$.

We claim that $\overline{G}$ contains at most two non-trivial components. Otherwise, suppose that G_1, G_2 are non-trivial components distinct from F. Since $F \cup 2P_3 \cup 2K_1 \not\subset \overline{G}$, $F \cup P_3 \cup K_2 \cup 3K_1 \not\subset \overline{G}$ and $\omega(G) = 8$, Fact 26 implies that both G_1 and G_2 are complete. Consequently, $F \cup 2K_2 \cup 4K_1 \subset \overline{G}$, which contradicts $\lambda_2(G) \leqslant \sigma$. Thus, $\overline{G}$ contains at most two non-trivial components, as claimed.

Assume that $\overline{G}$ is not an induced subgraph of $F \cup H$ for $H \in \{3K_1 \cup \overline{W}_{3,3}, 4K_1 \cup C_5, W_{6,6}\}$. Then, $\overline{G}$ contains exactly two non-trivial components, as $\omega(G) = 8$ and $F \cup$

$6K_1 \subset F \cup W_{6,6}$. Let G_1 be the other non-trivial component. By the assumption, we have $G_1 \notin \{\overline{W}_{3,3}, C_5, W_{6,6}\}$. Since $F \cup D_{2,2} \not\subset \overline{G}$ and $F \cup 4K_1 \cup (K_1 \vee P_3) \not\subset \overline{G}$, we have $G_1 \cong W_{c,j}$ for $0 \leqslant j \leqslant c$ by Fact 25, as $G_1 \notin \{\overline{W}_{3,3}, C_5\}$.

We claim that $j \in \{0, c-1, c\}$. Otherwise, there would be $\omega(\overline{W}_{c,j}) = j+1$ and $F \cup W_{3,1} \cup 4K_1 \subset F \cup W_{c,j} \cup (5-j)K_1 \cong \overline{G}$, as $\omega(G) = 8$ and $W_{3,1} \cup (j-1)K_1 \subset W_{c,j}$. This contradicts $W_{3,1} \cup 4K_1 \cup F \not\subset \overline{G}$. Thus, $j \in \{0, c-1, c\}$, and this implies that $\overline{G}$ is isomorphic to either $F \cup K_c \cup 5K_1$ for $c \geqslant 2$, or $F \cup W_{c,c-1} \cup (6-c)K_1$ for $2 \leqslant c \leqslant 6$, or $F \cup W_{c,c} \cup (6-c)K_1$ for $2 \leqslant c \leqslant 6$. Combining this with $\overline{G} \not\subset F \cup W_{6,6}$, we obtain $H \cong K_c$ for $c \geqslant 2$.

It remains to consider F. If $F \cong D_{4,4}$, then $\overline{G} \subset D_{4,4} \cup 5K_1 \cup K_4$, as $D_{4,4} \cup 5K_1 \cup K_5 \not\subset \overline{G}$. Otherwise, we have $F \cong D_{3,6}$. Since $D_{3,6} \cup 5K_1 \cup K_3 \not\subset \overline{G}$, it holds $\overline{G} \subset D_{3,6} \cup 5K_1 \cup K_2 \subset D_{3,6} \cup 4K_1 \cup C_5$, which contradicts the assumption of $\overline{G}$. This completes the proof. □

Now, we set $a = 2$.

Fact 28. *Let $D_{2,b}$ be a component of $\overline{G}_0$. If $b \geqslant 19$, then $\overline{G}$ is an induced subgraph of some graph of $\{D_{2,27} \cup 6K_1, D_{2,21} \cup W_{6,6}, D_{2,21} \cup \overline{W}_{3,3} \cup 3K_1, D_{2,21} \cup C_5 \cup 4K_1, D_{2,19} \cup K_4 \cup 5K_1\}$.*

Proof. We denote $H \cong D_{2,b}$. By Fact 25, we have $G_0 \cong G$ even for $b \geqslant 4$. Since $b \geqslant 19$ and $7K_1 \cup D_{2,14} \not\subset \overline{G}$, we have $q = 8$.

We claim that $\overline{G}$ contains at most two non-trivial components. Otherwise, suppose that G_1, G_2 are two non-trivial components distinct from H. Note that $D_{2,19} \cup 2K_2 \cup 4K_1 \not\subset \overline{G}$. Since $D_{2,19} \cup 2P_3 \cup 2K_1 \not\subset \overline{G}$, $D_{2,19} \cup P_3 \cup K_2 \cup 3K_1 \not\subset \overline{G}$ and $\omega(G) = 8$, G_1 and G_2 are complete by Fact 26, which leads to the impossible scenario $D_{2,19} \cup 2K_2 \cup 4K_1 \subset \overline{G}$.

If $D_{2,t}$ is the unique non-trivial component of $\overline{G}$, then $\overline{G} \subset D_{2,27} \cup 6K_1$, as $D_{2,28} \cup 6K_1 \not\subset \overline{G}$. Next, let G_1 be the other (apart from H) non-trivial component. Since $D_{2,12} \cup D_{2,2} \not\subset \overline{G}$ and $D_{2,13} \cup G_1 \cup 4K_1 \not\subset \overline{G}$ for $G_1 \in \{W_{3,1}, K_1 \vee P_3\}$, by Fact 25 we have

$$G_1 \in \{C_5, \overline{W}_{3,3}, W_{c,c-1}, W_{c,c}, K_c\}, \text{ for a proper } c \geqslant 2. \tag{8}$$

For $G_1 \cong \overline{W}_{3,3}$, since $D_{2,22} \cup \overline{W}_{3,3} \cup 3K_1 \not\subset \overline{G}$, we obtain $b \leqslant 21$. It follows that $\overline{G} \subset D_{2,21} \cup \overline{W}_{3,3} \cup 3K_1$. For $G_1 \cong C_5$, from $D_{2,22} \cup C_5 \cup 4K_1 \not\subset \overline{G}$, we deduce $b \leqslant 21$, and thus $\overline{G} \subset D_{2,21} \cup C_5 \cup 4K_1$. For $G_1 \in \{W_{c,c}, W_{c,c-1}\}$ for some $c \geqslant 2$, we have $b \leqslant 21$, as follows from $D_{2,22} \cup P_3 \cup 4K_1 \not\subset \overline{G}$ and Fact 26. This implies $\overline{G} \subset D_{2,21} \cup W_{6,6}$.

The remaining case of (8) is $G_1 \cong K_c$, for $c \geqslant 2$. Since $D_{2,22} \cup K_2 \cup 5K_1 \not\subset \overline{G}$, we have $b \leqslant 21$. When $20 \leqslant b \leqslant 21$, from $D_{2,20} \cup K_3 \cup 5K_1 \not\subset \overline{G}$ we have $c = 2$. Then $\overline{G} \subset D_{2,21} \cup K_2 \cup 5K_1 \subset D_{2,21} \cup W_{6,6}$. When $b = 19$, from $D_{2,19} \cup K_5 \cup 5K_1 \not\subset \overline{G}$ we have $c \leqslant 4$. Then $\overline{G} \subset D_{2,19} \cup K_4 \cup 5K_1$.

Gathering the obtained possibilities for $\overline{G}$, we arrive at the desired result. □

We are in position to prove Theorem 7.

Proof of Theorem 7. The sufficiency for (i) follows from Corollary 6, whereas for (ii)–(iv) it is confirmed by direct computation.

We proceed with the necessity, i.e., we assume that G is as in the statement of the theorem. As noted before Fact 25, we have $G \cong G_0 \vee (K_h | W_{h,h})$ with $V(G_0) = V(G) \setminus$

$N_{K_q}[V_1]$. If $\overline{G}_0$ does not contain $D_{a,b}$ as a component, then each component of $\overline{G}_0$ is an induced subgraph of either $W_{c,c}$, or $\overline{W}_{3,3}$, or $K_1 \vee C_5$, as follows from Fact 25. Therefore, there exists a sufficiently large $s \geqslant h$, such that $G \subset H_s \vee (K_s|W_{s,s})$ where $\overline{H}_s = s((K_1 \vee C_5) \cup \overline{W}_{3,3} \cup W_{s,s})$. In other words, G is an induced subgraph of some graph of $\mathcal{D}$, as in (i).

We next suppose that $D_{a,b}$ is a component of $\overline{G}_0$. For $b \geqslant 19$ and $a = 2$, or $b \geqslant a \geqslant 4$, or $b \geqslant 6$ and $a = 3$, Facts 27 and 28 lead to (ii)–(iv). If either $a = 2$ and $4 \leqslant b \leqslant 18$, or $a = 3 \leqslant b \leqslant 5$, then $G \cong G_0$ by Fact 25. This implies that $\overline{G}$ contains a special component, which contradicts the assumption of this theorem. The remaining possibility is $a = 2 \leqslant b \leqslant 3$. Once again, by Fact 25, each component of $\overline{G}_0$ is an induced subgraph of either $W_{c,c}$, or $D_{2,3}$, or $\overline{W}_{3,3}$, or $K_1 \vee C_5$. As before, this leads to the conclusion that G is as in (i). The proof is completed. □

Corollary 29 (**Necessity in Theorem 2**). *Let G be a σ-graph satisfying either*

(i) $\omega(G) \geqslant 54$ or

(ii) $\omega(G) \geqslant 8$ and G has a pendant vertex.

Then G is an induced subgraph of some graph of $\mathcal{D} \cup \{\overline{D}_{2,4} \vee K_{52}\}$.

Proof. We first suppose that G satisfies (ii). If $\overline{G}_0$ contains $D_{a,b}$ as a component for $a + b \geqslant 6$, then Fact 25 yields $V_1 = \emptyset$, and thus $V(G) = V_2 \cup V(K_q)$. Since every vertex of V_2 is adjacent to at least two vertices of K_q, G has no pendant vertex, which contradicts the assumption of this corollary. It remains to consider the case in which $D_{a,b}$, for $a+b \geqslant 6$, does not appear as a component of $\overline{G}_0$. Then, by virtue of Fact 25, for every component H of $\overline{G}_0$ we have either $H \cong W_{t,j}$ with $0 \leqslant j \leqslant t$ and $t \geqslant 1$, or $H \cong D_{a,b}$ with $2 \leqslant a \leqslant b \leqslant 3$, or $H \in \{K_1 \vee P_3, K_1 \vee P_4, K_1 \vee C_5, C_5, \overline{W}_{3,3}\}$. In the first case we have $H \subset W_{t,t}$; in the second case, we have $H \subset D_{2,3}$; in the third case, we have $H \subset K_1 \vee C_5$ or $H \subset \overline{W}_{3,3}$. Summa summarum, G is an induced subgraph of some graph of $\mathcal{D}$.

In the remainder of the proof we suppose that G satisfies item (i) of the corollary. If $\overline{G}$ has no any special component, then one of items (i)–(iv) of Theorem 7 holds. Moreover, if G is as in Theorem 7(ii)–(iv), then $\omega(G) < 54$ (even more, it is at most 8) contrary to the assumption of the corollary. The remaining possibility (that is Theorem 7(i)) states that G is an induced subgraph of some graph of $\mathcal{D}$.

Otherwise, $\overline{G}$ contains a special component $D_{a,b}$. If $b \geqslant a \geqslant 3$, then $17K_1 \cup D_{3,3} \subset \overline{G}$ (as $\omega(G) \geqslant 54$ and $\omega(\overline{D}_{a,b}) = 2$), but this is impossible since $\lambda_2(K_{17} \vee \overline{D}_{3,3}) > 0.619 > \sigma$. Hence, $b \geqslant 4$ and $a = 2$. Together with $53K_1 \cup D_{2,4} \not\subset \overline{G}$, this implies $\omega(G) = 54$. Next, from $\omega(G) = 54$ and $19K_1 \cup D_{2,5} \not\subset \overline{G}$, we obtain $b = 4$. For $(a, b) = (2, 4)$, Fact 25 implies $G \cong G_0$. Thus, we only need to determine the structure of G_0.

We claim that $D_{2,4}$ is the unique non-trivial component of $\overline{G} \cong \overline{G}_0$. Otherwise, suppose that H is another non-trivial component. If H is a complete graph, then we have $F_1 \cong D_{2,4} \cup K_2 \cup 51K_1 \subset \overline{G}$, since $\omega(G) = 54$ and $\omega(\overline{D}_{2,4} \vee \overline{H}) = 3$. If H is non-complete, applying Fact 26 to H and $\overline{G}$ (in the role of $\overline{G}_0$), we arrive at $F_2 \cong D_{2,4} \cup P_3 \cup 50K_1 \subset \overline{G}$,

since $\omega(G) = 54$ and $\omega(\overline{D_{2,4} \cup P_3}) = 4$. Both possibilities are eliminated because $\overline{F_1}$ and $\overline{F_2}$ are not σ-graphs as confirmed directly.

Since $D_{2,4}$ is the unique non-trivial component of $\overline{G}$, we have $\overline{G} \cong D_{2,4} \cup kK_1$. From $\omega(G) = 54$ and $\omega(\overline{D}_{2,4}) = 2$, we obtain $k = 52$, and thus $\overline{G} \cong D_{2,4} \cup 52K_1$. The proof is completed. □

5 Concluding remarks

Here we mention some details observed during the research, give directions for future works and make more comparisons with the existing results. To make the reading easier, for some notions introduced in the previous sections we refer to the first occurrence in the text.

We have determined the σ-graphs whose clique number is at least 54. Simultaneously, we have established all σ-graphs whose clique number is at least 8, under the additional assumption that they contain at least one pendant vertex. At the first glance, someone would expect a long list of the resulting graphs, but it occurs that they fall into the induced subgraphs of exactly two structured types (if we consider the class $\mathcal{D}$ as one of them and the single graph $\overline{D}_{2,4} \vee K_{52}$ as the other one).

The next natural step would be to consider the remaining σ-graphs whose clique number is at least 8, where 'remaining' refers to those without pendant vertices. Theorem 7 can be seen as a first step in this direction, as it provides the desired σ-graphs G under the caveat that $\overline{G}$ has no any special component, where a special component is defined upon the same theorem. Next, if $\overline{G}$ has a special component, then by Fact 25, we have $G \cong G_0$; again, G_0 is defined upon the same fact. With slight modifications in the proofs of Facts 27 and 28, one may extend the result of Theorem 7. For example, the case in which $\overline{G}$ has the special component $D_{2,18}$ can be easily resolved, since there $\omega(G) = 8$ must hold (provided by $7K_1 \cup D_{2,14} \not\subset \overline{G}$). However, it seems that extending Facts 27 and 28, and consequently Theorem 2, to cover all the remaining special components would be a rather difficult task.

Besides, σ-graphs G satisfying $8 \leqslant \omega(G) \leqslant 53$ can be considered from the following perspective. By Theorem 7, we may suppose that $\overline{G}$ contains at least one special component (say $D_{a,b}$). In this case, by Fact 25, we have $V_1 = \emptyset$ and $G \cong G_0$. Since $D_{2,4} \cup D_{3,3} \not\subset \overline{G}$, $2D_{2,4} \not\subset \overline{G}$ and $2D_{3,3} \not\subset \overline{G}$, we deduce that $\overline{G}$ contains exactly one special component. Now, from Fact 25, we obtain that $\overline{G}$ is isomorphic to

$$D_{a,b} \cup a_1(K_1 \vee P_3) \cup a_2(K_1 \vee P_4) \cup a_3(K_1 \vee C_5) \cup a_4 C_5 \cup a_5 \overline{W_{3,3}} \cup a_6 D_{2,2} \cup a_7 D_{2,3} \cup \bigcup_{i=1}^{a_8} W_{t_i,j_i} \cup \bigcup_{i=1}^{a_9} K_{s_i},$$

where $a_i \geqslant 0$ for $1 \leqslant i \leqslant 9$, $t_i \geqslant j_i \geqslant 1$ for $0 \leqslant i \leqslant a_8$, $s_i \geqslant 1$ for $0 \leqslant i \leqslant a_9$ and $D_{a,b}$ is a special component of $\overline{G}$ (with a convention that $\bigcup_{i=1}^{0} F_i$ is an empty graph).

On the basis of Fact 25, we determine connected graphs with given clique number and $\lambda_2 \leqslant \frac{1}{2}$.

Proposition 30. *Let G be a connected graph with clique number at least 19. Then $\lambda_2(G) < \frac{1}{2}$ if and only if each component of $\overline{G}$ is either K_r with $r \geqslant 1$, or $W_{2,1}$, or $W_{3,1}$.*

Proof. By using the Courant-Weyl Inequalities, we get $\lambda_2(G) + \lambda_{\min}(\overline{G}) \leqslant \lambda_2(K_n) = -1$. One can easily check that $\lambda_{\min}(H) > -\frac{3}{2}$ holds for $H \in \{K_r, W_{2,1}, W_{3,1}\}$. Therefore, $\lambda_2(G) < \frac{1}{2}$ holds for every graph given in the statement of this proposition.

For the necessity, we always suppose that $\omega(G) = q \geqslant 19$ and K_q is a fixed maximum clique of G.

Since $\lambda_2(G) < \frac{1}{2} < \frac{\sqrt{5}-1}{2}$, Fact 25 remains valid for G. Since the set V_1, of vertices in $V(G) \setminus V(K_q)$ having exactly one neighbour in K_q, is empty (as follows directly by taking into account $q \geqslant 19$ and $\lambda_2 < \frac{1}{2}$), we may reformulate this fact as follows.

Fact 17′. *For any component H of $\overline{G}$, there is either $H \cong W_{t,j}$ with $0 \leqslant j \leqslant t$ and $t \geqslant 1$, or $H \cong D_{a,b}$ with $b \geqslant a \geqslant 2$, or*

$$H \in \{K_1 \vee P_3, K_1 \vee P_4, K_1 \vee C_5, C_5, \overline{W}_{3,3}\}.$$

We discuss the possibilities for H. If $H \cong K_r$ for some $r \geqslant 1$, we are done. Next, we assume that H is not a complete graph. By Fact 17′, either $H \cong W_{t,j}$ with $1 \leqslant j \leqslant t$ and $t \geqslant 2$ (note that $W_{t,0} \cong K_t$ and $W_{1,1} \cong K_2$), or $H \cong D_{a,b}$ with $b \geqslant a \geqslant 2$, or $H \in \{K_1 \vee P_3, K_1 \vee P_4, K_1 \vee C_5, C_5, \overline{W}_{3,3}\}$.

Since $\lambda_2(\overline{P_4}) = \frac{\sqrt{5}-1}{2} > \frac{1}{2}$, we obtain $P_4 \not\subset \overline{G}$. So, the case $H \in \{K_1 \vee P_4, K_1 \vee C_5, C_5, \overline{W}_{3,3}\}$ cannot occur. Observing that $\omega(\overline{D_{a,b}}) = \omega(\overline{K_1 \vee P_3}) = 2$ and taking into account the restriction $q \geqslant 19$, we obtain $H \cong W_{t,j}$ with $1 \leqslant j \leqslant t$ and $t \geqslant 2$, as $\lambda_2(\overline{D_{2,2} \cup 5K_1}) > \frac{1}{2}$ and $\lambda_2(\overline{(K_1 \vee P_3) \cup 2K_1}) > \frac{1}{2}$.

Since $P_4 \not\subset \overline{G}$, we have $j = 1$ and $t \geqslant 2$. We also have $\omega(\overline{W_{t,1}}) = 2$, along with $\lambda_2(\overline{W_{4,1} \cup 17K_1}) > \frac{1}{2}$. Hence, $t \leqslant 3$, which implies $H \cong W_{3,1}$ for $t = 3$ and $H \cong W_{2,1}$ for $t = 2$. □

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Spectral characterization of the complete graph removing a cycle



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ABSTRACT

A graph is determined by its spectrum if there is not another graph with the same spectrum. Cámara and Haemers proved that the graph $K_n \setminus C_k$, obtained from the complete graph K_n with n vertices by deleting all edges of a cycle C_k with k vertices, is determined by its spectrum for $k \in \{3, 4, 5\}$, but not for $k = 6$. In this paper, we show that $k = 6$ is the unique exception for the spectral determination of $K_n \setminus C_k$.

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1. Introduction

For a graph $G = G(V, E)$, we denote by n the number of its vertices (also known as the *order* of G) and by $A(G)$ its adjacency matrix. The *eigenvalues* of G are the eigenvalues of $A(G)$, and they form the multiset $S(G)$ known as the *spectrum* of G. Since $A(G)$ is real and symmetric, the eigenvalues $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ of G are real. Throughout the paper we assume that the eigenvalues are indexed non-increasingly.

If G and H share the same spectrum, then we say that they are *cospectral*. We say that a graph G is determined by its spectrum if every graph cospectral with G is isomorphic to G. In this case we briefly say that G is a *DS graph*.

We denote the complete graph, complete bipartite graph, the path and the cycle with n vertices by K_n, $K_{s,t}$ (with $s + t = n$), P_n and C_n, respectively. In particular, $K_{1,n-1}$ denotes a star with n vertices. If H is a subgraph of G, then we write $G \setminus H$ to denote the graph obtained from G by deleting all the edges of H.

Cámara and Haemers [2] conjectured that $K_n \setminus P_k$ is *DS* for every $2 \leq k \leq n$. The conjecture has been confirmed for $k = n$ [8], $2 \leq k \leq 6$ [2], $7 \leq k \leq 9$ [20], and $k \geq 20$ [19]. Recently, the remaining case $10 \leq k \leq 19$ has been settled in [18], and thus the conjecture is resolved positively.

The authors of [2] also proved that, except for exactly one pair of non-isomorphic cospectral graphs, every graph obtained from the complete graph by deleting at most five edges is *DS*. This implies that $K_n \setminus C_k$ is *DS* for $k \in \{3, 4, 5\}$. However, they also discovered that for $n \geq 7$ the graph $K_n \setminus C_6$ is not *DS*, as it is cospectral with $K_n \setminus Z_{2,2,2}$ (where $Z_{2,2,2}$ is the graph illustrated in the forthcoming Fig. 3). Since $K_6 \setminus C_6$ is regular and every graph cospectral with a regular graph is also regular [7, Proposition 2], we can easily see that $K_6 \setminus C_6$ is *DS*. In this paper, we show that $k = 6$ is the only exception for the spectral determination of $K_n \setminus C_k$, i.e., we prove that $K_n \setminus C_k$ is *DS* provided $k \geq 7$.

Our main result and the concept of its proof are given in Section 2. Section 3 contains the additional terminology and notation along with some known and some initial results. The proof is given in Sections 4–9 and the Appendix. Some concluding remarks are given in Section 10.

2. Main result and the concept of its proof

Our main result reads as follows.

Theorem 2.1. *For $k \geq 3$ and $k \neq 6$, if Γ is a graph cospectral with $K_n \setminus C_k$, then Γ and $K_n \setminus C_k$ are isomorphic.*

Throughout the paper we exclusively reserve the symbol Γ for a graph described in the previous theorem. The concept of our proof does not deviate from those used in [2, 8,18–20], i.e., we derive some structural and spectral properties of Γ and its complement $\overline{\Gamma}$, and then use them to narrow down the search on Γ. The proof is considerably long

and straightforward in some parts, but nevertheless we present the full details on all theoretical considerations. However, we frequently deal with the particular eigenvalues of some comparatively small graphs without a reference. We believe that they can easily be computed, and that such details should be omitted.

Contrary to the DS-problem for $K_n \setminus P_k$ [8,18–20], where computing the spectrum of $K_n \setminus P_k$ has been a difficult challenge, the spectrum for $K_n \setminus C_k$ is determined directly (see the forthcoming Lemma 5.1). However, even if we know the spectrum, the proof that $K_n \setminus C_k$ is DS for $k \neq 6$ has instances that do not appear for $K_n \setminus P_k$; the main task is the elimination of a comparatively large number of candidates for cospectral graphs. To deal with this task, we develop several techniques and particular approaches. In relation to this, we note that finding a simple method for dealing with spectral determination of graphs obtained by removing a sparse subgraph from K_n remains as an interesting challenge for future research.

Here is the outline of the proof. Each part is separated in the corresponding section.

1. Throughout the paper we use certain forbidden induced subgraphs defined in Section 4.
2. Section 5 is a preparatory one. There we compute the spectrum of $K_n \setminus C_k$. We also prove that there must be $\lambda_2(\overline{\Gamma}) < 2$ and $\lambda_n(\Gamma) > -3$. On the basis of these results, we prove that $\overline{\Gamma}$ can eventually be a graph that consists of a c-cyclic graph Γ^* and a forest whose components are paths and the particular trees that fall into the four fixed types. The case in which the maximum vertex degree in $\overline{\Gamma}$ does not exceed 2 is resolved in this section; it results in $\Gamma = K_n \setminus C_k$. Additional structural properties of Γ^* are given.
3. In Section 6 we narrow down the possibilities for Γ^* by excluding all except a unicyclic graph or a tree.
4. In Section 7 we exclude the possibility that Γ^* is a tree.
5. In Section 8 we prove that Γ^* is not a unicyclic graph whose girth is at least 4 if the maximum vertex degree of $\overline{\Gamma}$ is greater than 2. Thus, under the assumption on the maximum vertex degree, it remains that Γ^* can eventually be a unicyclic graph with a triangle.
6. In Section 9 we eliminate the last possibility for Γ^* and finalize the proof.
7. The proofs of some lemmas formulated in Sections 6 and 9 are long, technical and similar to the proofs of the other statements. Therefore, we separate them in the Appendix. In this way we present the proofs of all results, but put the focus on the most relevant ones and make reading the text easier.

3. Preliminaries

We write I_n and J_n for the identity matrix and the all-1 matrix of size $n \times n$, respectively. We use $G \cup H$ to denote the disjoint union of graphs G and H. In particular, the disjoint union of k copies of G is denoted by kG. We denote the degree of a vertex u

of a graph G by $d_G(u)$. A *t-vertex* is a vertex with degree t, and a *t-regular graph* is a graph in which every vertex is a t-vertex. A 0-vertex and a 1-vertex are referred to as an *isolated vertex* and a *pendant vertex*, respectively. An isolated vertex considered as a component of a disconnected graph is called a *trivial component*. We denote by $\Delta(G)$ and $\delta(G)$ the maximum and the minimum vertex degree in G, respectively. We write $\eta(G)$ to denote the number of non-trivial components of a graph G, and $\varepsilon(F)$ for the number of non-trivial paths considered as components of a forest F.

Further, we denote by $\tau(G)$, $m_1(G)$, $m_2(G)$, $m_3(G)$ and $m_4(G)$ the numbers of distinct (not necessarily induced) subgraphs of G that are isomorphic to C_3, P_3, $2K_2$, P_4 and C_4, respectively.

A connected graph is said to be *c-cyclic* if it has $n + c - 1$ edges and n vertices. In particular a 0-cyclic, a 1-cyclic, a 2-cyclic and a 3-cyclic graph are referred to as a *tree*, a *unicyclic graph*, a *bicyclic graph* and a *tricyclic graph*, respectively. The *girth* of a unicyclic graph is the number of vertices in its unique cycle. A cycle in a graph with an even (resp. odd) number of vertices is referred to as an *even* (*odd*) cycle.

For a graph G, we denote by $\overline{G}$ its *complement* and we denote by $G[X]$ the subgraph induced by the vertex subset $X \subseteq V(G)$. We write $\mathrm{rank}(G)$ to denote the rank of the adjacency matrix of G.

A hereditary property of G is a property that is also a property of each induced subgraph of G. For example, $\Delta(G) < s$ and $\lambda_1(G) \leq s$, for $s \in \mathbb{N}$, are such properties. On the other hand, if G does not pose a given hereditary property, then it is referred to as a *forbidden induced subgraph* for that property.

Suppose that u is a non-internal vertex of a path P, and v is a vertex of a graph G, where P and G are vertex-disjoint. By inserting the edge uv we get a graph *obtained by attaching the path P to the vertex v of G*. A path $P_s = u_1u_2\cdots u_s$ with $s \geq 2$ is called a *pendant path* of G if $d_G(u_s) = 1 < d_G(u_{s-1}) = d_G(u_{s-2}) = \cdots = d_G(u_2) = 2 < d_G(u_1)$. Next, u_1 is referred to as an *initial vertex* of P_s.

Throughout the paper, let Δ_4, Δ_5, Δ_6, H_1, H_2, $\ldots$, H_{14} and Θ_{s_1,s_2,s_3} be the graphs illustrated in Fig. 1, and let L_1, L_2, $\ldots$, L_{16} be the graphs illustrated in Fig. 2.

We proceed by defining more particular graphs.

Definition 3.1.

(i) Let W_q ($q \geq 6$) be the tree with q vertices obtained from the path $P_{q-2} = u_1u_2\cdots u_{q-2}$ and two isolated vertices u_{q-1} and u_q by adding two edges u_2u_{q-1} and $u_{q-3}u_q$.

(ii) Let $Z_{s_1,s_2,\ldots,s_t}$ be the tree obtained by attaching t ($t \geq 3$) paths $P_{s_1}, P_{s_2}, \ldots, P_{s_t}$ to a single vertex. Next, if $s_1 \geq s_2 \geq \cdots \geq s_t$, then $Z_{s_1,s_2,\ldots,s_t}(j)$ is the graph obtained from $Z_{s_1,s_2,\ldots,s_t}$ by attaching an isolated vertex to the 2-vertex at distance j from the initial vertex of the pendant path P_{s_1}.

(iii) Let $U_{3;s,t}$ be the unicyclic graph obtained from a triangle C_3 by attaching one path P_s to a vertex of C_3, and then attaching another path P_t to a different vertex of

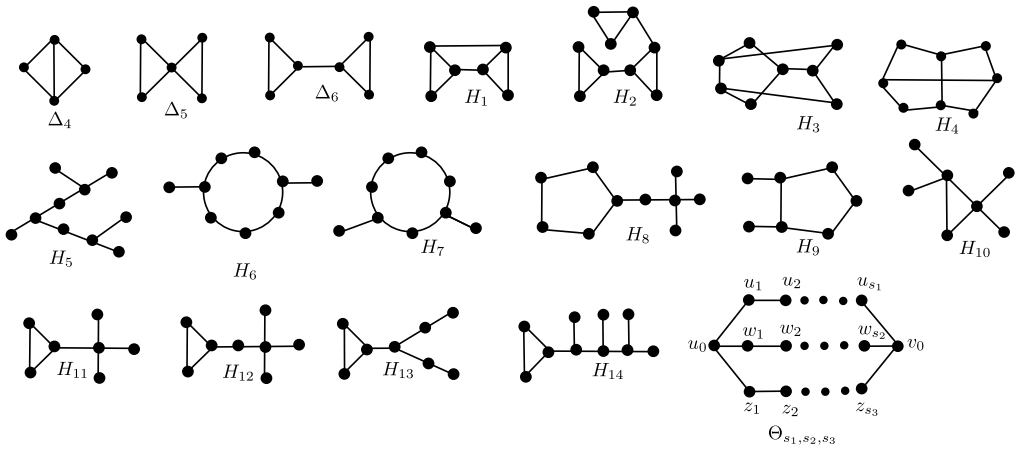


Fig. 1. The graphs Δ_4, Δ_5, Δ_6, H_1, H_2, ..., H_{14} and Θ_{s_1,s_2,s_3}.

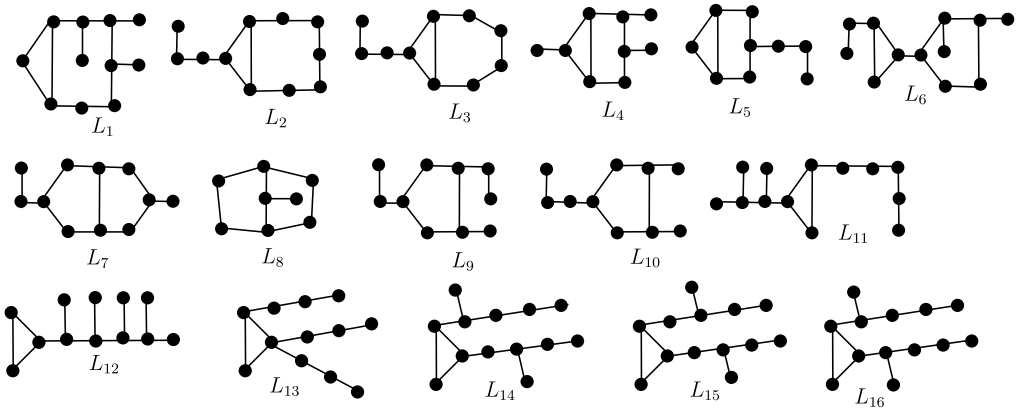


Fig. 2. The graphs L_1, L_2, ..., L_{16}.

C_3. Next, if $s \geq t$, then $U_{3;s,t}(j)$ is the graph obtained from $U_{3;s,t}$ by attaching an isolated vertex to the 2-vertex at distance j from the initial vertex of the pendant path P_s.

(iv) Let $U^g_{s_1,s_2,\ldots,s_t}$ be the unicyclic graph obtained from a cycle C_g by attaching t paths P_{s_1}, $P_{s_2}, \ldots, P_{s_t}$ to a vertex of C_g. Next, if $s_1 \geq s_2 \geq \cdots \geq s_t$, then $U^g_{s_1,s_2,\ldots,s_t}(j)$ is the graph obtained from $U^g_{s_1,s_2,\ldots,s_t}$ by attaching an isolated vertex to the 2-vertex at distance j from the initial vertex of the pendant path P_{s_1}.

(v) For $q \leq d$, denote by $U^5_{q;d}$ the unicyclic graph obtained from U^5_d by attaching a path P_q to a 2-vertex of C_5 at distance 2 from the unique 3-vertex. Next, $U^5_{q;d}(j)$ is the unicyclic graph obtained from $U^5_{q;d}$ by attaching an isolated vertex to the 2-vertex at distance j from the initial vertex of the pendant path P_d.

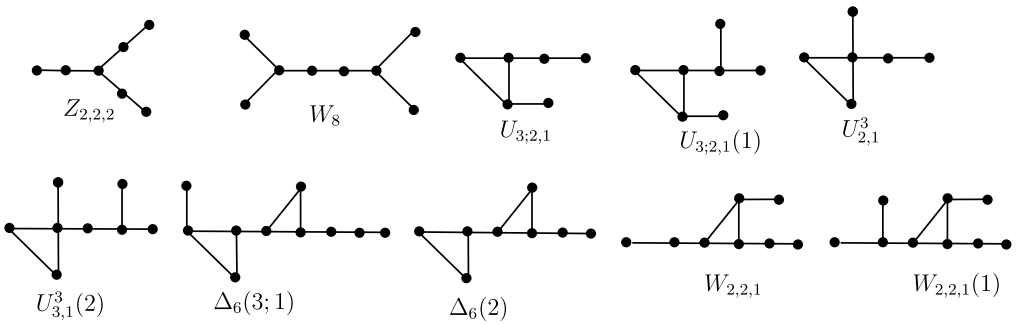


Fig. 3. The graphs $Z_{2,2,2}$, W_8, $U_{3;2,1}$, $U_{3;2,1}(1)$, $U^3_{2,1}$, $U^3_{3,1}(2)$, $\Delta_6(3;1)$, $\Delta_6(2)$, $W_{2,2,1}$ and $W_{2,2,1}(1)$.

(vi) Let $\Delta_6(s)$ be the bicyclic graph obtained from Δ_6 by attaching a path P_s to a 2-vertex of Δ_6; Let $\Delta_6(s;t)$ be the bicyclic graph obtained from Δ_6 by attaching two paths P_s and P_t to two non-adjacent 2-vertices of Δ_6, respectively.

(vii) Let W_{s_1,s_2,s_3} be the unicyclic graph obtained from a triangle C_3 with $V(C_3) = \{w_1, w_2, w_3\}$ by attaching the path P_{s_i} to the vertex w_i, where $i \in \{1, 2, 3\}$. Next, if $s_1 \geq s_2 \geq s_3 \geq 1$, then $W_{s_1,s_2,s_3}(j)$ is the unicyclic graph obtained from W_{s_1,s_2,s_3} by attaching an isolated vertex to the 2-vertex at distance j from the initial vertex of the pendant path P_{s_1}.

(viii) Let $B_1(g, 3)$ be the bicyclic graph obtained from the cycles C_g and C_3 by adding an edge u_1w_1, and let $B_2(g, 3)$ be the bicyclic graph obtained from the same cycles by identifying the vertices u_1 and w_1, where $C_g = w_1w_2 \cdots w_g$ and $C_3 = u_1u_2u_3$.

For an illustration, the graphs $Z_{2,2,2}$, W_8, $U_{3;2,1}$, $U_{3;2,1}(1)$, $U^3_{2,1}$, $U^3_{3,1}(2)$, $\Delta_6(3;1)$, $\Delta_6(2)$, $W_{2,2,1}$, $W_{2,2,1}(1)$ are depicted in Fig. 3. It is easy to see that $\Delta_5 = B_2(3, 3)$, $\Delta_6 = B_1(3, 3)$ and $W_8 = Z_{4,1,1}(3)$.

Definition 3.2.

(i) For a connected graph G with at least one cycle, we define the *base* $\mathcal{R}(G)$ of G to be the graph obtained from G by a successive deleting of pendant vertices, until no pendant vertex remains. For trees, this base is empty.

(ii) Let G be a graph with a non-empty base. A vertex u of G is said to be a *special vertex* if $d_G(u) \geq 3$ and u has at least one neighbour not in $\mathcal{R}(G)$. If G is a tree, then every vertex with degree at least 3 is also called as a *special vertex* of G. We denote by $q(G)$ the number of special vertices of G.

(iii) A cycle C_q of a graph G is a *pendant cycle* if it has exactly one vertex with degree at least three.

By the previous definition we see that if G is c-cyclic with $c \geq 1$, then $\mathcal{R}(G)$ is the unique c-cyclic subgraph of G such that $\mathcal{R}(G)$ contains no pendant vertices, and

$\mathcal{R}(G) = G$ if G contains no pendant vertices. We also have $\mathcal{R}(U_{3;2,1}) = \mathcal{R}(U^3_{2,1}) = C_3$, $q(U_{3;2,1}) = 2$ and $q(U^3_{2,1}) = 1$. Moreover, the unique triangle of $U^3_{2,1}$ is a pendant triangle.

We proceed by quoting some well-known results. As before we denote by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ the eigenvalues of a real symmetric matrix or a graph.

Lemma 3.3. (Courant-Weyl Inequalities, [1, p. 29]) *Let A and B be some $n \times n$ real symmetric matrices. For $1 \leq i, j \leq n$, we have:*

(i) If $i + j - 1 \leq n$, then $\lambda_{i+j-1}(A + B) \leq \lambda_i(A) + \lambda_j(B)$;
(ii) If $i + j - 1 \geq n$, then $\lambda_{i+j-n}(A + B) \geq \lambda_i(A) + \lambda_j(B)$.

We denote by $m_G(\lambda)$ the multiplicity of an eigenvalue λ of $A(G)$.

Lemma 3.4. [19] *Let G be a graph with n vertices. Then for any real number α, we have*

$$m_G(\alpha) - 1 \leq m_{\overline{G}}(-1 - \alpha) \leq m_G(\alpha) + 1.$$

Lemma 3.5. (Cauchy Interlacing, [11, Corollary 2.2]) *Let A be an $n \times n$ real symmetric matrix and let A_q be a principal submatrix of A. Then for $i \in \{1, 2, \ldots, q\}$, we have*

$$\lambda_{n-q+i}(A) \leq \lambda_i(A_q) \leq \lambda_i(A).$$

By setting $i = q - j$ in the previous lemma, we get the following consequence.

Corollary 3.6. *Let G be a graph with n vertices and H be an induced subgraph of G with q vertices. Then, for $j \in \{0, 1, \ldots, q-1\}$, we have $\lambda_{n-j}(G) \leq \lambda_{q-j}(H) \leq \lambda_{q-j}(G)$.*

Lemma 3.7 *([25]). Let G be a connected graph. Then, $\lambda_1(G) < 2$ if and only if either G is a path or $G \in \{Z_{n-3,1,1}, Z_{2,2,1}, Z_{3,2,1}, Z_{4,2,1}\}$ with $n \geq 4$.*

On the basis of the previous result we formulate the following definition which concludes this section.

Definition 3.8. If $T \in \{Z_{q,1,1}, Z_{2,2,1}, Z_{3,2,1}, Z_{4,2,1}\}$ for $q \geq 1$, then T is called a *first-type tree*.

4. Some forbidden induced subgraphs

This section contains some general results that are not restricted to neither Γ nor $\overline{\Gamma}$. We start with the following lemma and then continue with lists of forbidden induced subgraphs for graphs whose complements have particular spectral properties.

Lemma 4.1. *If $\lambda_2(G) < 2$, then $G = G^* \cup F \cup \big(|V(G)| - |V(G^*)| - |V(F)|\big)K_1$, where G^* is some c-cyclic graph with no induced union of two disjoint cycles, F is a forest consisting of exactly $\varepsilon(F)$ non-trivial paths and $\eta(G) - \varepsilon(F) - 1$ first-type trees.*

Proof. Since $\lambda_2(G) < 2$, G cannot contain the union of two disjoint cycles, and then the result follows from Lemma 3.7. □

Remark 4.2. We note in passing that the previous lemma deals with the so-called *reflexive graphs* (i.e., graphs whose second largest eigenvalue does not exceed 2). They represent the Lorentzian counterparts of the spherical and Euclidean graphs which occur in the theory of reflection groups [23]. Reflexive trees and reflexive bipartite regular graphs are known [13,22], while the remaining results refer to reflexive graphs with a small number of cycles or a particular structure [21]. Any further result on this topic is welcome.

We now give some forbidden induced subgraphs for $\overline{G}$ having the property $\lambda_2(G) \leq 1$.

Lemma 4.3. *If either W_6 or $Z_{2,2,2}$ is an induced subgraph of $\overline{G}$, then $\lambda_2(G) \geq 1$. Moreover, if any of the graphs listed in the following items is an induced subgraph of $\overline{G}$, then $\lambda_2(G) > 1$.*

(i) $Z_{3,2,2}$, $Z_{4,4,1}$, $Z_{4,3,1} \cup 2P_2 \cup K_1$, $Z_{4,3,1} \cup P_3 \cup P_2$, $Z_{2,1,1,1} \cup 2P_2 \cup K_{1,3}$, $Z_{3,1,1,1} \cup P_2 \cup 2P_3$, $Z_{4,1,1,1} \cup P_2 \cup K_1$, $Z_{6,2,1} \cup P_2 \cup K_1$, $Z_{6,3,1}$, $Z_{7,2,1} \cup P_2$, $Z_{2,2,1,1} \cup K_1$;

(ii) $Z_{2,2,1}(1)$, $Z_{3,2,1}(2) \cup P_2 \cup P_5$, $Z_{3,2,1}(2) \cup P_2 \cup K_{1,3}$, $Z_{3,2,1}(2) \cup 2P_2 \cup P_3$, $Z_{3,3,1}(2) \cup K_{1,3}$, $Z_{3,3,1}(2) \cup P_6$, $Z_{4,2,1}(2)$, $Z_{4,2,1}(3)$, $Z_{5,3,1}(4) \cup P_2$, $Z_{5,2,1}(4) \cup P_2 \cup K_1$, $Z_{6,1,1}(2) \cup P_2$, $Z_{6,2,1}(4)$, $Z_{6,2,1}(5)$, $Z_{2,1,1,1}(1)$, $Z_{3,1,1,1}(2) \cup 2P_2 \cup P_3$, $Z_{2,1,1,1,1} \cup P_2 \cup K_1$;

(iii) $U_1^4 \cup P_2$, $U_5^5 \cup P_2 \cup K_1$, U_6^5, $U_3^5(2) \cup 2P_2$, $U_{3,2}^3 \cup 3P_2$, $U_{1,1}^5 \cup 2P_2 \cup P_3$, $U_{4;1}^5 \cup P_2 \cup K_1$, $U_{3;2}^5 \cup P_2 \cup K_1$, $U_5^3(1)$, $U_6^3(3)$, $U_6^3(2) \cup P_2$, $U_{3;3,3}(1) \cup 2P_2$, $U_{3;5,1}(2) \cup 2P_2$, $K_{1,5} \cup 5P_2$, $K_{2,3} \cup P_2$, $H_5 \cup 2P_2$, $H_{11} \cup 2P_2$, H_{13}, $U_1^9 \cup P_2 \cup K_1$.

Proof. If W_6 or $Z_{2,2,2}$ is an induced subgraph of $\overline{G}$, then $\lambda_2(K_6 \setminus W_6) = \lambda_2(K_7 \setminus Z_{2,2,2}) = 1$, and thus the result follows from Lemma 3.5. The remainder of the proof follows by direct computation of the second largest graph eigenvalue. □

The following result can be found in [1].

Lemma 4.4.

(i) $S(C_q) = \left\{2\cos\left(\frac{2j\pi}{q}\right),\ \text{where } j = 0, 1, \ldots, q-1\right\}$;

(ii) $S(P_q) = \left\{2\cos\left(\frac{j\pi}{q+1}\right),\ \text{where } j = 1, 2, \ldots, q\right\}$;

(iii) $S(Z_{q,1,1}) = \left\{2\cos\left(\frac{j\pi}{2(q+2)}\right),\ \text{where } j = 1, 3, \ldots, 2q+3\right\}$.

An eigenvalue is called *main* if it has no eigenvector orthogonal to the all-1 vector $\mathbf{j}$; for otherwise, it is *non-main*. Observe that if λ is a non-main eigenvalue of $\overline{G}$ afforded by an eigenvector $\mathbf{x}$, then $A(G)\mathbf{x} = J_n\mathbf{x} - A(\overline{G})\mathbf{x} - I_n\mathbf{x} = (-\lambda - 1)\mathbf{x}$, which implies that $-\lambda - 1$ is an eigenvalue of G with the same eigenvector. We now prove the next result.

Lemma 4.5. *The following statements hold:*

(i) If $\lambda_2(G) < 1$, then $\overline{G}$ has no induced even cycle;
(ii) If $\lambda_2(G) \leq 1$, then both U_1^g (where $g \geq 6$ is even) and $U_1^4 \cup P_2$ are forbidden induced subgraphs for $\overline{G}$.

Proof. (i): Assume by way of contradiction that C_g is an induced even cycle of $\overline{G}$. For $j \in \{1, 2, \ldots, g-1\}$, $2\cos\left(\frac{2j\pi}{g}\right)$ is a non-main eigenvalue of $S(C_g)$ by Lemma 4.4(i), as C_g is 2-regular. It follows that $-1 - 2\cos\left(\frac{2j\pi}{g}\right)$ is an eigenvalue of $S(K_g \setminus C_g)$. Since $K_g \setminus C_g$ is $(g-3)$-regular, we have $\lambda_1(K_g \setminus C_g) = g - 3 \geq 1$. From Corollary 3.6 we get that $\lambda_2(G) \geq \lambda_2(K_g \setminus C_g) = 1$, a contradiction.

(ii): First, $U_1^4 \cup P_2$ is forbidden by Lemma 4.3(iii). Assume that U_1^g is an induced subgraph of $\overline{G}$ for some even g. If $g \geq 10$, then $Z_{4,4,1}$ is an induced subgraph of $\overline{G}$, contrary to Lemma 4.3(i). Since $\lambda_2(K_{g+1} \setminus U_1^g) > 1$ for $g \in \{6, 8\}$, the result follows by the interlacing argument (Corollary 3.6). □

Let G_1 and G_2 be induced subgraphs of $\overline{G}$ such that $V(G_1) \cap V(G_2) = \emptyset$. Denote by $E_{\overline{G}}(G_1, G_2) = \{uv \in E(\overline{G})$: where $u \in V(G_1)$ and $v \in V(G_2)\}$. The following result is obtained by slight modifications of the proof of [19, Lemma 4.5].

Lemma 4.6. *Let G_1 be a c-cyclic (not necessarily induced) subgraph of $\overline{G}$ with t vertices and G_2 be an induced forest of $\overline{G}$ having p vertices and s non-trivial trees, where G_1 and G_2 are vertex-disjoint and $E_{\overline{G}}(G_1, G_2) = \emptyset$. If $c \geq 2$ and $\lambda_n(G) > -3$, then $(c-1)p^2 < st^2$.*

The following corollary is immediate. We recall that the graphs Δ_t are illustrated in Fig. 1.

Corollary 4.7. *Suppose that, for $t \in \{4, 5, 6\}$, Δ_t is a (not necessarily induced) subgraph of $\overline{G}$ and T is an induced tree of $\overline{G}$ with p vertices, where Δ_t and T are vertex-disjoint and $E_{\overline{G}}(\Delta_t, T) = \emptyset$. If $\lambda_n(G) > -3$, then $p < t$.*

By virtue of the previous result we get some forbidden induced subgraphs for $\overline{G}$ having the property $\lambda_n(G) > -3$.

Lemma 4.8. *If any of the graphs listed in the following items is an induced subgraph of $\overline{G}$, then $\lambda_n(G) \leq -3$.*

(i) $\Delta_4 \cup 3P_2$, $\Delta_4 \cup P_2 \cup P_3$, $\Delta_5 \cup P_3 \cup P_2 \cup K_1$, $\Delta_5 \cup 2P_3$, $\Delta_5 \cup P_4$, $\Delta_5 \cup K_{1,3}$, $\Delta_6 \cup 2P_2 \cup 2P_3$, $\Delta_6 \cup 3P_3$, $\Delta_6 \cup 2P_2 \cup P_4$, $\Delta_6 \cup P_4 \cup P_3$, $\Delta_6 \cup P_5$, $\Delta_6 \cup K_{1,3}$, $\Delta_6(2;2)$, $\Delta_6(3;1)$;

(ii) $\Theta_{7,0,1} \cup P_2 \cup P_3$, $\Theta_{2,0,1} \cup 2P_2 \cup P_3$, $\Theta_{2,0,1} \cup 2P_3$, $\Theta_{2,0,1} \cup P_4$, $\Theta_{3,0,3} \cup P_2 \cup 2P_3 \cup P_4$, $\Theta_{3,0,3} \cup P_2 \cup P_3 \cup K_{1,3}$, $\Theta_{3,0,3} \cup 2P_2 \cup P_5$, $\Theta_{2,1,2} \cup P_2 \cup P_5$, $\Theta_{2,1,2} \cup 3P_3 \cup 3P_2$, $\Theta_{2,1,2} \cup P_3 \cup K_{1,3}$, $C_3 \cup K_{1,4} \cup 2P_2$, $C_5 \cup K_{1,4}$;

(iii) $U_1^3 \cup P_5 \cup 2P_2$, $U_1^3 \cup P_5 \cup P_3$, $U_1^3 \cup P_6$, $U_1^3 \cup K_{1,3} \cup P_2 \cup P_3$, $U_1^3 \cup P_4 \cup K_{1,3}$, $U_1^3 \cup 2K_{1,3}$, $U_1^3 \cup Z_{2,1,1}$, $U_{1,1}^3 \cup 2P_3 \cup P_2$, $U_{1,1}^3 \cup P_4 \cup P_2$, $U_{1,1}^3 \cup K_{1,3}$, $U_{3;1,1} \cup K_{1,3}$, $U_{3;1,1} \cup 2P_3 \cup 2P_2$, $U_{3;1,1} \cup 3P_3$, $U_{3;1,1} \cup 2P_2 \cup P_4$, $U_{3;1,1} \cup P_4 \cup P_3$, $U_{3;1,1} \cup P_5$, $U_{1,1,1}^3 \cup 2P_2 \cup P_3$.

(iv) $U_2^3 \cup 2P_4$, $U_3^3 \cup 2P_2 \cup P_3 \cup P_4$, $U_{3;6,1} \cup P_2$, $U_2^3(1) \cup P_5$, $U_2^3(1) \cup 2P_2 \cup K_{1,3}$, $U_2^3(1) \cup 3P_3 \cup P_2$, $U_1^5 \cup P_8$, $U_1^5 \cup Z_{3,1,1}$, $U_1^5 \cup Z_{2,2,1}$, $U_1^5 \cup Z_{2,1,1} \cup P_6$, $U_{1;1}^5 \cup P_2 \cup Z_{2,1,1}$, $U_{1;1}^5 \cup P_7$, $U_{1;1}^5 \cup P_6 \cup P_3$, $U_{1;1}^5 \cup P_6 \cup 2P_2$;

(v) $H_1 \cup P_2 \cup P_3$, $H_9 \cup P_6 \cup P_2$, $H_9 \cup Z_{2,1,1} \cup P_2$, $H_{10} \cup 2P_2 \cup P_3$, $W_{1,1,1} \cup 2P_3 \cup P_2$, $W_{1,1,1} \cup P_4 \cup P_2$, $W_{4,1,1} \cup 2P_2 \cup P_3$, $W_{5,1,1} \cup 2P_2$.

Proof. If H is some of the listed graphs with $|V(H)| = s$ and H is an induced subgraph of G, then $\lambda_n(G) \le \lambda_s\big(K_s \setminus H\big) \le -3$ follows from Corollary 3.6 and the computation of the least eigenvalue of $K_s \setminus H$. □

5. Properties of $\mathbf{\Gamma}$ and $\overline{\mathbf{\Gamma}}$

We first compute the spectrum of $K_n \setminus C_k$. In the exponential notation, the exponent stands for the multiplicity of the corresponding eigenvalue. By [5, Theorem 2.1.2] and Lemma 4.4(i), we get

$$S\big(K_k \setminus C_k\big) = \left\{k-3,\ -1-2\cos\left(\frac{2j\pi}{k}\right), \text{ where } 1 \le j \le k-1\right\}. \tag{1}$$

Lemma 5.1. *If* $3 \le k \le n-1$, *then*

$$S(K_n \setminus C_k) = \left\{\frac{1}{2}\left(n-4 \pm \sqrt{(n+2)^2-8k}\right), -1^{(n-k-1)}, -1-2\cos\left(\frac{2j\pi}{k}\right), \right.$$
$$\left. 1 \le j \le k-1\right\}.$$

Proof. It is easy to see that $K_n \setminus C_k = K_{n-k} \vee \big(K_k \setminus C_k\big)$, that is, $K_n \setminus C_k$ is the join of K_{n-k} and $K_k \setminus C_k$. Let $\lambda_1 > \lambda_2$ be the roots of $(x-k+3)(x+k+1-n) - k(n-k)$, i.e.,

$$\lambda_1, \lambda_2 = \frac{1}{2}\left(n-4 \pm \sqrt{(n+2)^2-8k}\right).$$

Since $S(K_{n-k}) = \big\{n-k-1, -1^{(n-k-1)}\big\}$, by combining (1) and [5, Theorem 2.1.8], we obtain

$$S\big(K_{n-k} \vee (K_k \setminus C_k)\big) = \big(S(K_{n-k}) \setminus \{n-k-1\}\big) \cup \big(S(K_k \setminus C_k) \setminus \{k-3\}\big) \cup \big\{\lambda_1, \lambda_2\big\}$$
$$= \left\{ \frac{1}{2}\left(n-4 \pm \sqrt{(n+2)^2-8k}\right), -1^{(n-k-1)}, -1-2\cos\left(\frac{2j\pi}{k}\right), 1 \le j \le k-1 \right\},$$

as desired. □

On the basis of Lemmas 3.4 and 5.1, we obtain the following corollary.

Corollary 5.2. *Let k and n be positive integers with $4 \le k \le n-1$.*

(i) If $4 \nmid k$, then $n-k-2 \le m_{\overline{\Gamma}}(0) \le n-k$;
(ii) If $4 \mid k$, then $n-k \le m_{\overline{\Gamma}}(0) \le n-k+2$.

Proof. Note that under the initial assumption on k and n we have

$$\frac{1}{2}\left(n-4-\sqrt{(n+2)^2-8k}\right) \neq -1.$$

(i): When $1 \le j \le k-1$, since $0 < \frac{2j\pi}{k} < 2\pi$ and $4 \nmid k$, we have $\cos\left(\frac{2j\pi}{k}\right) \neq 0$, and thus $m_\Gamma(-1) = n-k-1$, by Lemma 5.1. Now, from Lemma 3.4, we have $n-k-2 \le m_{\overline{\Gamma}}(0) \le n-k$.

(ii): If $1 \le j \le k-1$, then $0 < \frac{2j\pi}{k} < 2\pi$. Suppose that $k = 4s$, where $s \ge 1$. Since $\cos\left(\frac{2s\pi}{4s}\right) = \cos\left(\frac{6s\pi}{4s}\right) = 0$, we get $m_\Gamma(-1) = n-k+1$, again by Lemma 5.1. Similarly, from Lemma 3.4, we have $n-k \le m_{\overline{\Gamma}}(0) \le n-k+2$, as desired. □

We now give some spectral constraints on Γ and $\overline{\Gamma}$.

Lemma 5.3. *The following inequalities hold for $5 \le k \le n$.*

(i) $2\cos\left(\frac{2\pi}{k}\right) \le \lambda_2(\overline{\Gamma}) < 2$, and

$$\lambda_n(\Gamma) = \min\left\{ \frac{1}{2}\left(n-4-\sqrt{(n+2)^2-8k}\right), -1-2\cos\left(\frac{2\pi}{k}\right) \right\} > -3;$$

(ii) If k is odd, then $\lambda_2(\Gamma) = \lambda_3(\Gamma) = 2\cos\left(\frac{\pi}{k}\right) - 1 < 1$, and $\lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right)$;
(iii) If k is even, then $\lambda_3(\Gamma) = \lambda_4(\Gamma) = 2\cos\left(\frac{2\pi}{k}\right) - 1 < 1 = \lambda_2(\Gamma)$, and $\lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right)$.

Proof. By using (1), Lemmas 3.3 and 4.4(i), we get

$$2\cos\left(\frac{2\pi}{k}\right) = \lambda_3(C_k) = \lambda_3\big(C_k \cup (n-k)K_1\big)$$
$$\le -1 - \lambda_{n-1}\big(K_n \setminus C_k\big) = -1 - \lambda_{n-1}\big(\Gamma\big)$$

$$\leq \lambda_2(\overline{\Gamma}) \leq -1 - \lambda_n(\Gamma)$$
$$= -1 - \min\left\{\frac{1}{2}\left(n-4-\sqrt{(n+2)^2-8k}\right), -1-2\cos\left(\frac{2\pi}{k}\right)\right\} < 2.$$

By Lemma 5.1 and (1), we have

$$-3 < \min\left\{\frac{1}{2}\left(n-4-\sqrt{(n+2)^2-8k}\right), -1-2\cos\left(\frac{2\pi}{k}\right)\right\} = \lambda_n(K_n \setminus C_k) = \lambda_n(\Gamma).$$

Thus, (i) holds.

If k is odd, by (1) and Lemma 5.1, we get $\lambda_2(\Gamma) = \lambda_3(\Gamma) = 2\cos\left(\frac{\pi}{k}\right) - 1 < 1$. Combining this with Lemma 3.3, we arrive at

$$-2\cos\left(\frac{\pi}{k}\right) = -1 - \lambda_2(\Gamma) \leq \lambda_{n-1}(\overline{\Gamma}) \leq -1 - \lambda_3(\Gamma) = -2\cos\left(\frac{\pi}{k}\right),$$

and thus (ii) holds.

If k is even, by (1) and Lemma 5.1, we get $\lambda_3(\Gamma) = \lambda_4(\Gamma) = 2\cos\left(\frac{2\pi}{k}\right) - 1 < 1 = \lambda_2(\Gamma)$. As before, by employing Lemma 3.3, we obtain

$$-2\cos\left(\frac{2\pi}{k}\right) = -1 - \lambda_3(\Gamma) \leq \lambda_{n-2}(\overline{\Gamma}) \leq -1 - \lambda_4(\Gamma) = -2\cos\left(\frac{2\pi}{k}\right),$$

and thus (iii) holds. □

We proceed with some structural examinations on $\overline{\Gamma}$. First, Lemma 5.3(i) tells us that $\lambda_2(\overline{\Gamma}) < 2$, and therefore by Lemma 4.1, we may suppose that

$$\overline{\Gamma} = \Gamma^* \cup F \cup \big(|V(\overline{\Gamma})| - |V(\Gamma^*)| - |V(F)|\big)K_1, \tag{2}$$

where Γ^* is a c-cyclic graph with no induced union of two disjoint cycles and F is a forest which consists of $\varepsilon(F)$ non-trivial paths and $\eta(\overline{\Gamma}) - \varepsilon(F) - 1$ first-type trees (introduced in Definition 3.8). Throughout the remainder of the text we will frequently use the fact that $\overline{\Gamma}$ has the form (2), along with the corresponding notation.

At this point we define

$$\Phi(G) = \big(8n-20\big)m_1(G) + 16m_2(G) - 8m_3(G) + 8m_4(G),$$

where the quantities on the right hand side are defined in Section 3.

Lemma 5.4. [2] *If G is a graph with n vertices and e edges, then the number of closed 4-walks of $\overline{G}$ is equal to $(n-1)^4 + (n-1) - (8n^2 - 32n + 34)e + (8n-20)m_1(G) + 16m_2(G) - 8m_3(G) + 8m_4(G)$.*

For $k \geq 5$ it is not difficult to verify that $m_1(C_k) = k$, $m_2(C_k) = \frac{1}{2}k(k-3)$, $m_3(C_k) = k$ and $m_4(C_k) = 0$. Since Γ is cospectral with $K_n \setminus C_k$, they have the same number of closed 4-walks, and thus we have the following consequence of the previous lemma.

Corollary 5.5. *If $k \geq 5$, then $\Phi(\overline{\Gamma}) = \Phi(C_k \cup (n-k)K_1) = (8n-20)k + 8k(k-4)$.*

We now quote the following result.

Lemma 5.6. [12] *Let G be a connected graph with n vertices, e edges and minimum degree $\delta \geq 1$. Then*

$$\lambda_1(G) \leq \frac{1}{2}\left(\delta - 1 + \sqrt{(\delta+1)^2 + 8e - 4n\delta}\right).$$

Equality holds if and only if G is either a regular graph or a bidegreed graph in which the degree of each vertex is equal to either δ or $n-1$.

Lemma 5.7. *The statement of Theorem 2.1 holds for $\Delta(\overline{\Gamma}) \leq 2$ and $k \geq 7$.*

Proof. We assume that the statement of the corresponding theorem does not hold under the given constraints. We easily conclude that Γ is connected with $\delta(\Gamma) \geq n-3$. Note that $x - 1 + \sqrt{(x+1)^2 + 8|E(\Gamma)| - 4nx}$ strictly decreases in $x \geq 1$ (see [12]). Therefore, from (1), Lemmas 5.1 and 5.6, we get

$$\lambda_1(K_n \setminus C_k) = \lambda_1(\Gamma) \leq \frac{1}{2}\left(n - 4 + \sqrt{(n+2)^2 - 8k}\right) = \lambda_1(K_n \setminus C_k),$$

and thus Γ is either a d-regular or a bidegreed graph with vertex degrees $n-3$ and $n-1$.

In the latter case $\overline{\Gamma}$ consists of exactly one cycle with k edges and $n-k$ isolated vertices by (2), which in turn leads to $\Gamma = K_n \setminus C_k$. If Γ is d-regular, then $nd = 2|E(\Gamma)| = n(n-1) - 2k$ and $2d = 2\lambda_1(\Gamma) = n - 4 + \sqrt{(n+2)^2 - 8k}$, and so $k = n$ and $d = n-3$. Therefore $\Gamma = K_n \setminus C_n$ or $\overline{\Gamma}$ is the union of at least two disjoint cycles, but the latter possibility contradicts (2), and we are done. □

Corollary 5.8. *The statement of Theorem 2.1 holds for $k = n$.*

Proof. Since a graph cospectral with a regular graph is regular with the same vertex degree [7, Proposition 2], we get that $\overline{\Gamma}$ is 2-regular. Thus, $\overline{\Gamma}$ is the union of some cycles, and then the result follows from (2). □

We proceed by quoting the following two results.

Lemma 5.9. [19, Corollary 3.9] *Let G be a c-cyclic graph with n vertices and $q(G)$ special vertices. If $c \geq 1$, then*

$$\sum_{i=1}^{n} d_i^2(G) \geq 4n + 10(c-1) + 2q(G),$$

with equality if and only if each special vertex of G is a 3-vertex and $\mathcal{R}(G)$ contains exactly $2(c-1)$ vertices of degree three.

Lemma 5.10. [8] *If G is a graph with n vertices and e edges, then*

$$\tau\left(\overline{G}\right) + \tau(G) = \binom{n}{3} - (n-1)e + \frac{1}{2}\sum_{i=1}^{n} d_i^2(G),$$

where τ denotes the number of triangles in the corresponding graph.

Using the previous results we prove the following one.

Corollary 5.11. *If Γ^* is a c-cyclic graph and $k \geq 7$, then*

$$\sum_{i=1}^{|V(\Gamma^*)|} d_i\big(\Gamma^*\big)\big(d_i(\Gamma^*) - 2\big) = 2\big(\tau(\Gamma^*) + \varepsilon(F)\big). \tag{3}$$

Moreover, if $c \geq 1$, then $\tau(\Gamma^*) \geq 3(c-1) + q\big(\Gamma^*\big) - \varepsilon(F)$, with equality if and only if each special vertex of Γ^* is a 3-vertex and $\mathcal{R}(\Gamma^*)$ contains exactly $2(c-1)$ vertices of degrees three.

Proof. By Lemma 5.10, we have $\tau\big(K_n \backslash C_k\big) = \binom{n}{3} - (n-3)k$ and

$$\tau\big(\Gamma\big) = \binom{n}{3} - (n-1)k + \frac{1}{2}\sum_{i=1}^{n} d_i^2(\overline{\Gamma}) - \tau(\overline{\Gamma}).$$

Since Γ is cospectral with $K_n \backslash C_k$, we have $\tau\big(K_n \backslash C_k\big) = \tau\big(\Gamma\big)$ (see [7, Lemma 4]), and thus $\sum_{i=1}^{n} d_i^2(\overline{\Gamma}) = 2\tau(\overline{\Gamma}) + 4k$. Combining this with $\sum_{i=1}^{n} d_i(\overline{\Gamma}) = 2k$ and (2), we get

$$\sum_{i=1}^{n} d_i\big(\overline{\Gamma}\big)\big(d_i(\overline{\Gamma}) - 2\big) = 2\tau(\overline{\Gamma}) = 2\tau(\Gamma^*). \tag{4}$$

If T is a tree of F with $\Delta(T) \geq 3$, by (2), we conclude that T is a first-type tree, i.e. $T \in \big\{Z_{p,1,1},\, Z_{2,2,1},\, Z_{3,2,1},\, Z_{4,2,1}\big\}$. This implies that

$$\sum_{i=1}^{n} d_i\big(\overline{\Gamma}\big)\big(d_i(\overline{\Gamma}) - 2\big) = \sum_{i=1}^{|V(\Gamma^*)|} d_i\big(\Gamma^*\big)\big(d_i(\Gamma^*) - 2\big) - 2\varepsilon(F). \tag{5}$$

Now, (3) follows from (4) and (5).

If $c \geq 1$, by Lemma 5.9, we have $\sum_{i=1}^{|V(\Gamma^*)|} d_i^2(\Gamma^*) \geq 4|V(\Gamma^*)| + 10(c-1) + 2q(\Gamma^*)$. By combining this with $\sum_{i=1}^{|V(\Gamma^*)|} d_i(\Gamma^*) = 2(|V(\Gamma^*)| + c - 1)$ and (3), we conclude the proof. □

6. Γ^* is not c-cyclic with $c \geq 2$

In this and the subsequent sections we assume that $\overline{\Gamma}$ has the structure described in (2). Once again, we recall for the reader that Theorem 2.1 has been settled for $3 \leq k \leq 6$ and $k = n$ (Corollary 5.8), and so we assume that $7 \leq k \leq n-1$. The main result of this section is formulated in Theorem 6.12.

Since $\overline{\Gamma}$ contains exactly $n - |V(\Gamma^*)| - |V(F)|$ isolated vertices, by Corollary 5.2, we have

$$n - k - 2 \leq m_{\Gamma^*}(0) + m_F(0) + n - |V(\Gamma^*)| - |V(F)| = m_{\overline{\Gamma}}(0) \leq n - k \text{ if } 4 \nmid k, \quad (6)$$

$$n - k \leq m_{\Gamma^*}(0) + m_F(0) + n - |V(\Gamma^*)| - |V(F)| = m_{\overline{\Gamma}}(0) \leq n - k + 2 \text{ if } 4 \mid k. \quad (7)$$

Since $-3 < \lambda_n(\Gamma) \leq \lambda_2(\Gamma) \leq 1$ (by Lemma 5.3), the graphs listed in Lemmas 4.3 and 4.8 are forbidden induced subgraphs for $\overline{\Gamma}$.

We start by transferring another result of [19].

Lemma 6.1. [19, Lemma 3.8] *Let G be a forest without isolated vertices. If G has n vertices, s components and $q(G)$ special vertices, then*

$$\sum_{i=1}^{n} d_i^2(G) \geq 4n - 6s + 2q(G),$$

with equality if and only if each special vertex of G is a 3-vertex.

We now prove the following three lemmas.

Lemma 6.2. *The statement of Theorem 2.1 holds if $\eta(\overline{\Gamma}) = 1$ and $k \geq 7$.*

Proof. Since $\eta(\overline{\Gamma}) = 1$ and $|E(\Gamma^*)| = k$, we have $|V(\Gamma^*)| \leq k+1$ and $F = \emptyset$.

Case 1: $|V(\Gamma^*)| = k+1$. Obviously, in this case, Γ^* is a tree. By Lemma 6.1, we have

$$\sum_{i=1}^{k+1} d_i^2(\Gamma^*) \geq 4k - 2 + 2q(\Gamma^*), \quad (8)$$

where equality holds if and only if each special vertex of Γ^* is a 3-vertex. Now, since $\varepsilon(F) = \tau(\Gamma^*) = 0$, the equality (3) implies that

$$\sum_{i=1}^{k+1} d_i^2(\Gamma^*) = 2\sum_{i=1}^{k+1} d_i(\Gamma^*) = 4k,$$

and thus we have $q(\Gamma^*) \leq 1$ by (8). Hence, $\Gamma^* = P_{k+1}$ $\big(q(\Gamma^*) = 0\big)$ or Γ^* contains exactly one special vertex, which is a 3-vertex.

Since the former possibility is resolved in Lemma 5.7, we may suppose that $q(\Gamma^*) = 1$, and so $\Gamma^* = Z_{s,p,k-s-p}$. If $\min\{s, p, k-s-p\} \geq 2$, then $\Gamma^* = Z_{2,2,2}$, as $Z_{3,2,2}$ is forbidden by Lemma 4.3(i). This implies that $k = |E(\Gamma^*)| = 6$, a contradiction. Thus, we may suppose that $\Gamma^* = Z_{1,p,k-1-p}$ with $k-1-p \geq p \geq 1$. Since $m_1(Z_{1,p,k-1-p}) = k = m_1(C_k)$, $m_2(Z_{1,p,k-1-p}) = \frac{1}{2}k(k-3) = m_2(C_k)$, $m_3(Z_{1,p,k-1-p}) \leq k-1 < m_3(C_k)$ and $m_4(Z_{1,p,k-1-p}) = 0 = m_4(C_k)$, we have $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, which contradicts Corollary 5.5.

Case 2: $|V(\Gamma^*)| = k$. In this case, Γ^* is a unicyclic graph with k vertices. By Corollary 5.11, we have $1 \geq \tau(\Gamma^*) \geq q(\Gamma^*)$, and so either $q(\Gamma^*) = 0$ or $q(\Gamma^*) = 1$.

If $q(\Gamma^*) = 0$, then $\Gamma^* = C_k$, which leads to the desired result. For otherwise, we have $\tau(\Gamma^*) = 1$, and thus $\Gamma^* = U^3_{k-3}$. Since $m_1\big(U^3_{k-3}\big) = k+1$, $m_2\big(U^3_{k-3}\big) = \frac{1}{2}(k^2-3k-2)$, $m_3\big(U^3_{k-3}\big) = k-1$ and $m_4\big(U^3_{k-3}\big) = 0$, we have $\Phi(\overline{\Gamma}) = \Phi\big(U^3_{k-3} \cup (n-k)K_1\big) = (8n-20)(k+1) + 8(k^2-4k-1) > (8n-20)k + 8k(k-4) = \Phi\big(C_k \cup (n-k)K_1\big)$, which again contradicts Corollary 5.5.

Case 3: $|V(\Gamma^*)| \leq k-1$. In this case, $\overline{\Gamma}$ contains at least $n-k+1$ isolated vertices and thus $4 \mid k$ by (6). From (7) we have $k-2 \leq |V(\Gamma^*)| \leq k-1$, and thus Γ^* is either a bicyclic or a tricyclic graph. If Γ^* is a bicyclic graph, Corollary 5.11 and $\varepsilon(F) = 0$ lead to the impossible scenario $3 \leq \tau(\Gamma^*) \leq 2$. If Γ^* is a tricyclic graph, then $6 \leq \tau(\Gamma^*) \leq 4$ by Corollary 5.11, and we are done. □

Lemma 6.3. *If either P_2 or P_5 is a component of F, then $3 \mid k$.*

Proof. Suppose that $V(\overline{\Gamma}) = \{u_1, u_2, \ldots, u_n\}$ and that $P_s = u_1u_2\cdots u_s$ is a component of F. If $s = 2$, then $\mathbf{f}_1 = \big(1, -1, \mathbf{0}^{\intercal}_{n-2}\big)^{\intercal}$ (where $\mathbf{0}_{n-2}$ is the $(n-2)\times 1$ all-0 vector) is an eigenvector afforded by the eigenvalue -1 of $A(\overline{\Gamma})$. Since $A(\Gamma) = J_n - A(\overline{\Gamma}) - I_n$, it is easy to see that $\mathbf{f}_1$ is an eigenvector of 0 of $A(\Gamma)$. If $s = 5$, then $\mathbf{f}_2 = \big(1, -1, 0, 1, -1, \mathbf{0}^{\intercal}_{n-5}\big)^{\intercal}$ is an eigenvector afforded by the eigenvalue -1 of $A(\overline{\Gamma})$, and thus $\mathbf{f}_2$ is an eigenvector of 0 of $A(\Gamma)$. Therefore, in both cases 0 is an eigenvalue of $A(\Gamma)$. If $n-4-\sqrt{(n+2)^2-8k} = 0$, then $k = \frac{3(n-1)}{2}$, contrary to the assumption that $7 \leq k \leq n-1$. Thus, by Lemma 5.1, $\cos\big(\frac{2j\pi}{k}\big) = -\frac{1}{2}$ for some $j \in \{1, 2, \ldots, k-1\}$. This implies that either $\frac{2j\pi}{k} = \frac{2\pi}{3}$ or $\frac{2j\pi}{k} = \frac{4\pi}{3}$, and thus $3 \mid k$. □

Lemma 6.4. *The following statements hold:*

(i) If $2P_2$ is a component of F, then Γ^* has no pendant triangle;
(ii) F contains at most two components isomorphic to P_2.

Proof. Here we only prove (i), as (ii) can be proved by the same argument. Suppose that $V(\overline{\Gamma}) = \{u_1, u_2, \ldots, u_n\}$ and $V(2P_2) = \{u_1, u_2, u_3, u_4\}$, where $2P_2 = u_1u_2 \cup u_3u_4$.

Assume by way of contradiction that Γ^* contains a pendant triangle. Let u_5, u_6 be the 2-vertices of C_3. Since $\left(1,-1,\mathbf{0}_{n-2}^\intercal\right)^\intercal$, $\left(0,0,1,-1,\mathbf{0}_{n-4}^\intercal\right)^\intercal$ and $\left(\mathbf{0}_4^\intercal,1,-1,\mathbf{0}_{n-6}^\intercal\right)^\intercal$ (where $\mathbf{0}_s$ is the $s\times 1$ all-0 vector) are the orthogonal eigenvectors belonging to the eigenspace of -1 in $A(\overline{\Gamma})$ and since $A(\Gamma)=J_n-A(\overline{\Gamma})-I_n$, the same vectors are afforded by the eigenvalue 0 of $A(\Gamma)$. By Lemma 5.1, we have $n-4-\sqrt{(n+2)^2-8k}=0$, and thus $k=\frac{3(n-1)}{2}$, contradicting $7\le k\le n-1$. □

Remark 6.5. From Lemma 6.4(ii), if $\eta(\overline{\Gamma})\ge 4$ or $\varepsilon(F)\ge 3$, then F must contains $2P_2\cup P_3$ as an induced subgraph. We will repeatedly make use of this observation in what follows.

We recall from Section 3 that $\mathrm{rank}(G)$ denotes the rank of $A(G)$. It is easy to see that $\mathrm{rank}(P_q)=q-1$ for q odd, $\mathrm{rank}(P_q)=q$ for q even and $\mathrm{rank}(K_{1,q-1})=2$ for $q\ge 2$ [4]. A *skew palindromic vector* $(x_1,x_2,\ldots,x_n)$, satisfies $(x_1,x_2,\ldots,x_n)=-(x_n,x_{n-1},\ldots,x_1)$.

Lemma 6.6. *For $q\notin\{1,3\}$, $\overline{\Gamma}$ has no three components isomorphic to P_q.*

Proof. By way of contradiction, we assume that $\overline{\Gamma}$ contains at least three copies of a non-trivial path P_q, where $q\notin\{1,3\}$. The case $q=2$ follows from Lemma 6.4(ii). For $q\ge 4$, since $\lambda_1(\Gamma)>1\ge\lambda_2(\Gamma)$ (by Lemma 5.3), in the light of Lemma 5.1, to arrive at contradiction it suffices to find two eigenvalues of Γ both of multiplicity at least 3 and distinct from -1.

Now, on the basis of [8, Lemma 1] we get that P_q has $\lfloor\frac{q}{2}\rfloor$ independent skew palindromic eigenvectors. Combining this with the facts that $\mathrm{rank}(P_q)\ge q-1$ and that P_q has no repeated eigenvalues, we conclude that, for $q\ge 6$, P_q has at least two distinct non-zero and non-main eigenvalues with independent skew palindromic eigenvectors, and thus Γ contains at least two eigenvalues distinct from -1. Moreover, the same conclusion holds for $q=4$ as $\mathrm{rank}(P_4)=4$. For $q=5$, $(1,-1,0,1,-1,\mathbf{0}_{n-5})^\intercal$ and $(1,1,0,-1,-1,\mathbf{0}_{n-5})^\intercal$ are eigenvectors of the non-main eigenvalues -1 and 1 of $\overline{\Gamma}$, respectively. This implies that the mentioned eigenvectors correspond to 0 and -2 of Γ, and we are done. □

Lemma 6.7. *Assume that Γ is non-isomorphic to $K_n\setminus C_k$ for an odd k. If $7\le k\le n-1$, then neither $\lambda_{n-1}(\overline{\Gamma})$ nor $\lambda_n(\overline{\Gamma})$ is an eigenvalue of any path of F. Moreover, if $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*)\ne\lambda_{n-1}(\overline{\Gamma})=-2\cos\left(\frac{\pi}{k}\right)$, then we have either*

- *$Z_{q,2,1}$ is a component of F with $q\ge 2$, or*
- *$Z_{q,1,1}$ is a component of F with $q\ge\frac{k}{2}-2$.*

Proof. Assume that either $\lambda_{n-1}(\overline{\Gamma})$ or $\lambda_n(\overline{\Gamma})$ is an eigenvalue of some path P_q of F. By Lemmas 4.4(ii) and 5.3(ii),

$$-2\cos\left(\frac{\pi}{q+1}\right)=\lambda_q(P_q)\le\lambda_{n-1}(\overline{\Gamma})=-2\cos\left(\frac{\pi}{k}\right)$$

and thus $q \geq k-1 \geq 6$. This implies that $|E(\Gamma^*)| \leq 2$, and thus $\Gamma^* \in \{P_2, P_3\}$, which contradicts Lemma 5.7. Thus, neither $\lambda_{n-1}(\overline{\Gamma})$ nor $\lambda_n(\overline{\Gamma})$ is an eigenvalue of any path of F.

We assume that $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \neq \lambda_{n-1}(\overline{\Gamma})$. Then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) > \lambda_{n-1}(\overline{\Gamma})$, and thus $\lambda_{|V(T)|}(T) \leq \lambda_{n-1}(\overline{\Gamma})$ for some first-type tree T of F.

If $T \neq Z_{q,2,1}$ with $q \geq 2$, then $T = Z_{q,1,1}$ by (2). By Lemmas 4.4(iii) and 5.3(ii), $-2\cos\left(\frac{\pi}{2q+4}\right) = \lambda_{q+3}(Z_{q,1,1}) \leq \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right)$, and thus $q \geq \frac{k}{2} - 2$. □

Lemma 6.8. *Assume that Γ is non-isomorphic to $K_n \backslash C_k$ for an even k with $7 \leq k \leq n-1$.*

(i) If P_q is a path of F, then $\lambda_{q-1}(P_q) > \lambda_{n-2}(\overline{\Gamma})$;
(ii) If $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \neq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right)$, then we have either
- *P_q is a component of F with $q \geq \frac{k}{2} - 1$, or*
- *$Z_{q,1,1}$ is a component of F with $q \geq \frac{k}{4} - 2$, or*
- *$Z_{q,2,1}$ is a component of F with $q \geq 2$.*

Proof. We first assume that $\lambda_{q-1}(P_q) \leq \lambda_{n-2}(\overline{\Gamma})$ for some path P_q of F. By Lemmas 4.4(ii) and 5.3(iii), we have $-2\cos\left(\frac{2\pi}{q+1}\right) = \lambda_{q-1}(P_q) \leq -2\cos\left(\frac{2\pi}{k}\right)$, and thus $q \geq k-1$. This implies that $\Gamma^* \in \{P_2, P_3\}$, which contradicts Lemma 5.7. Thus, (i) holds.

We second turn to show (ii). If $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \neq \lambda_{n-2}(\overline{\Gamma})$, then $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) > \lambda_{n-2}(\overline{\Gamma})$, and thus $\lambda_{|V(T)|}(T) \leq \lambda_{n-2}(\overline{\Gamma})$ for some tree T of F. We assume that $T \neq Z_{q,2,1}$ with $q \geq 2$. Then $T = P_q$ or $T = Z_{q,1,1}$. If $T = P_q$, by Lemmas 4.4(ii) and 5.3(iii), $-2\cos(\frac{\pi}{q+1}) = \lambda_q(P_q) \leq -2\cos(\frac{2\pi}{k})$, and thus $q \geq \frac{k}{2} - 1$. Otherwise, $T = Z_{q,1,1}$. Then, by Lemmas 4.4(iii) and 5.3(iii), $-2\cos\left(\frac{\pi}{2q+4}\right) = \lambda_{q+3}(Z_{q,1,1}) \leq -2\cos\left(\frac{2\pi}{k}\right)$, and thus $q \geq \frac{k}{4} - 2$. □

We proceed with further characterizations of $\overline{\Gamma}$, i.e., of its subgraph F. The proofs of the next three lemmas are given in the Appendix.

Lemma 6.9. *At most three non-trivial components of F are isomorphic. Moreover, if $\tau(\Gamma^*) \geq 2$, then no two non-trivial components of F are isomorphic.*

We recall that Γ^* is a c-cyclic graph and in the next two lemmas consider the interplay between c and the parameters $\eta(\overline{\Gamma})$ (the number of non-trivial components of $\overline{\Gamma}$) and $\tau(\overline{\Gamma})$ (the number of triangles in $\overline{\Gamma}$).

Lemma 6.10. *If $c \geq 2$, then $\eta(\overline{\Gamma}) \geq 4$.*

Lemma 6.11. *If $c \geq 2$, then $\overline{\Gamma}$ does not contain a triangle.*

Here is the main result of this section.

Theorem 6.12. Γ^* *is not a c-cyclic graph, with* $c \geq 2$.

Proof. Assume that $c \geq 2$, and let C_g be the shortest cycle of Γ^*. Since $\tau(\overline{\Gamma}) = 0$ (by Lemma 6.11), we have $g \geq 4$, and then Corollary 5.11 implies that

$$\varepsilon(F) \geq 3 + q(\Gamma^*) \geq 3. \tag{9}$$

We prove the following claim.

Claim A. *Under the previous assumptions, we have* $g = 5$.

Proof of Claim A. First, if $g = 4$, then either $U_1^4 \cup P_2$ or $K_{2,3} \cup P_2$ is an induced subgraph of $\overline{\Gamma}$ by (9), but this contradicts Lemma 4.3(iii). Hence, $g \geq 5$. Since U_1^g is forbidden for an even integer $g \geq 6$ by Lemma 4.5(ii), it follows that g is odd. Now, $g \geq 9$, together with (9), implies that $Z_{4,3,1} \cup 2P_2 \cup K_1$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(i). If $g = 7$, then U_2^7 is an induced subgraph of Γ^*, since C_7 is the shortest cycle of Γ^* and $c \geq 2$. This implies that $Z_{3,2,2}$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(i). Thus $g = 5$, and this completes the proof of Claim A.

We now distinguish the two cases depending on whether $U_2^5(1)$ is a subgraph of Γ^* or not.

Case 1: $U_2^5(1)$ *is a subgraph of* Γ^*. Since C_5 is the shortest cycle of Γ^* and $Z_{2,2,1}(1)$ is forbidden (by Lemma 4.3(ii)), we get that H_3 is an induced subgraph of Γ^*. On the base of Corollary 3.6, we have $\lambda_3(\Gamma) \geq \lambda_3(K_8 \setminus H_3) = 1$, which contradicts Lemma 5.3.

Case 2: $U_2^5(1)$ *is not a subgraph of* Γ^*. Let C_q be the second shortest cycle of Γ^*, and let $C_5 = w_1 w_2 \cdots w_5$. If $d_{\Gamma^*}(w_i) \geq 4$ for some i, then (9) leads to the conclusion that $U_{1,1}^5 \cup 2P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(iii). Thus, $2 \leq d_{\Gamma^*}(w_i) \leq 3$ for each i. Combining this with (2) and the fact that $U_2^5(1)$ is not a subgraph of Γ^*, we can choose $G\big[V(C_5) \cup V(C_q)\big] = \Theta_{s_1,s_2,s_3}$ as an induced subgraph of $\overline{\Gamma}$ such that $s_1 \geq s_3 \geq s_2$, $q = s_1 + s_2 + 2$, $s_2 + s_3 = 3$, $0 \leq s_2 \leq 1$ and $d_{\Gamma^*}(u_0) = d_{\Gamma^*}(v_0) = 3$, where u_0 and v_0 are distinguished in Fig. 1. Since U_1^q is forbidden for even integers $q \geq 6$ (by Lemma 4.5(ii)), we get that q is odd and $q \geq 5$. Let further P_s be a longest path of F (if any).

Subcase 2.1: $s_2 = 0$. Then $s_3 = 3$. If $s_1 \geq 4$, then $Z_{2,2,1}(1)$ is an induced subgraph of Γ^* (since $\Theta_{s_1,0,3}$ is an induced subgraph of $\overline{\Gamma}$), contrary to Lemma 4.3(ii). Thus, $s_1 = 3$, and so $q = 5$. This implies that $\Theta_{3,0,3}$ is an induced subgraph of Γ^*.

If $c \geq 3$, then $\varepsilon(F) \geq 6$ (by Corollary 5.11), and thus $\Theta_{3,0,3} \cup P_2 \cup 2P_3 \cup P_4$ is an induced subgraph of $\overline{\Gamma}$, by Lemmas 6.6 and 6.9, which in turn contradicts Lemma 4.8(ii). Hence, $c = 2$ giving $k = |E(\Gamma^*)| + |E(F)| \geq 13$ by (9).

Since W_6 is forbidden if k is odd (by Lemma 4.3), and since $\Theta_{3,0,3}$ is an induced subgraph of Γ^*, we get that k is even. Since $\Theta_{3,0,3} \cup P_2 \cup P_3 \cup K_{1,3}$, $\Theta_{3,0,3} \cup 2P_2 \cup P_5$ are forbidden (by Lemma 4.8(ii)), we have $\Delta(F) = 2$ (by (9)) and each path of F contains at most four vertices, that is, $s \leq 4$. Taking into account Lemma 6.8, the inequality $s \leq 4 < \frac{k}{2} - 1$, we get

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{7}\right) < -1.80.$$

Now, since $Z_{2,2,1}(1)$, $Z_{4,3,1} \cup P_2 \cup P_3$ are forbidden (by Lemma 4.3(i) and (ii)), Γ^* is an induced subgraph of L_7. On the basis of Corollary 3.6, we have $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_9(L_7) > -1.79$, a contradiction.

Subcase 2.2: $s_2 = 1$. Then $s_3 = 2$. Since $q = s_1 + s_2 + 2 = s_1 + 3$ is odd, s_1 is even. If $s_1 \geq 6$, then $Z_{4,3,1} \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$ by (9), contrary to Lemma 4.3(i). Thus, $s_1 \in \{2, 4\}$. Let, as in Fig. 1, $\{u_0, w_1, v_0\}$ be the common vertices of C_q and C_5. In this case, $q = s_1 + 3$ and C_{s_1+4} is an induced even cycle of Γ^*. Combining this with Lemma 4.5(i), we conclude that k is even.

Let first $s_1 = 4$. Then $q = 7$ and Γ^* is obtained from $\Theta_{4,1,2}$ by attaching a path P_t to w_1; otherwise, as $q = 7$ and $g = 5$, U_1^8 would be an induced subgraph of Γ^*, but this contradicts Lemma 4.5(ii). Recall that $Z_{3,2,2}$ is forbidden by Lemma 4.3(i) and $q = 7$. Thus, $t = 0$ and so $\Gamma^* = \Theta_{4,2,1}$.

In this case, $k = |E(\Theta_{4,2,1})| + |E(F)| \geq 14$ by Lemma 6.6 and (9). Since $U_{1;1}^5 \cup P_6 \cup 2P_2$ is forbidden (by Lemma 4.8(iv)), we have $s \leq 5$. Since

$$\lambda_7(\Theta_{4,2,1}) > -1.42 > -1.8 > -2\cos\left(\frac{\pi}{7}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma}) \tag{10}$$

(see Lemma 5.3(iii)), we have $\lambda_{|V(F)|}(F) \leq \lambda_{n-2}(\overline{\Gamma})$. Since $s \leq 5 < \frac{k}{2} - 1$, by Lemma 6.8 and (10) we conclude that $Z_{2,1,1}$ is an induced subgraph of some first-type tree T of F by Lemma 6.8. Combining this with (9), we get that $U_{1;1}^5 \cup Z_{2,1,1} \cup P_2$ is an induced subgraph of $\overline{\Gamma}$, but this contradicts Lemma 4.8(iv).

Let now $s_1 = 2$. Then $q = 5$. Since $\Theta_{2,1,2} \cup P_3 \cup K_{1,3}$, $\Theta_{2,1,2} \cup P_2 \cup P_5$ are forbidden (by Lemma 4.8(ii)), we conclude that $\Delta(F) = 2$ and each path of F contains at most four vertices, that is $s \leq 4$. Since $k \geq |E(\Theta_{2,1,2})| + |E(F)| \geq 12$ by (9), we have $s \leq 4 < \frac{k}{2} - 1$. By Lemma 6.8, we obtain

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{6}\right) < -1.73.$$

If $c \geq 3$, then $\varepsilon(F) \geq 6$ (by Corollary 5.11). This implies that $\Theta_{2,1,2} \cup 3P_3 \cup 3P_2$ is an induced subgraph of Γ^*, but this contradicts Lemma 4.8(ii) and Lemma 6.6. Thus, $c = 2$. Since U_1^6 and $Z_{3,2,2}$ are forbidden by Lemma 4.5(ii) and Lemma 4.3(i), Γ^* is obtained from $\Theta_{2,1,2}$ by attaching a path P_t to w_1 and $0 \leq t \leq 1$. This implies that Γ^* is an induced subgraph of L_8. By direct computation based on Corollary 3.6, we get $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_6(L_8) = -1$, a final contradiction. □

7. Γ^* is not a tree

The main result of this section is Theorem 7.7 in which we eliminate the possibility that Γ^* is a tree. A sequence of auxiliary lemmas is needed.

Lemma 7.1. *Let $G = K_{1,4} \cup P_{s_1} \cup P_{s_2}$ and $t = s_1 + s_2 + 2$. If $s_1 \geq s_2 \geq 2$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$ and $m_3(G) < m_3(C_t)$.*

Proof. It is not difficult to see that $|E(G)| = |E(C_t)|$. Further, $m_1(G) = s_1+s_2+2 = t = m_1(C_t)$, $m_2(G) = 4\big(s_1+s_2-2\big)+(s_1-1)(s_2-1)+\frac{1}{2}\big(s_1-2\big)\big(s_1-3\big)+\frac{1}{2}\big(s_2-2\big)\big(s_2-3\big) = \frac{1}{2}\big(s_1+s_2+2\big)\big(s_1+s_2-1\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \leq s_1+s_2-4 = t-6 < t = m_3(C_t)$. □

Lemma 7.2. *Let $G = Z_{p_1,p_2,1} \cup Z_{q_1,q_2,1}$ and $t = p_1 + p_2 + q_1 + q_2 + 2$. If $p_1 \geq p_2 \geq 1$ and $q_1 \geq q_2 \geq 1$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$ and $m_3(G) < m_3(C_t)$.*

Proof. As in the previous proof, we easily get $|E(G)| = |E(C_t)|$, $m_1(G) = p_1+p_2+q_1+q_2+2 = t = m_1(C_t)$, $m_2(G) = p_1+p_2+q_1+q_2-4+\frac{1}{2}(p_1+p_2-1)(p_1+p_2-2)+\frac{1}{2}(q_1+q_2-1)(q_1+q_2-2)+(p_1+p_2+1)(q_1+q_2+1) = \frac{1}{2}\big(p_1+p_2+q_1+q_2+2\big)\big(p_1+p_2+q_1+q_2-1\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \leq p_1+p_2+q_1+q_2 = t-2 < t = m_3(C_t)$. □

Lemma 7.3. *Let $G = W_q \cup P_s$ and $t = q+s-2$. If $q \geq 6$ and $s \geq 2$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$ and $m_3(G) < m_3(C_t)$.*

Proof. As before, $|E(G)| = |E(C_t)|$, $m_1(G) = q+s-2 = t = m_1(C_t)$, $m_2(G) = q-4+q-5+\frac{1}{2}(q-4)(q-5)+(q-1)(s-1)+\frac{1}{2}(s-2)(s-3) = \frac{1}{2}\big(q+s-5\big)\big(q+s-2\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \leq q+s-4 = t-2 < t = m_3(C_t)$. □

Lemma 7.4. *Let $G = Z_{p_1,p_2,1} \cup Z_{2,2,2}$ and $t = p_1 + p_2 + 7$. If $p_1 \geq p_2 \geq 1$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$ and $m_3(G) < m_3(C_t)$.*

Proof. Again, we have $|E(G)| = |E(C_t)|$, $m_1(G) = p_1+p_2+7 = t = m_1(C_t)$, $m_2(G) = 9+6(p_1+p_2+1)+p_1+p_2-2+\frac{1}{2}(p_1+p_2-1)(p_1+p_2-2) = \frac{1}{2}\big(p_1+p_2+7\big)\big(p_1+p_2+4\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \leq p_1+p_2+6 = t-1 < t = m_3(C_t)$. □

Remark 7.5. Prior to Lemmas 7.1–7.4, since $t \geq 6$, it is easily checked that $m_4(G) = m_4(C_t) = 0$.

Lemma 7.6. *Let $G = Z_{p_1,p_2,1} \cup C_q$ and $t = p_1 + p_2 + q + 1$. If $p_1 \geq p_2 \geq 1$ and $q \geq 3$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$,*

- *$m_3(G) \leq t-1 < t = m_3(C_t)$, with $m_3(G) = t-1$ if and only if $p_2 \geq 2$ and $q \geq 4$, and*
- *$m_4(C_t) = 0$ and $m_4(G) \leq 1$, with equality if and only if $q = 4$.*

Proof. The proof is similar to the previous ones. We clearly have $|E(G)| = |E(C_t)|$. Moreover, $m_1(G) = p_1+p_2+q+1 = t = m_1(C_t)$, $m_2(G) = p_1+p_2-2+\frac{1}{2}(p_1+p_2-1)(p_1+$

$p_2-2)+(p_1+p_2+1)q+\frac{1}{2}q(q-3) = \frac{1}{2}\big(p_1+p_2+q+1\big)\big(p_1+p_2+q-2\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \le p_1+p_2+q = t-1 < t = m_3(C_t)$. Obviously, the equality $m_3(G) = t-1$ holds if and only if $p_2 \ge 2$ and $q \ge 4$. Finally, we have $m_4(C_t) = 0$ and $m_4(G) \le 1$, with equality if and only if $q = 4$. □

We are ready to prove the announced result.

Theorem 7.7. *Γ^* is not a tree.*

Proof. By way of contradiction, we assume that Γ^* is a tree. Here is the additional setting. Under the previous assumption and by virtue of (2), we have that every component of $\overline{\Gamma}$ is a tree. In addition, Lemma 5.7 allows us to assume that $\Delta(\overline{\Gamma}) \ge 3$. Therefore, without loss of generality we can also assume that $\Delta(\Gamma^*) \ge 3$ and that Γ^* has the largest spectral radius among all components with maximum vertex degree at least 3.

Since $\tau(\Gamma^*) = 0$, by Lemma 6.1 and (3), we have

$$\sum_{i=1}^{|V(\Gamma^*)|} d_i(\Gamma^*)\big(d_i(\Gamma^*)-2\big) = 2\varepsilon(F) \ge 4|V(\Gamma^*)|-6+2q(\Gamma^*)-4\big(|V(\Gamma^*)|-1\big) = 2\big(q(\Gamma^*)-1\big),$$

and so

$$\varepsilon(F) \ge q(\Gamma^*) - 1, \tag{11}$$

with equality if and only if every special vertex of Γ^* is a 3-vertex. Let further P_s be a longest path of F (if any).

Case 1: $\Delta(\Gamma^*) \ge 4$. If $q(\Gamma^*) \ge 2$, then $\varepsilon(F) \ge 2$ by (11). Since $Z_{2,1,1,1}(1)$, $Z_{2,2,1,1} \cup K_1$, $Z_{4,1,1,1} \cup P_2 \cup K_1$ are forbidden (by Lemma 4.3(i) and (ii)), we conclude that $Z_{3,1,1,1}(2)$ is an induced subgraph of Γ^* and $q(\Gamma^*) = 2$. Combining the latter with $\Delta(\Gamma^*) \ge 4$, we get $\varepsilon(F) \ge 3$ by (3). Thus, $Z_{3,1,1,1}(2) \cup 2P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$ (by Lemma 6.6), but this contradicts Lemma 4.3(ii). Hence, $q(\Gamma^*) = 1$. This implies that Γ^* is a star-like tree, that is it has exactly one vertex with degree at least three.

By (3) and $\tau(\Gamma^*) = 0$, we have

$$\varepsilon(F) = \frac{1}{2}\Delta(\Gamma^*)\big(\Delta(\Gamma^*)-3\big) \ge 2. \tag{12}$$

Since $Z_{2,2,1,1} \cup K_1$, $Z_{2,1,1,1,1} \cup P_2 \cup K_1$, $Z_{4,1,1,1} \cup P_2 \cup K_1$ are forbidden (by Lemma 4.3 (i)–(ii)) and $\Delta(\Gamma^*) \ge 4$, it follows from (12) that either Γ^* is a star, or $\Gamma^* = Z_{2,1,1,1}$, or $\Gamma^* = Z_{3,1,1,1}$. We now consider these possibilities.

Subcase 1.1: $\Gamma^* \in \{Z_{2,1,1,1}, Z_{3,1,1,1}\}$. Since $Z_{2,1,1,1} \cup 2P_2 \cup K_{1,3}$ is forbidden (by Lemma 4.3(i)) and $\varepsilon(F) = 2$ by (12), we get $\eta(\overline{\Gamma}) = \varepsilon(F)+1 = 3$ and $F = P_s \cup P_t$, where $2 \le t \le s$. Since $k \ge 7$, on the basis of Lemma 5.3 and Corollary 3.6 we compute

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_6(Z_{3,1,1,1}) > -1.26 > -2\cos\left(\frac{\pi}{4}\right) \geq -2\cos\left(\frac{2\pi}{k}\right).$$

Thus, k is even by Lemma 6.7 and

$$\lambda_s(P_s) = \lambda_{|V(F)|}(F) \leq \lambda_{|V(F)|-1}(F) \leq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right). \tag{13}$$

Since $\lambda_{|V(F)|}(F) \leq \lambda_{|V(F)|-1}(F) \leq \lambda_{n-2}(\overline{\Gamma}) < \lambda_{s-1}(P_s)$ (by (13) and Lemma 6.8), we have $\lambda_t(P_t) \leq \lambda_{n-2}(\overline{\Gamma})$, and so $s \geq t \geq \frac{k}{2} - 1$ (see the proof of Lemma 6.8). This implies that $k = |E(\Gamma^*)| + |E(F)| \geq 3 + s + t \geq k + 1$, a contradiction.

Subcase 1.2: $\Gamma^* = K_{1,q}$, *where* $q \geq 4$. If $q \geq 5$, then $\varepsilon(F) \geq 5$ by (12), and thus $K_{1,5} \cup 5P_2$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(iii). Hence, $\Gamma^* = K_{1,4}$ and so $\varepsilon(F) = 2$ by (12). By (2), F consists of two non-trivial paths and $\eta(\overline{\Gamma}) - 3$ first-type trees. Let F_1 be the set of those first-type trees, and let P_t and P_s be the two non-trivial paths of F. (Note that, by Corollary 5.5 and Lemma 7.1, we have $F_1 \neq \emptyset$.) By Lemmas 7.1 and 7.6, we have $m_1(\overline{\Gamma}) = m_1(C_k \cup (n-k)K_1)$, $m_2(\overline{\Gamma}) = m_2(C_k \cup (n-k)K_1)$, $m_3(\overline{\Gamma}) < m_3(C_k \cup (n-k)K_1)$ and $m_4(\overline{\Gamma}) = m_4(C_k \cup (n-k)K_1) = 0$. This implies that $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, but the latter contradicts Corollary 5.5.

Case 2: $\Delta(\Gamma^*) = 3$.

Subcase 2.1: $q(\Gamma^*) \geq 2$. Here we have $\varepsilon(F) = q(\Gamma^*) - 1 \geq 1$ by (11). If $Z_{2,2,2}$ is an induced subgraph of Γ^*, then since $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)) and $q(\Gamma^*) \geq 2$, we have that $Z_{2,2,1}(1)$ is an induced subgraph of Γ^*, contrary to Lemma 4.3(ii). Hence, we may suppose that $Z_{p_1,p_2,1}$ is an induced subgraph of Γ^* such that p_2 takes the largest possible value, and subject to this, $p_1 + p_2$ takes the largest possible value, along with $p_1 \geq p_2 \geq 1$.

Since $q(\Gamma^*) \geq 2$, we have $p_1 \geq 2$. If $p_1 = 2$, then $\Gamma^* = W_6$, as $Z_{2,2,1}(1)$ is forbidden by Lemma 4.3(ii). In this case, $\varepsilon(F) = 1$. By Lemmas 7.3 and 7.6, we have $m_1(\overline{\Gamma}) = m_1\big(C_k \cup (n-k)K_1\big)$, $m_2(\overline{\Gamma}) = m_2\big(C_k \cup (n-k)K_1\big)$, $m_3(\overline{\Gamma}) < m_3\big(C_k \cup (n-k)K_1\big)$ and $m_4(\overline{\Gamma}) = m_4\big(C_k \cup (n-k)K_1\big) = 0$, which implies that $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, contrary to Corollary 5.5. Thus, $p_1 \geq 3$. If $p_2 = 1$, by the choice of p_2 and (11), we have $\Gamma^* = W_q$ and $\varepsilon(F) = 1$. From Lemmas 7.3 and 7.6 we get $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, again contrary to Corollary 5.5. Combining this with the fact that $Z_{4,4,1}$ is forbidden (by Lemma 4.3(i)), we conclude that

$$2 \leq p_2 \leq 3 \leq p_1.$$

Subsubcase 2.1.1: $p_2 = 3$. Then $3 \leq p_1 \leq 5$, as $Z_{6,3,1}$ is forbidden by Lemma 4.3(i). Moreover, since $Z_{2,2,1}(1)$, $Z_{4,2,1}(2)$, $Z_{4,2,1}(3)$, $Z_{5,3,1}(4) \cup P_2$, $Z_{6,1,1}(2) \cup P_2$, $Z_{3,2,2}$ are forbidden (by Lemma 4.3(i)–(ii)), we have $p_1 = 3$ and $\Gamma^* \in \big\{H_5, Z_{3,3,1}(2)\big\}$.

If $\Gamma^* = H_5$, then $\varepsilon(F) = q(\Gamma^*) - 1 = 2$, and thus $H_5 \cup 2P_2$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(iii). Thus, $\Gamma^* = Z_{3,3,1}(2)$, along with $\varepsilon(F) = 1$. Combining this with the fact that $Z_{3,3,1}(2) \cup K_{1,3}$, $Z_{3,3,1}(2) \cup P_6$ are forbidden (by Lemma 4.3(ii)), we obtain $F = P_s$ with $2 \leq s \leq 5$. In this case, $k = |E(\Gamma^*)| + |E(F)| \geq 9$.

If k is odd, then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_8\big(Z_{3,3,1}(2)\big) > -1.6 > -2\cos\big(\frac{\pi}{9}\big) \geq -2\cos\big(\frac{\pi}{k}\big) = \lambda_{n-1}(\overline{\Gamma})$ (by Lemma 5.3(ii)), contrary to Lemma 6.7. If k is even, then in the same way we get $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_8\big(Z_{3,3,1}(2)\big) > -1.6 > -2\cos\big(\frac{\pi}{5}\big) \geq -2\cos\big(\frac{2\pi}{k}\big) = \lambda_{n-2}(\overline{\Gamma})$, which implies $\lambda_{s-1}(P_s) \leq \lambda_{n-2}(\overline{\Gamma})$, contrary to Lemma 6.8(i).

Subsubcase 2.1.2: $p_2 = 2$. Since $Z_{7,2,1} \cup P_2$ is forbidden (by Lemma 4.3(i)), we have $3 \leq p_1 \leq 6$.

We first suppose that $p_1 = 6$. Since $Z_{6,2,1} \cup P_2 \cup K_1$ is forbidden (by Lemma 4.3(i)) and $\varepsilon(F) \geq 1$, we have $F \in \{P_2, P_3\}$. From (11) we also have $q(\Gamma^*) = 2$, and so $\Gamma^* = Z_{6,2,1}(j)$ for $2 \leq j \leq 5$, as $Z_{3,2,2}$ and $Z_{2,2,1}(1)$ are forbidden by Lemma 4.3(i)–(ii). However, $Z_{4,2,1}(2)$, $Z_{4,2,1}(3)$, $Z_{6,2,1}(4)$, $Z_{6,2,1}(5)$ are forbidden (by Lemma 4.3(ii)), a contradiction.

We now suppose that $4 \leq p_1 \leq 5$. Since $Z_{4,2,1}(2)$, $Z_{4,2,1}(3)$, $Z_{2,2,1}(1)$, $Z_{3,2,2}$ are forbidden (again by Lemma 4.3(i)–(ii)), we have $\Gamma^* = Z_{5,2,1}(4)$, and so $\varepsilon(F) = 1$ by (11). Since $Z_{5,2,1}(4) \cup P_2 \cup K_1$ is forbidden (by Lemma 4.3(ii)), we have $F \in \{P_2, P_3\}$. In this case, since $10 \leq k = |Z_{5,2,1}(4)| + E(F)| \leq 11$, we have $F = P_3$ and $k = 11$ by Lemma 6.3. A straightforward computation leads to $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_9\big(Z_{5,2,1}(4)\big) > -1.79 > -2\cos\big(\frac{\pi}{11}\big) = \lambda_{n-1}(\overline{\Gamma})$, which contradicts Lemma 6.7.

It remains to consider the possibility that $p_1 = 3$. Since $Z_{2,2,1}(1), Z_{3,2,1}(2) \cup P_2 \cup K_{1,3}$ are forbidden (by Lemma 4.3(ii)), we have $\Gamma^* = Z_{3,2,1}(2)$ and $F = P_s$ by (11). Since $Z_{3,2,1}(2)$ is an induced subgraph of $Z_{3,3,1}(2)$, by Corollary 3.6 we have $\lambda_{n-1}(\overline{\Gamma}) = -2\cos\big(\frac{\pi}{k}\big) \leq -2\cos\big(\frac{\pi}{7}\big) < -1.8 < -1.6 < \lambda_8\big(Z_{3,3,1}(2)\big) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*)$, and thus k is even by Lemma 6.7. If $k \geq 10$, then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_8\big(Z_{3,3,1}(2)\big) > -1.6 > -2\cos\big(\frac{\pi}{5}\big) \geq \lambda_{n-2}(\overline{\Gamma})$, while by Lemma 5.3(iii) and Corollary 3.6, we have $\lambda_{s-1}(P_s) \leq \lambda_{n-2}(\overline{\Gamma})$, contrary to Lemma 6.8. Thus, $k = 8$ and $s = 2$, but this contradicts Lemma 6.3.

Subcase 2.2: $q(\Gamma^*) = 1$. First, $\Gamma^* \neq Z_{p_3,p_4,1}$, where $p_3 \geq p_4 \geq 1$. Otherwise, (3) implies that $\overline{\Gamma}$ contains $\eta(\overline{\Gamma}) - 1$ first-type trees. Since $\eta(\overline{\Gamma}) \geq 2$ (by Lemma 6.2), from Lemmas 7.2 and 7.6 we get that $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, contrary to Corollary 5.5. Secondly, since $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)), we obtain $\Gamma^* = Z_{2,2,2}$ and $\varepsilon(F) = 0$ by (11). In this case, since $\eta(\overline{\Gamma}) \geq 2$, from Lemmas 7.4 and 7.6 we obtain $m_1(\overline{\Gamma}) = m_1\big(C_k \cup (n-k)K_1\big)$, $m_2(\overline{\Gamma}) = m_2\big(C_k \cup (n-k)K_1\big)$, $m_3(\overline{\Gamma}) < m_3\big(C_k \cup (n-k)K_1\big)$ and $m_4(\overline{\Gamma}) = m_4\big(C_k \cup (n-k)K_1\big) = 0$, which implies that $\Phi(\overline{\Gamma}) > \Phi\big(C_k \cup (n-k)K_1\big)$, but this contradicts Corollary 5.5. □

8. If $\Delta(\overline{\Gamma}) \geq 3$, then Γ^* is not a unicyclic graph with girth ≥ 4

The main result of this section is Theorem 8.7. In the following text, we abbreviate $\Delta(\Gamma^*)$ to Δ and assume that Γ^* is a unicyclic graph with the unique cycle C_{g_0}.

Lemma 8.1. *The statement of Theorem 2.1 holds for* $\Gamma^* = C_{g_0}$.

Proof. We assume that the statement of the corresponding theorem does not hold for $\Gamma^* = C_{g_0}$. Under the assumption of this lemma, by (3), we have $\tau(\Gamma^*) = \varepsilon(F) = 0$, and thus non-trivial paths are not components of F and $g_0 \geq 4$. Then obviously $g_0 \neq k$, as

$\Delta(\overline{\Gamma}) \geq 3$. If $g_0 \geq 5$, by a successive application of Lemma 7.6, we get $\Phi(\overline{\Gamma}) > \Phi\big(G\big)$, but this contradicts Corollary 5.5. Hence, $g_0 = 4$.

Similarly to the proof of Lemma 7.6, we have $|E(\overline{\Gamma})| = |E\big(G\big)|$, $m_1(\overline{\Gamma}) = m_1\big(G\big) = k$, $m_2(\overline{\Gamma}) = m_2\big(G\big) = \frac{1}{2}k(k-3)$, $m_3(\overline{\Gamma}) \leq k-1 < k = m_3(G)$ and $m_4(\overline{\Gamma}) = 1 > 0 = m_4(G)$. Thus, $\Phi(\overline{\Gamma}) > \Phi(G)$, contrary to Corollary 5.5. □

By virtue of the previous lemma, we may suppose that $\Delta \geq 3$ and thus $U_1^{g_0}$ is an induced subgraph of Γ^*. Since $\varepsilon(F) \geq q(\Gamma^*) - \tau(\Gamma^*)$ by Corollary 5.11, Lemma 4.5(ii) tells us that g_0 is odd.

Since F contains $|V(F)| + 1 - \eta(\overline{\Gamma})$ edges, if $g_0 \geq 4$ then by Corollary 5.11 we have

$$|V(\Gamma^*)| = |E(\Gamma^*)| = k - 1 + \eta(\overline{\Gamma}) - |V(F)|,\ \tau(\overline{\Gamma}) = 0 \text{ and } \varepsilon(F) \geq q(\Gamma^*), \tag{14}$$

with equality if and only if each special vertex of Γ^* is a 3-vertex.

We proceed with the following lemmas. Their proofs are very similar to the proofs of the sequence of lemmas from the beginning of the previous section. Therefore, we give the proof of the first lemma, and omit the remaining ones.

Lemma 8.2. *Let $G = H_6 \cup P_{q_1} \cup P_{q_2}$ and $t = q_1 + q_2 + 7$. If $q_1 \geq q_2 \geq 2$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$, $m_4(G) = m_4(C_t) = 0$ and $m_3(G) \leq m_3(C_t)$, with equality if and only if $q_1 = q_2 = 2$.*

Proof. Evidently, we have $|E(G)| = |E(C_t)|$. Moreover, $m_1(G) = q_1 + q_2 + 7 = t = m_1(C_t)$, $m_2(G) = 25+9(q_1+q_2-2)+(q_1-1)(q_2-1)+\frac{1}{2}(q_1-2)(q_1-3)+\frac{1}{2}(q_2-2)(q_2-3) = \frac{1}{2}\big(q_1+q_2+7\big)\big(q_1+q_2+4\big) = \frac{1}{2}t(t-3) = m_2(C_t)$ and $m_3(G) \leq q_1+q_2+7 = t = m_3(C_t)$. The equality in the latter expression holds if and only if $q_1 = q_2 = 2$. □

Lemma 8.3. *Let $G = U_1^7 \cup P_q$ and $t = q + 7$. If $q \geq 2$, then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$, $m_4(G) = m_4(C_t) = 0$ and $m_3(G) \leq m_3(C_t)$, with equality if and only if $q = 2$.*

Lemma 8.4. *Let $G = U_d^5 \cup P_q \cup Z_{p_1,p_2,1}$ and $t = d + q + 5 + p_1 + p_2$, with $q \geq 2$, $d \geq 1$ and $p_1 \geq p_2 \geq 1$. Then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$, $m_4(G) = m_4(C_t) = 0$ and*

- *for $d \geq 2$, $m_3(G) \leq t = m_3(C_t)$, with equality if and only if $q = 2$ and $p_1 \geq p_2 \geq 2$,*
- *for $d = 1$, $m_3(G) < t = m_3(C_t)$.*

Lemma 8.5. *Let $G = U_d^5 \cup P_q$ and $t = d + q + 4$, with $q \geq 2$ and $d \geq 1$. Then $|E(G)| = |E(C_t)|$, $m_1(G) = m_1(C_t)$, $m_2(G) = m_2(C_t)$ and $m_4(G) = m_4(C_t) = 0$ and*

- *for $d \geq 2$, $m_3(G) \geq t = m_3(C_t)$, with equality if and only if $q \geq 3$,*
- *for $d = 1$, $m_3(G) \leq t = m_3(C_t)$, with equality if and only if $q = 2$.*

We now return to the initial settings of this section (given before and after Lemma 8.1).

Lemma 8.6. $g_0 \notin \mathbb{N} \setminus \{3,5\}$.

Proof. Recall that g_0 is odd. Assume that $g_0 \geq 7$. Since $q(\Gamma^*) \geq 1$ (by Lemma 8.1), we see from (14) that $\varepsilon(F) \geq 1$, with the equality if and only if Γ^* contains exactly one special vertex, which is a 3-vertex. Since $Z_{4,4,1}$ is forbidden by Lemma 4.3(i), we have $g_0 \in \{7,9\}$. In what follows we consider these possibilities one-by-one.

Case 1: $g_0 = 9$. Since $U_1^9 \cup P_2 \cup K_1$ is forbidden (by Lemma 4.3(iii)) and $\varepsilon(F) \geq 1$, we have $F = P_s$ with $s \leq 3$. This follows that $\varepsilon(F) = q(\Gamma^*) = 1$ and $\Delta = 3$ by (14). Note that $Z_{3,2,2}$ is forbidden by Lemma 4.3(i). Thus, $\Gamma^* = U_1^9$. In this case, $k = |E(U_1^9)| + |E(F)| \geq 11$. If k is odd, by using Lemma 6.7 we compute have $-1.88 < \lambda_9(U_1^9) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) < -1.91$, a contradiction. Otherwise, k is even. Since $\lambda_8(U_1^9) > -1.18 > -2\cos\left(\frac{\pi}{6}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$, by using Lemma 5.3(iii), we get $s \geq 5$ by Lemma 6.8, a contradiction.

Case 2: $g_0 = 7$. Since $Z_{3,2,2}$ is forbidden by (Lemma 4.3(i)), we get that U_2^7 is also forbidden for $\overline{\Gamma}$. Combining this with the fact that $Z_{2,2,1,1} \cup K_1$ is forbidden (by Lemma 4.3(i)), we conclude that $\Delta = 3$, and thus $\varepsilon(F) = q(\Gamma^*) \geq 1$ by (14). Let P_s be a longest path of F.

Claim A. *H_7 is forbidden.*

Proof of Claim A. Assume that H_7 is an induced subgraph of Γ^*. Since $Z_{3,2,1}(2) \cup K_{1,3} \cup P_2$ is forbidden (by Lemma 4.3(ii)), we have $\Delta(F) = 2$. Moreover, since $Z_{3,2,1}(2) \cup 2P_2 \cup P_3, Z_{2,2,1}(1), Z_{3,2,2}$ are forbidden (by Lemma 4.3(i)–(ii)) and $\varepsilon(F) = q(\Gamma^*)$, we have $\Gamma^* = H_7$ and $\varepsilon(F) = 2$, by Lemma 6.6. Thus, $k = |E(\Gamma^*)| + |E(F)| \geq 11$. If k is odd, then Lemma 6.7 gives $-1.88 < \lambda_8(H_7) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) < -1.91$, a contradiction. Otherwise, $k \geq 12$ is even. Since $\lambda_7(H_7) = -1 > -2\cos\left(\frac{\pi}{6}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$, we have $s \geq 5$ by Lemma 6.8. Thus, $Z_{3,2,1}(2) \cup P_2 \cup P_5$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3(ii). This completes the proof of Claim A.

Claim B. *H_6 is forbidden.*

Proof of Claim B. As before, assume that H_6 is an induced subgraph of Γ^*. Since H_7 is forbidden by Claim A and since $Z_{2,2,1}(1)$, $Z_{3,2,2}$ are forbidden (by Lemma 4.3 (i)–(ii)), we have $\Gamma^* = H_6$, and thus $\varepsilon(F) = 2$ by (14). From Lemmas 7.6, 8.2 and Corollary 5.5 we conclude that $F = 2P_2$. In this case, $k = |E(\Gamma^*)| + |E(F)| = 11$, contrary to Lemma 6.3. This completes the proof of Claim B.

In view of Claims A and B, we have $\Gamma^* = U_1^7$, as $Z_{2,2,1}(1)$ and $Z_{3,2,2}$ are forbidden. Thus, $\varepsilon(F) = 1$ by (14). By Lemmas 7.6 and 8.3 and Corollary 5.5, we get $\overline{\Gamma} = U_1^7 \cup P_2$ and $k = 9$. By direct computation, we obtain $\lambda_7(U_1^7) > -1.81 > -2\cos\left(\frac{\pi}{9}\right) = \lambda_{n-1}(\overline{\Gamma})$, which contradicts Lemma 6.7. □

We arrive at the main result of this section.

Theorem 8.7. *If $\Delta(\overline{\Gamma}) \geq 3$, then Γ^* is not a unicyclic graph with girth at least 4.*

Proof. By way of contradiction, we assume that $g_0 \geq 4$, i.e., by taking into account the previous lemma, that $g_0 = 5$.

We first eliminate the possibility that $\Delta = \Delta(\Gamma^*) \neq 3$, i.e., by taking into account Lemma 8.1, that $\Delta \geq 4$. If $q(\Gamma^*) = 1$, then $\varepsilon(F) \geq 3$ by (3). If $q(\Gamma^*) \geq 2$, then $\varepsilon(F) \geq 3$ by (14). Thus, we always have $\varepsilon(F) \geq 3$. Since $U^5_{1,1} \cup 2P_2 \cup P_3$, $C_5 \cup K_{1,4}$, $Z_{2,2,1}(1)$ are forbidden (by Lemmas 4.3(ii)–(iii) and 4.8(ii)), we get that $\Gamma^* \cup F$ contains $H_8 \cup 2P_2 \cup P_3$ as an induced subgraph by Lemma 6.6. On the other hand, $Z_{3,1,1,1}(2) \cup 2P_2 \cup P_3$ is forbidden by Lemma 4.3(ii), a contradiction.

Let further $\Delta = 3$. In this case, Γ^* contains U^5_1 as an induced subgraph. By (14), it follows that

$$\varepsilon(F) = q(\Gamma^*) \geq 1. \tag{15}$$

Let U^5_d be an induced subgraph of Γ^* such that d has the largest possible value, and let P_s be the longest path of F.

Claim A. *If $q(\Gamma^*) \geq 2$, then $d \leq 4$ and Γ^* is an induced subgraph of L_9.*

Proof of Claim A. For $d \leq 2$, since $Z_{2,2,1}(1)$ is forbidden (by Lemma 4.3(ii)), we conclude that Γ^* is an induced subgraph of L_9. Thus, to complete the proof of this claim, it suffices to show that $d \leq 2$. By (15), we have $\varepsilon(F) \geq 2$.

Assume that $d \geq 3$. We immediately get that $d \leq 4$, as $U^5_5 \cup P_2 \cup K_1$ is forbidden (by Lemma 4.3(iii)). Moreover, $d = 4$ is impossible, as $Z_{4,2,1}(2), Z_{4,2,1}(3), Z_{2,2,1}(1), U^5_{4;1} \cup P_2 \cup K_1$ are forbidden by Lemma 4.3(ii)–(iii). Hence, $d = 3$.

Since $U^5_3(2) \cup 2P_2, Z_{2,2,1}(1), U^5_{3;2} \cup P_2 \cup K_1$ are forbidden (by Lemma 4.3(ii)–(iii)) and $\varepsilon(F) \geq 2$, we have $\Gamma^* \in \{U^5_{3;1}, L_{10}\}$.

If $\Gamma^* = L_{10}$, then k is even by Lemma 4.3 (as W_6 is an induced subgraph of L_{10}). In this case, $\varepsilon(F) = q(\Gamma^*) \geq 3$, and thus $k = |E(\Gamma^*)| + |E(F)| \geq 14$. Since $\lambda_8(L_{10}) > -1.31 > -2\cos\left(\frac{\pi}{7}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$, we have $\lambda_{|V(T)|}(T) \leq \lambda_{n-2}(\overline{\Gamma})$ for some tree $T \in F$. Since $U^5_{1;1} \cup Z_{2,1,1} \cup P_2$ is forbidden (by Lemma 4.8(iv)), we have $s \geq \frac{k}{2} - 1 \geq 6$ by Lemma 6.8, contrary to the fact that $U^5_{1;1} \cup 2P_2 \cup P_6$ is forbidden by Lemma 4.8(iv).

If $\Gamma^* = U^5_{3;1}$, then $\varepsilon(F) = q(\Gamma^*) = 2$. In this case, $k = |E(\Gamma^*)| + |E(F)| \geq 11$.

Assume that k is odd. Since $\lambda_8(U^5_{3;1}) > -1.84 > -2\cos\left(\frac{\pi}{11}\right) \geq -2\cos\left(\frac{\pi}{k}\right) = \lambda_{n-1}(\overline{\Gamma})$, we get that $U^5_{1;1} \cup Z_{2,1,1} \cup P_2$ is an induced subgraph of $\overline{\Gamma}$ (by Lemma 6.7), contrary to Lemma 4.8(iv).

Assume now that k is even. If $k \geq 14$, then $\lambda_7(U^5_{3;1}) > -1.28 > -2\cos\left(\frac{\pi}{7}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$, and thus $\lambda_{|V(T)|}(T) \leq \lambda_{n-2}(\overline{\Gamma})$ for some tree T of F. Combining this with Lemma 6.8 and the fact that $U^5_{1;1} \cup Z_{2,1,1} \cup P_2$ is forbidden (by Lemma 4.8(iv)), we obtain $T = P_s$ with $s \geq \frac{k}{2} - 1$. Since $U^5_{1;1} \cup P_7$ is forbidden (by Lemma 4.8(iv)), we have $s \leq 6$, precisely $k = 14$ and $s = 6$. However, $k = |E(\Gamma^*)| + |E(F)| \geq 9 + s \geq \frac{k}{2} + 8$, a contradiction.

If $k = 12$ then $F = P_2 \cup P_3$, which yields

$$\lambda_{n-2}(\overline{\Gamma}) = \lambda_{12}\left(U^5_{3;1} \cup P_2 \cup P_3\right) = \lambda_3(P_3) > -1.42 > -2\cos\left(\frac{\pi}{6}\right),$$

contrary to Lemma 5.3(iii). This completes the proof of Claim A.

Claim B. *If* $q(\Gamma^*) = 1$, *then* $d \le 4$.

Proof of Claim B. Assume that $d \ge 5$. Since $U_5^5 \cup P_2 \cup K_1$ and U_6^5 are forbidden (by Lemma 4.3(iii)), we have $F = P_s$ with $s \le 3$ and $\Gamma^* = U_5^5$. If $s = 2$, then $k = 11$, contrary to Lemma 6.3. Thus, $s = 3$ and $k = 12$. By using Lemma 5.3(iii) we compute $-1.62 < \lambda_{11}\big(U_5^5 \cup P_3\big) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction. This completes the proof of Claim B.

We now return to the settings before Claim A and distinguish the two cases depending on the parity of k.

Case 1: k is odd. We first suppose that $k \ge 11$. If $q(\Gamma^*) \ge 2$, since W_6 is forbidden (by Lemma 4.3), we have that Γ^* is an induced subgraph of $U_{2;2}^5$ by Claim A. If $q(\Gamma^*) = 1$, then Γ^* is an induced subgraph of U_4^5 by Claim B. In both cases, on the basis of Corollary 3.6 and Lemma 5.3(ii) we compute

$$\begin{aligned}\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) &\ge \min\left\{\lambda_8(U_{2;2}^5), \lambda_8(U_4^5)\right\} > -1.88 > -1.91 > -2\cos\left(\frac{\pi}{11}\right)\\ &\ge -2\cos\left(\frac{\pi}{k}\right) = \lambda_{n-1}(\overline{\Gamma}).\end{aligned}$$

Combining this with Lemma 6.7, we deduce that either $Z_{3,1,1}$ or $Z_{2,2,1}$ is an induced subgraph of F, contrary to the fact that $U_1^5 \cup Z_{3,1,1}$, $U_1^5 \cup Z_{2,2,1}$ are forbidden (by Lemma 4.8(iv)).

We now suppose that $k \le 9$. If $q(\Gamma^*) \ge 2$, then $\Gamma^* = U_{1;1}^5$ and $F = 2P_2$, as $\varepsilon(F) \ge 2$ by (15). In this case, by Lemma 6.7, we have $-1.81 < \lambda_6(U_{1;1}^5) = \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = -2\cos(\frac{\pi}{9}) < -1.87$, a contradiction. Thus $q(\Gamma^*) = 1$. Since $k \le 9$ and $\varepsilon(F) = 1$ by (15), we have $\Gamma^* \cup F = U_d^5 \cup P_s$. In this case, since Γ^* is an induced subgraph of U_4^5 (by Claim B), Corollary 3.6 leads to the conclusion that $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \ge \lambda_8(U_4^5) \ge -1.62 > -2\cos(\frac{\pi}{7}) \ge -2\cos(\frac{\pi}{k}) = \lambda_{n-1}(\overline{\Gamma})$, but this contradicts Lemma 6.7.

Case 2: k is even. If $k = 8$, then $\varepsilon(F) = q(\Gamma^*) = 1$ by (15). Note that we have $s \ne 2$ by Lemma 6.3, and thus $\Gamma^* \cup F = U_1^5 \cup P_3$. Since $s = 3$, by Lemma 8.5, we have $\Phi(\overline{\Gamma}) = \Phi\big(U_1^5 \cup P_3 \cup (n-9)K_1\big) > \Phi\big(C_8 \cup (n-8)K_1\big)$, contrary to Corollary 5.5. Hence, $k \ge 10$.

If $q(\Gamma^*) \ge 2$, then Γ^* is an induced subgraph of L_9 by Claim A. If $q(\Gamma^*) = 1$, then Γ^* is an induced subgraph of U_4^5 by Claim B. In both cases, by using Corollary 3.6, Lemma 5.3(iii), we get

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \ge \min\left\{\lambda_8(L_9), \lambda_7(U_4^5)\right\} > -1.49 > -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma}). \quad (16)$$

Subcase 2.1: $q(\Gamma^*) \ge 2$. Since $\varepsilon(F) = q(\Gamma^*) \ge 2$ by (15), we have $k = |E(\Gamma^*)| + |E(F)| \ge 12$ by Lemma 6.3 (as $3 \nmid 10$). By Claim A, Γ^* is an induced subgraph of L_9, which implies that either $U_{1;1}^5$ or H_9 is an induced subgraph of Γ^*. Since $U_{1;1}^5 \cup Z_{2,1,1} \cup P_2$, $H_9 \cup Z_{2,1,1} \cup P_2$, $U_{1;1}^5 \cup P_7$, $H_9 \cup P_2 \cup P_6$ are forbidden (by Lemma 4.8(iv)–(v)), we have

$$s \leq 6 \text{ and } T = K_{1,3} \text{ whenever } \Delta(T) = 3 \text{ and } T \in F. \tag{17}$$

From (16), (17) and Lemma 6.8 we have $k \in \{12, 14\}$. If $k = 14$, then $P_2 \notin F$ by Lemma 6.3. Since $U_{1;1}^5 \cup P_3 \cup P_6$ and $H_9 \cup P_2 \cup P_6$ are forbidden (by Lemma 4.8(iv)–(v)), we have $s \leq 5 < \frac{k}{2} - 1$. Combining this with (16) and Lemma 6.8, we conclude that $Z_{2,1,1}$ is an induced subgraph of F, contrary to (17).

Let $k = 12$. If $\Gamma^* = U_{1;1}^5$, by using Lemmas 3.5, and 5.3(iii), we get

$$0.79 < \lambda_3\big(K_8 \setminus (U_{1;1}^5 \cup K_1)\big) \leq \lambda_3(\Gamma) = 2\cos\left(\frac{\pi}{6}\right) - 1 < 0.74,$$

a contradiction. Hence, $\Gamma^* \neq U_{1;1}^5$.

We first suppose that $\Delta(F) = 2$. By Lemma 6.8 and (16), we have $s \geq \frac{k}{2} - 1 = 5$. Combining this with $|E(\Gamma^*)| \geq 7$ and $\varepsilon(F) = q(\Gamma^*) \geq 2$, we get $F = P_2 \cup P_5$ and $\Gamma^* = H_9$, as $\Gamma^* \neq U_{1;1}^5$. In this case, since $\Gamma^* = H_9$, Lemma 5.3(iii) leads to $-1.68 < \lambda_{12}\big(H_9 \cup P_2 \cup P_5\big) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction. Hence, $\Delta(F) = 3$.

It follows that $F = K_{1,3} \cup 2P_2$ and $\Gamma^* = H_9$. In this case, Lemma 5.3(iii) also leads to $-1.68 < \lambda_{13}\big(H_9 \cup 2P_2 \cup K_{1,3}\big) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction.

Subcase 2.2: $q(\Gamma^*) = 1$. Then $\varepsilon(F) = 1$ and Γ^* is an induced subgraph of U_4^5 by Claim B and (15). Recall that $k \geq 10$. We first suppose that $k \geq 12$. By using Corollary 3.6 and Lemma 5.3(iii), we get

$$\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_8(U_4^5) > -1.62 > -2\cos\left(\frac{\pi}{6}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma}),$$

and thus $\lambda_{|V(F)|}(F) \leq \lambda_{|V(F)|-1}(F) \leq \lambda_{n-2}(\overline{\Gamma})$. Combining this with $\lambda_{s-1}(P_s) > \lambda_{n-2}(\overline{\Gamma})$ (by Lemma 6.8), the fact that $U_1^5 \cup Z_{2,2,1}$ is forbidden (by Lemma 4.8(iv)) and Lemma 6.8, we conclude that $P_s \cup Z_{q,1,1}$ is an induced subgraph of F, where $s \geq \frac{k}{2} - 1$ and $q \geq \frac{k}{4} - 2$. Since $U_1^5 \cup Z_{2,1,1} \cup P_6$ is forbidden (by Lemma 4.8(iv)), we have $k = 12$, and thus $s \geq 5$ and $q \geq 1$. This implies that $k = |E(\Gamma^*)| + |E(F)| \geq 13$, a contradiction.

We now suppose that $k = 10$. Then $P_2 \notin F$ and $P_5 \notin F$ by Lemma 6.3. This implies that $\Delta(F) = 2$ and so $F = P_s$. Since $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) > \lambda_{n-2}(\overline{\Gamma})$ (by (16)), Lemma 6.8 gives $s \geq 4$. Combining this with $s \neq 5$, we obtain $\Gamma^* \cup F = U_2^5 \cup P_4$. Now, from Corollary 3.6, Lemma 5.1, we get

$$-0.13 < \lambda_5\big(K_{11} \setminus (U_2^5 \cup P_4)\big) \leq \lambda_5\big(\Gamma\big) = -2\cos\left(\frac{3\pi}{5}\right) - 1 < -0.38,$$

a final contradiction. □

9. The completion of the proof of Theorem 2.1

In this section we finalize the proof of our main result. According to the previous results, it remains to consider the case in which the component Γ^* of a putative graph

$\overline{\Gamma}$ is a unicyclic graph with a proper induced triangle C_3. We denote the vertices of C_3 by w_1, w_2 and w_3, and assume that $d_{\Gamma^*}(w_1) \geq d_{\Gamma^*}(w_2) \geq d_{\Gamma^*}(w_3) \geq 2$ and $d_{\Gamma^*}(w_1) \geq 3$ by Lemma 8.1. In what follows, we also denote by U_d^3 the induced subgraph of Γ^* such that d has the largest possible value, and by P_s the longest path of F (if one exists). The forthcoming statements are formulated under the previous assumptions.

Since $U_1^3 \cup P_6$ is forbidden (by Lemma 4.8(iii)), from Corollary 5.11 we get

$$d \leq 7,\ s \leq 5 \text{ and } \varepsilon(F) \geq q(\Gamma^*) - 1, \tag{18}$$

where $\varepsilon(F) = q(\Gamma^*) - 1$ if and only if each special vertex of Γ^* is a 3-vertex.

Lemma 9.1. *If $\Delta = \Delta(\Gamma^*) \geq 4$, then the vertices of Γ^* distinct from w_1 are of degree at most 3.*

Proof. Assume that there is another vertex of Γ^* distinct from w_1 have degree at least four. Then, $q(\Gamma^*) \geq 2$. Suppose that H_{10} is an induced subgraph of Γ^*. If $q(\Gamma^*) \geq 3$, then $\varepsilon(F) \geq 3$ by (18). If $q(\Gamma^*) = 2$, then $\varepsilon(F) \geq 3$ follows from (3). This implies that $H_{10} \cup 2P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.8(v). Thus, H_{10} is forbidden. Also, $C_3 \cup K_{1,4} \cup 2P_2$ is forbidden by Lemma 4.8(ii) and $H_{11} \cup 2P_2$ is forbidden by Lemma 4.3(iii), and thus by analysing the structure of Γ^*, we conclude that H_{12} is its induced subgraph, as $\varepsilon(F) \geq q(\Gamma^*) \geq 2$ by (18).

If $\varepsilon(F) \geq q(\Gamma^*) = 2$, then Γ^* contains a pendant triangle and thus $P_2 \cup P_3$ is an induced subgraph of F by Lemma 6.4. Otherwise, $\varepsilon(F) \geq q(\Gamma^*) \geq 3$, and then $P_2 \cup P_3$ is also an induced subgraph of F by Lemma 6.6. In both cases, $P_2 \cup P_3$ is also an induced subgraph of F.

Since $C_3 \cup K_{1,4} \cup 2P_2$, $Z_{2,2,1}(1)$, $Z_{2,2,1,1} \cup K_1, U_1^3 \cup K_{1,3} \cup P_2 \cup P_3$ are forbidden by (Lemmas 4.3(i)–(ii) and 4.8(ii)–(iii)), we have $\Gamma^* = H_{12}$ and $\Delta(F) = 2$. By (3), we have $\varepsilon(F) = 3$. Combining this with the conclusion that C_3 must be a pendant triangle of Γ^*, by Lemma 6.4, we obtain that $H_{12} \cup P_2 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$, which contradicts the fact that $Z_{3,1,1,1} \cup 2P_3 \cup P_2$ is forbidden by Lemma 4.3(i). □

The proofs of the next three lemmas are given in the Appendix.

Lemma 9.2. $d \notin \{5, 6, 7\}$.

Now we limit the degree of w_1 in $\overline{\Gamma}$.

Lemma 9.3. $d_{\overline{\Gamma}}(w_1)$ *is not larger than* 3.

And here we fix the degree of w_2.

Lemma 9.4. $d_{\overline{\Gamma}}(w_2) = 2$.

We are ready to complete the proof of Theorem 2.1.

Proof of Theorem 2.1. It is sufficient to prove the statement of the theorem for $7 \leq k \leq n-1$. In the light of Lemmas 5.7, 9.1 and 9.3, we need to prove that Γ does not exist under the assumption that $\Delta = \Delta(\Gamma^*) = 3$. We assume the contrary, and then by Lemmas 9.1–9.4, we conclude that Γ^* is a subgraph of H_{14}, as $Z_{3,2,2}$ and H_{13} are forbidden by Lemma 4.3 (i) and (iii). By (18), $\varepsilon(F) = q(\Gamma^*) - 1$. Let P_s be a longest path of F (if exists).

Case 1: k is odd. Since $k \geq 7$, $\lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{7}\right) < -1.80 < -1.56 < \lambda_9(H_{14}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*)$ by Lemma 5.3(ii) and Corollary 3.6. Combining this with Lemma 6.7, we deduce that $U_1^3 \cup Z_{2,1,1}$ is an induced subgraph of $\overline{\Gamma}$, but this contradicts Lemma 4.8(iii).

Case 2: k is even. Since $U_1^3 \cup Z_{2,1,1}$, $U_1^3 \cup 2K_{1,3}, U_1^3 \cup P_6$ are forbidden (by Lemma 4.8(iii)), we have $s \leq 5$, and if $\Delta(T) = 3$ for some tree T of F, then $T = K_{1,3}$ and F contains at most one copy of $K_{1,3}$.

Subcase 2.1: $k \geq 10$. By Corollary 3.6, we have $\lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{5}\right) < -1.61 < \lambda_9(H_{14}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*)$, and thus

$$\lambda_{|V(F)|}(F) \leq \lambda_{|V(F)|-1}(F) \leq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) < -1.618. \tag{19}$$

Combining this with the above conclusion on $K_{1,3}$, we get $\lambda_s(P_s) \leq \lambda_{n-2}(\overline{\Gamma})$, and thus $s \geq \frac{k}{2} - 1 \geq 4$ (see the proof of Lemma 6.8). Moreover, since $U_1^3 \cup P_4 \cup K_{1,3}$ is forbidden (by Lemma 4.8(iii)), we have $\Delta(F) = 2$. Since (19) and $\lambda_{s-1}(P_s) > \lambda_{n-2}(\overline{\Gamma})$ by Lemma 6.8, we further get that $2P_4$ is an induced subgraph of F and $\varepsilon(F) \geq 2$. Since $q(\Gamma^*) - 1 = \varepsilon(F) \geq 2$, we also have that $U_2^3 \cup 2P_4$ is an induced subgraph of $\Gamma^* \cup F$, but this contradicts Lemma 4.8(iv).

Subcase 2.2: $k = 8$. In this case, $P_2 \notin F$ by Lemma 6.3, and thus $s \geq 3$ if P_s exists. If $q(\Gamma^*) \geq 2$, then $\varepsilon(F) \geq 1$ by (18), and thus $\Gamma^* \cup F = U_2^3(1) \cup P_3$. We compute $\lambda_{n-2}(\overline{\Gamma}) = \lambda_7\big(U_2^3(1) \cup P_3\big) = -1 > -2\cos\left(\frac{\pi}{4}\right)$, which contradicts Lemma 5.3(iii). If $q(\Gamma^*) = 1$ then $F = K_{1,3}$, as $\varepsilon(F) = 0$ and $\eta(\overline{\Gamma}) \geq 2$ by Lemma 6.2. This implies $\Gamma^* = U_2^3$. Thus, we have $\lambda_{n-2}(\overline{\Gamma}) = \lambda_7\big(U_2^3(1) \cup K_{1,3}\big) = -1 > -2\cos\left(\frac{\pi}{4}\right)$, which contradicts Lemma 5.3(iii), and the proof is complete. □

10. Concluding remarks

In [2], Cámara and Haemers conjectured that the graph $K_n \setminus P_k$ is determined by its spectrum. The conjecture is addressed positively through several steps reported in [2,8,18–20]. The main subject of [2] was the spectral determination of almost complete graphs, and it is also showed that $K_n \setminus C_k$ are DS for $k \in \{3, 4, 5\}$, but not for $k = 6$. In this paper we proved that this particular case is the unique exception.

In view of Lemma 5.3, we have $-3 < \lambda_n(K_n \setminus C_k) \leq \lambda_2(K_n \setminus C_k) \leq 1$ for $5 \leq k \leq n$. By [19, Lemma 4.1], $-3 < \lambda_n(K_n \setminus P_k) \leq \lambda_2(K_n \setminus P_k) < 1$ holds for $5 \leq k \leq n$.

This relates our and the corresponding results to the so-called Hoffman problem (cf. [6]) asking for a characterization of connected graphs whose second largest eigenvalue does not exceed 1. This is a very difficult problem, and after the four decades of intensive investigations by many experts, we have a significant number of partial results but not the full characterization. Some related references are [3,9,10,16,17,24,26–28]. One more relation with graphs whose second largest eigenvalue is bounded by a comparatively small constant is mentioned in Remark 4.2.

The foregoing chains of inequalities relate our paper to an other spectral problem: Characterize graphs whose spectrum is bounded from below by a fixed constant, in our case -3. A nice survey on recent progress in this direction can be found in [14]. We also refer the reader to [15,29].

Combining the previous research problems, we arrive at the following one.

Problem 1. Characterize connected graphs whose spectrum is bounded by -3 and second largest eigenvalue does not exceed 1.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A

Here we give the proofs of six lemmas from Sections 6 and 9.

- **Lemmas from Section 6.**

Proof of Lemma 6.9. If $\overline{\Gamma}$ contains at least four copies of a non-trivial tree T, then $m_{\overline{\Gamma}}(\pm\lambda) \geq 4$ holds for some eigenvalue $\lambda > 0$ of $\overline{\Gamma}$, and then we have $m_{\Gamma}(-1 \pm \lambda) \geq 3$ by Lemma 3.4, which contradicts Lemma 5.1.

Next we suppose that $\tau(\Gamma^*) \geq 2$. Since $\overline{\Gamma}$ does not contain a union of two disjoint cycles as an induced subgraph (by (2)), $\overline{\Gamma}$ contains Δ_t (of Fig. 1) as a subgraph, where $t \in \{4, 5, 6\}$. Suppose that F contains at least two copies of a tree T. Then $T \in \{P_2, P_3, P_4, K_{1,3}\}$, due to Lemma 4.6. We distinguish the three cases depending on t.

Case 1: $t = 4$. From Lemma 4.6 we have $T = P_2$ and Δ_4 is an induced subgraph of Γ^*. Since $\Delta_4 \cup 3P_2$ is forbidden (by Lemma 4.8(i)), we have $F = 2P_2$ and $\varepsilon(F) = 2$. From (3) we have $\Gamma^* \neq \Delta_4$ and thus $q(\Gamma^*) \geq 1$. Moreover, by Lemma 4.6, K_4 is not an induced subgraph of Γ^*, and thus in a c-cyclic graph Γ^* we have $c \geq \tau(\Gamma^*) \geq 3(c-1)+q(\Gamma^*)-2 \geq 3c-4$ (by Corollary 5.11). Hence, $c = 2$. Since $\Gamma^* \neq \Delta_4$, we have $q(\Gamma^*) \geq 1$. From the same corollary we conclude that Γ^* contains exactly one special vertex, which is a 3-vertex. Combining this with $|V(\Gamma^*)| = |E(\Gamma^*)| - 1 = k - 1 - |E(F)| = k - 3$, we get that Γ^* is obtained from Δ_4 by attaching a path P_{k-7} to a 2-vertex of Δ_4.

Once again, since $\Delta_4 \cup 3P_2$ is forbidden and $q(\Gamma^*) = 1$, we immediately get $k \in \{8, 9\}$. Moreover, since $F = 2P_2$, we have $k = 9$, by Lemma 6.3. In this case, by virtue of Lemmas 5.3(ii) and 6.7, we have $-1 = \lambda_5(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) = -2\cos\left(\frac{\pi}{9}\right) < -1.87$, a contradiction.

Case 2: $t = 5$. Since Δ_4 is not a subgraph of $\overline{\Gamma}$ (by the previous case), Δ_5 is an induced subgraph of $\overline{\Gamma}$. Note that $\Delta_5 \cup 2P_3$, $\Delta_5 \cup P_3 \cup P_2 \cup K_1$, $\Delta_5 \cup P_4$, $\Delta_5 \cup K_{1,3}$ are forbidden by (Lemma 4.8(i)), and then we have $T = P_2$ and $F = 2P_2$, by Lemma 6.6.

Since Δ_4 is not a subgraph of Γ^*, we have $c \geq \tau(\Gamma^*) > 3(c-1) + q(\Gamma^*) - 2 \geq 3c - 5$, by Corollary 5.11. Hence, $c = 2$, $q(\Gamma^*) = 0$ and $\tau(\Gamma^*) = 2$ (by the same corollary), which implies that $\Gamma^* = \Delta_5$. Now, $5 = |V(\Gamma^*)| = |E(\Gamma^*)| - 1 = k - 3$ and so $k = 8$, but this contradicts Lemma 6.3.

Case 3: $t = 6$. By the previous cases, Δ_4 and Δ_5 are not subgraphs of $\overline{\Gamma}$.

We claim that Δ_6 is an induced subgraph of Γ^*. Assuming the contrary, we get $c \geq 3$. Since Γ^* contains neither Δ_5 nor Δ_4 as a subgraph, we have $c \geq \tau(\Gamma^*) \geq 3(c-1) + q(\Gamma^*) - \varepsilon(F)$ (by Corollary 5.11), and so $\varepsilon(F) \geq 2c - 3 + q(\Gamma^*) \geq 3$. From Lemmas 4.6 and 6.6, we conclude that $c = 3$ and thus H_1 is an induced subgraph of Γ^*, as neither Δ_5 nor Δ_4 is a subgraph of Γ^*. This implies that $H_1 \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$ (by $\varepsilon(F) \geq 3$), but the latter contradicts Lemma 4.8(v). Therefore, Δ_6 is an induced subgraph of Γ^*.

Since $\Delta_6 \cup 2P_2 \cup 2P_3$ is forbidden (by Lemma 4.8(i)), from Lemma 6.6 we get $\varepsilon(F) \leq 3$. Combining this with the fact that Δ_4 is not a subgraph of Γ^* and taking into account Corollary 5.11, we compute

$$c \geq \tau(\Gamma^*) \geq 3(c-1) + q(\Gamma^*) - \varepsilon(F) \geq 3(c-2) + q(\Gamma^*) \geq 3(c-2), \tag{20}$$

which implies that $2 \leq c \leq 3$.

If $c = 3$, then $q(\Gamma^*) = 0$ and $\varepsilon(F) = \tau(\Gamma^*) = 3$, along with equalities in (20). By Corollary 5.11, Γ^* is a tricyclic graph with exactly four 3-vertices and no pendant vertices. Combining this with $c = 3$ and the conclusion that Δ_6 is an induced subgraph of Γ^*, we conclude that $\Gamma^* = H_2$, which contradicts (2), as H_2 contains a union of two disjoint triangles. Therefore, $c = 2$ and $\tau(\Gamma^*) = 2$.

Since $\Delta_6 \cup P_4 \cup P_3$, $\Delta_6 \cup K_{1,3}$ are forbidden (by Lemma 4.8(i)), we have $T \in \{P_2, P_3\}$. By Corollary 5.11, we further have

$$q(\Gamma^*) + 1 \le \varepsilon(F) \le 3. \tag{21}$$

We proceed by distinguishing the two subcases depending on T described in the beginning of the proof.

Subcase 3.1: $T = P_2$. Since Γ^* has no pendant triangle (by Lemma 6.4), we have $q(\Gamma^*) = 2$ and $\Gamma^* = \Delta_6(s;t)$, by (21). Since $\varepsilon(F) = 3$ and $\Delta_6 \cup 2P_2 \cup P_4$ is forbidden (by Lemma 4.8(i)), we have $F = 2P_2 \cup P_3$ by Lemma 6.6. Since $\Delta_6(2;2)$, $\Delta_6(3;1)$ are forbidden (by Lemma 4.8(i)), we get $\Gamma^* \in \{\Delta_6(2;1), \Delta_6(1;1)\}$. Since $F = 2P_2 \cup P_3$, we further deduce that $k = |E(\overline{\Gamma})| = 14$ if $\Gamma^* = \Delta_6(2;1)$, and $k = |E(\overline{\Gamma})| = 13$ if $\Gamma^* = \Delta_6(1;1)$. In each case, we get a contradiction to Lemma 6.3.

Subcase 3.2: $T = P_3$. Since $\Delta_6 \cup 3P_3$ is forbidden (by Lemma 4.8(i)), we have $F \in \{2P_3, 2P_3 \cup P_2\}$.

We first suppose that $F = 2P_3$. Then $|V(\Gamma^*)| + |V(F)| = k + 1$, and thus $\overline{\Gamma}$ contains $n - k - 1$ isolated vertices. Since $m_{\overline{\Gamma}}(0) \ge n - k - 1 + 2m_{P_3}(0) = n - k + 1$, (6) indicates that $4 \mid k$, and thus $\Gamma^* \ne \Delta_6$ as $|V(\Gamma^*)| = k - 5$. Combining this with (21) and $F = 2P_3$, we obtain $q(\Gamma^*) = 1$, and thus $\Gamma^* = \Delta_6(s)$ by Corollary 5.11. Since $4 \mid k$ and $\Delta_6 \cup 3P_3$ is forbidden (by Lemma 4.8(i)), we have $\Gamma^* = \Delta_6(1)$, and so $k = 12$. Using Lemma 5.3(iii), we compute $-1.42 < \lambda_{11}\big(\Delta_6(1) \cup 2P_3\big) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction.

Now let $F = 2P_3 \cup P_2$. Since $U^3_{1,1} \cup 2P_3 \cup P_2$, $W_{1,1,1} \cup 2P_3 \cup P_2$, $\Delta_6 \cup 2P_3 \cup 2P_2$, $U_{3;1,1} \cup 2P_3 \cup 2P_2$ are forbidden (by Lemma 4.8(i), (iii) and (v)), we have $\Gamma^* \in \{\Delta_6(1;1), \Delta_6(2), \Delta_6(1), \Delta_6\}$. In addition, since $P_2 \in F$, we have $3 \mid k$ by Lemma 6.3. Combining this with $k = |V(\Gamma^*)| + 6$ and the previous conclusion on Γ^*, we deduce that $\Gamma^* = \Delta_6$. As before, we compute $-1.42 < \lambda_{12}(\Delta_6 \cup 2P_3 \cup P_2) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction. □

Proof of Lemma 6.10. Due to Lemma 6.2, we may assume that $\eta(\overline{\Gamma}) \ge 2$. Suppose that $2 \le \eta(\overline{\Gamma}) \le 3$. Then $\varepsilon(F) \le \eta(\overline{\Gamma}) - 1 \le 2$. Since $c \ge 2$, by Corollary 5.11, we have

$$\tau\big(\overline{\Gamma}\big) = \tau\big(\Gamma^*\big) \ge 3(c-1) + q(\Gamma^*) - \varepsilon(F) \ge 1 + q(\Gamma^*) \ge 1. \tag{22}$$

We now consider the two cases depending on $\tau\big(\overline{\Gamma}\big)$.

Case 1: $\tau\big(\overline{\Gamma}\big) = 1$. By (22), $\varepsilon(F) = 2 = \eta(\overline{\Gamma}) - 1$, $q(\Gamma^*) = 0$, and $c = 2$. Next, by Corollary 5.11, Γ^* is a bicyclic graph with exactly two 3-vertices and $|V(\Gamma^*)| - 2$ vertices

of degree 2. Thus, $\Delta(\Gamma^*) = 3$. Let C_g be the second smallest cycle in Γ^*. Since $\tau(\overline{\Gamma}) = 1$ and $\varepsilon(F) = 2 = \eta(\overline{\Gamma}) - 1$, we may suppose that

$$\Gamma^* \in \{B_1(g,3), \Theta_{g-2,0,1}\} \text{ and } F = P_s \cup P_t, \text{ where } 2 \le t \le s.$$

Subcase 1.1: $\Gamma^* = B_1(g,3)$. Since $U_1^3 \cup P_5 \cup 2P_2$ is forbidden (by Lemma 4.8(iii)) and $\varepsilon(F) = 2$, we have $4 \le g \le 7$. Note that $U_1^4 \cup P_2$, U_1^6 are forbidden by Lemma 4.5(ii) and $Z_{3,2,2}$ is forbidden by Lemma 4.3(i). Thus, $g = 5$ and $\Gamma^* = B_1(5,3)$. This implies that

$$k = |E(\Gamma^*)| + |E(F)| \ge |E(\Gamma^*)| + 2 \ge 11.$$

If k is odd, by Lemma 6.7, we have $-1.62 < \lambda_7(B_1(5,3)) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \le -2\cos\left(\frac{\pi}{11}\right) < -1.91$, a contradiction. If k is even, since $\lambda_6(B_1(5,3)) = -1 > -1.73 > -2\cos\left(\frac{\pi}{6}\right) \ge -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$, we have $s \ge 5$ by Lemma 6.8. This implies that $B_1(5,3) \cup P_5$ is an induced subgraph of $\overline{\Gamma}$, which in turn contradicts the fact that $U_2^3(1) \cup P_5$ is forbidden by Lemma 4.8(iv).

Subcase 1.2: $\Gamma^* = \Theta_{g-2,0,1}$. Since $U_1^3 \cup P_5 \cup 2P_2$ is forbidden (by Lemma 4.8(iii)) and $\eta(\overline{\Gamma}) - 1 = \varepsilon(F) = 2$, we have $4 \le g \le 9$. If $g = 9$, then since $\Theta_{7,0,1} \cup P_2 \cup P_3$ is forbidden (by Lemma 4.8(ii)), we have $F = 2P_2$ and so $k = 13$, contrary to Lemma 6.3. Hence, $4 \le g \le 8$. Moreover, as $U_{3;1,1} \cup P_5$ and $\Theta_{2,0,1} \cup P_4$ are forbidden (by Lemma 4.8 (ii)–(iii)), we have $2 \le t \le s \le 4$. Note that $k = |E(\Gamma^*)| + |E(F)| \ge g + 4 \ge 8$. Thus, if k is odd, then $k \ge 9$ and then from Lemma 6.7 and $4 \le g \le 8$ we have $-1.81 < \lambda_7(\Theta_{5,0,1}) \le \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \le -2\cos\left(\frac{\pi}{9}\right) < -1.87$, a contradiction. Now, we can conclude that

$$4 \le g \le 8,\ 2 \le t \le s \le 4, \text{ and } k \ge 8 \text{ is even.}$$

Claim A. $s \ne 4$.

Proof of Claim A. Assume that $s = 4$. Since $U_{3;1,1} \cup P_3 \cup P_4$ and $\Theta_{2,0,1} \cup P_4$ are forbidden (by Lemma 4.8(ii)–(iii)), we have $F = P_2 \cup P_4$ and $g \ge 5$. Thus, $k = |E(\Gamma^*)| + |E(F)| = g + 6 \ge 12$ is even, which implies that $g \in \{6, 8\}$ and $k \in \{12, 14\}$. Combining this with $3 \mid k$ (by Lemma 6.3), we get $k = 12$ and $g = 6$.

On the basis of Lemma 5.3(iii) and $\lambda_4(P_4) = -2\cos\left(\frac{\pi}{5}\right) > -2\cos\left(\frac{\pi}{6}\right) = \lambda_{n-2}(\overline{\Gamma})$, we compute

$$-1 = \lambda_5(\Theta_{4,0,1}) = \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73,$$

a contradiction. This completes the proof of Claim A.

We now eliminate the possibility that $g \in \{5, 7\}$. Namely, since $k = |E(\Gamma^*)| + |E(F)| = g + s + t$ is even, we have $s = 3$ and $t = 2$, which implies that $k = g + 5 \ge 10$. Combining this with $3 \mid k$ (by Lemma 6.3), we get $k = 12$ and $g = 7$. Again, Lemma 5.3(iii) gives $-1.42 < \lambda_3(P_3) = \lambda_{11}(\Theta_{5,0,1} \cup P_2 \cup P_3) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \le -2\cos\left(\frac{\pi}{5}\right) < -1.61$, a contradiction.

Hence, $g \in \{4, 6, 8\}$, and then also $k = |E(\Gamma^*)| + |E(F)| = g + s + t \geq 8$. In this case, s and t have the same parity. Combining this with Claim A, we get $F \in \{2P_2, 2P_3\}$. If $F = 2P_2$, then $3 \mid k$ and $k = g + 4$, by Lemma 6.3. This implies that $g = 8$ and $k = 12$. Since $2 = s < \frac{k}{2} - 1$, on the basis of Lemma 6.8, we compute $-1.42 < \lambda_7(\Theta_{6,0,1}) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction. Hence, $F = 2P_3$. Since $\Theta_{2,0,1} \cup 2P_3$ is forbidden (by Lemma 4.8(ii)), we have $g \in \{6, 8\}$, and thus $k = g + 6 \in \{12, 14\}$. Since $3 = s < \frac{k}{2} - 1$, as before we compute $-1.42 < \min\{\lambda_7(\Theta_{6,0,1}), \lambda_5(\Theta_{4,0,1})\} \leq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction.

Case 2: $\tau(\overline{\Gamma}) \geq 2$. In this case, Γ^* contains Δ_t as a subgraph by (2), where $t \in \{4, 5, 6\}$.

Subcase 2.1: $t = 4$. If $\eta(\overline{\Gamma}) = 3$, then Lemma 4.6 implies that Δ_4 is an induced subgraph of Γ^* and thus $\Delta_4 \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 6.9, contrary to Lemma 4.8(i). Hence, $\eta(\overline{\Gamma}) = 2$. From Corollary 4.7 we have $F \in \{P_2, P_3\}$.

Claim B. *K_4 is forbidden for $\overline{\Gamma}$.*

Proof of Claim B. Assume that Γ^* contains K_4 as an induced subgraph. Then also $F = P_2$, by Lemma 4.6. Since $|V(\Gamma^*)| + c - 1 = |E(\Gamma^*)| = k - |E(F)| = k - 1$, we have $|V(\Gamma^*)| + |V(F)| = k + 2 - c$, and thus $\overline{\Gamma}$ contains $n + c - k - 2$ isolated vertices. By (6) and (7), we have $n + c - k - 2 \leq n - k + 2$, and thus $3 \leq c \leq 4$. Since K_4 is an induced subgraph of Γ^* and $c \leq 4$, we have $\tau(\Gamma^*) \leq 5$. Combining this with (22), we get that $1 = \varepsilon(F) \geq 3(c-1) + q(\Gamma^*) - \tau(\Gamma^*) \geq q(\Gamma^*) + 1$. Thus, $q(\Gamma^*) = 0$, $c = 3$ and $\Gamma^* = K_4$, implying that $k = 7$, but this contradicts Lemma 6.3. This completes the proof of Claim B.

By Claim B, we have $\tau(\Gamma^*) \leq c$. Together with $F \in \{P_2, P_3\}$ and (22), we have $c \geq \tau(\Gamma^*) \geq 3(c-1) + q(\Gamma^*) - \varepsilon(F) = 3c + q(\Gamma^*) - 4$, this leads to $c = 2$ and $q(\Gamma^*) = 0$, which further implies that $\Gamma^* = \Delta_4$. Since $7 \leq k = |E(\Gamma^*)| + |E(F)| \leq 7$, we have $F = P_3$ and $k = 7$. In this case, we compute $m_{\overline{\Gamma}}(0) = m_{\Delta_4}(0) + m_{P_3}(0) + n - 7 = n - 5 = n - k + 2$, but this contradicts (6).

Subcase 2.2: $t \in \{5, 6\}$. Since Δ_4 is not a subgraph of $\overline{\Gamma}$ (by Case 1), we conclude that $\tau(\Gamma^*) \leq c$. Combining this with (22) and $\varepsilon(F) \leq \eta(\overline{\Gamma}) - 1 \leq 2$, we obtain

$$2c - 3 + q(\Gamma^*) \leq \varepsilon(F) \leq 2 \text{ and so } 1 + q(\Gamma^*) \leq \tau(\Gamma^*) = c = 2. \tag{23}$$

This implies that Δ_t is an induced subgraph of Γ^* and $0 \leq q(\Gamma^*) \leq 1$. Note that $\Delta_t \cup K_{1,3}$ is forbidden by Lemma 4.8(i) for $t \in \{5, 6\}$. Thus, $\Delta(F) = 2$. In other words, every non-trivial tree of F is a path. Let P_s be a longest path of F.

Subsubcase 2.2.1: $q(\Gamma^*) = 0$. Then $\Gamma^* = \Delta_t$, for $t \in \{5, 6\}$. If k is odd, from Lemma 6.7 we have $-1 = \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{7}\right) < -1.8$, a contradiction. Hence, k is even, and so $k \geq 8$. Since $\Delta_t \cup P_5$ is forbidden by Lemma 4.8(i), we have $s \leq 4$. By Lemma 5.3(iii) and $k \geq 8$, we further obtain

$$-1 = \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) > -1.41 > -2\cos\left(\frac{\pi}{4}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma}).$$

Thus, $\lambda_{|V(F)|}(F) \leq \lambda_{|V(F)|-1}(F) \leq \lambda_{n-2}(\overline{\Gamma}) \leq -2\cos\left(\frac{\pi}{4}\right)$. Since $\Delta(F) = 2$, and $\lambda_{s-1}(P_s) > \lambda_{n-2}(\overline{\Gamma})$ by employing Lemma 6.8, we obtain $F = P_s \cup P_q$ (by (23)), where also $3 \leq q < s \leq 4$ by Lemmas 4.4(ii) and 6.9. This implies that $F = P_4 \cup P_3$. On the contrary, $\Delta_5 \cup 2P_3$ and $\Delta_6 \cup P_4 \cup P_3$ are forbidden by Lemma 4.8(i), a contradiction.

Subsubcase 2.2.2: $q(\Gamma^*) = 1$. Since we have equalities in (23), by Corollary 5.11 we get $\varepsilon(F) = 2$ and $\Gamma^* = \Delta_6(r)$. Since $\Delta_6 \cup 2P_2 \cup P_4$ and $\Delta_6 \cup P_5$ are forbidden (by Lemma 4.8(i)), we have $1 \leq r \leq 4$ and $s \leq 4$. Note that Γ^* contains a pendant triangle. Thus, $F \neq 2P_2$ (by Lemma 6.4), and so $k = |E(\Gamma^*)| + |E(F)| \geq 11$. If k is odd, then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) < -1.91$ by Lemma 6.7. However, Corollary 3.6 implies that $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_9\big(\Delta_6(4)\big) > -1.66$, a contradiction. If k is even, then $\lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{6}\right) < -1.73$, by Lemma 5.3(iii). On the contrary, since $s \leq 4 < \frac{k}{2} - 1$, Lemma 6.8 and Corollary 3.6 give

$$-1.25 < \lambda_8\big(\Delta_6(4)\big) \leq \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) < -1.73,$$

a final contradiction. □

Proof of Lemma 6.11. By virtue of the previous lemma we may assume that $\eta(\overline{\Gamma}) \geq 4$. We first assume that $\tau\big(\Gamma^*\big) \geq 2$. In this case Γ^* contains Δ_t as a subgraph by (2), where $t \in \{4, 5, 6\}$. Taking into account $\eta(\overline{\Gamma}) \geq 4$ and the fact that any two non-trivial trees of F are non-isomorphic (see Lemma 6.9), we get $|V(F)| \geq 9$. Combining this with Lemma 4.6, we conclude that Γ^* contains neither Δ_4 nor Δ_5 as its subgraph, which implies $t = 6$ and that Δ_6 is an induced subgraph of Γ^*. Thus, either $\Delta_6 \cup P_3 \cup P_4$ or $\Delta_6 \cup K_{1,3}$ is an induced subgraph of $\overline{\Gamma}$ (by Lemma 6.9), but this contradicts Lemma 4.8(i). Hence, $\tau\big(\Gamma^*\big) \leq 1$.

By way of contradiction, we further assume that $\tau\big(\Gamma^*\big) = 1$ and suppose that C_3 is the unique triangle of $\overline{\Gamma}$ and C_g is the second shortest cycle of Γ^*. Since $\tau(\overline{\Gamma}) = 1$, we have $g \geq 4$.

If $\Theta_{2,0,1}$ is a subgraph of Γ^*, then $\Theta_{2,0,1} \cup 2P_2 \cup P_3$ is an induced subgraph of the same graph (as $\eta(\overline{\Gamma}) \geq 4$), but this contradicts Lemma 4.8(ii). Hence, $\Theta_{2,0,1}$ is not a subgraph of Γ^*, and consequently U_2^3 is an induced subgraph of Γ^*, as $c \geq 2$.

Claim A. $\eta(\overline{\Gamma}) = 4$.

Proof of Claim A. We assume that $\eta(\overline{\Gamma}) \geq 5$. Since $\Theta_{2,0,1}$ is not a subgraph of Γ^* and $U_{3;1,1} \cup 2P_2 \cup 2P_3, U_{1,1}^3 \cup P_2 \cup 2P_3$ are forbidden (by Lemma 4.8(iii)), from Lemma 6.6 we get that Γ^* contains $B_1(g, 3)$ as an induced subgraph and C_3 is a pendant triangle of Γ^*. Since $U_1^4 \cup P_2$ is also forbidden by Lemma 4.5(ii), we have $g \geq 5$. This implies that $U_3^3(1)$ is an induced subgraph of Γ^*. Together with the previous conclusions of this claim, this yields that $U_2^3(1) \cup 3P_3 \cup P_2$ is an induced subgraph of $\overline{\Gamma}$ (see also Lemma 6.4), but the latter contradicts Lemma 4.8(iv), and the proof of Claim A is complete.

If $c \geq 3$, then $\varepsilon(F) \geq 3(c-1) + q(\Gamma^*) - 1 \geq 5$ (by Corollary 5.11), which is impossible by Claim A. Hence, $c = 2$. Combining this with $\varepsilon(F) \leq 3$ by Claim A, Corollary 5.11 and (2), we get

$$3 \geq \varepsilon(F) \geq 3c - 4 + q(\Gamma^*) = q(\Gamma^*) + 2, \text{ and } \mathcal{R}(\Gamma^*) \in \{\Theta_{g-2,0,1},\ B_1(g,3),\ B_2(g,3)\}. \tag{24}$$

(For $\mathcal{R}(\Gamma^*)$ see Definition 3.2.) We suppose that P_s is a longest path of F.

Case 1: $\mathcal{R}(\Gamma^*) = \Theta_{g-2,0,1}$. Since $\Theta_{2,0,1} \cup 2P_2 \cup P_3, U_{3;1,1} \cup 2P_2 \cup 2P_3, U_{3;1,1} \cup K_{1,3}$ are forbidden (by Lemma 4.8 (ii)–(iii)) and $\eta(\overline{\Gamma}) = 4$ (by Claim A), we have $g \in \{5,6,7,8\}$ and $\varepsilon(F) = 3$ (by Lemma 6.6). Further, since $U_{3;1,1} \cup 2P_2 \cup P_4, U_{3;1,1} \cup 3P_3$ are forbidden (by Lemma 4.8(iii)), we have $F \in \{P_2 \cup 2P_3, 2P_2 \cup P_3\}$, by Lemma 6.6. Thus, $s \leq 3$ and $3 \mid k$, by Lemma 6.3. Since $k = |E(F)| + |E(\Gamma^*)| \geq 4 + 7 = 11$ and $s \leq 3 < \frac{k}{2} - 1$, we have

$$\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) < -1.91 \text{ if } k \text{ is odd}, \tag{25}$$

by Lemma 6.7, and

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{6}\right) < -1.73 \text{ if } k \text{ is even}, \tag{26}$$

by Lemma 6.8.

If $\Gamma^* = \Theta_{g-2,0,1}$, then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_7(\Theta_{5,0,1}) > -1.81$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_7(\Theta_{6,0,1}) > -1.42$ by direct computation, contrary to (25) and (26). Hence, $q(\Gamma^*) = 1$, by (24). Since we have the equality in (24), from Corollary 5.11 we conclude that Γ^* is obtained from $\Theta_{g-2,0,1}$ by attaching a path P_t to a 2-vertex of $\Theta_{g-2,0,1}$, as $\varepsilon(F) = 3$. Note that $q(\Gamma^*) = 1$ and $U_{3;1,1} \cup 2P_2 \cup 2P_3$ is forbidden (by Lemma 4.8(iii)), and thus $1 \leq t \leq 3$. Since U_1^8 and $W_{4,1,1} \cup 2P_2 \cup P_3$ are forbidden by (Lemmas 4.5(ii) and 4.8(v)), we have $g \in \{5,6,7\}$. Let u_0 be the initial vertex of P_t.

If $g = 7$, then $\mathcal{R}(\Gamma^*) = \Theta_{5,0,1}$. If u_0 is in C_7, then $t = 1$, as $Z_{3,2,2}$ is forbidden for Γ^* by Lemma 4.3(i). In this case, Γ^* is obtained from $\Theta_{5,0,1}$ by attaching an isolated vertex to a 2-vertex of $\Theta_{5,0,1}$, and thus Γ^* is an induced subgraph of L_1 (see Fig. 2). By Corollary 3.6, we have $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_{10}(L_1) > -1.89$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_9(L_1) > -1.31$, contrary to (25) and (26). Otherwise, u_0 is in C_3. Since $1 \leq t \leq 3$, Γ^* is an induced subgraph of L_2. As before, we get $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_{10}(L_2) > -1.81$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_9(L_2) > -1.69$, contrary to (25) and (26).

If $g = 6$, then $\mathcal{R}(\Gamma^*) = \Theta_{4,0,1}$. Since U_1^6 is forbidden (by Lemma 4.5(ii)), u_0 is in C_3. Since $1 \leq t \leq 3$, Γ^* is an induced subgraph of L_3. From Corollary 3.6 we get $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_9(L_3) > -1.85$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_8(L_3) > -1.24$, contrary to (25) and (26).

Hence, $g = 5$, and so $\mathcal{R}(\Gamma^*) = \Theta_{3,0,1}$. If $F = 2P_2 \cup P_3$, then $12 \leq k = |E(\Gamma^*)| + |E(F)| \leq 14$ which follows from the aforementioned limit on t, $1 \leq t \leq 3$. Thus, $k = 12$ and $t = 1$, as $3 \mid k$ by Lemma 6.3. This implies that Γ^* is obtained from $\Theta_{3,0,1}$ by attaching an isolated vertex to a 2-vertex of $\Theta_{3,0,1}$. Thus, Γ^* is an induced subgraph of L_4. As before, we get $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_8(L_4) > -1.69$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_7(L_4) > -1.4$, contrary to (25) and (26).

So we have $F = 2P_3 \cup P_2$, and thus $13 \leq k = |E(\Gamma^*)| + |E(F)| \leq 15$, as $1 \leq t \leq 3$. This implies that $k = 15$ and $t = 3$, as $3 \mid k$. Since $W_{1,1,1} \cup 2P_3 \cup P_2$ and $Z_{3,2,2}$ are forbidden (by Lemmas 4.3(i) and 4.8(v)), we have $\Gamma^* = L_5$, which contradicts the fact that $U_{3;1,1} \cup 2P_2 \cup 2P_3$ is forbidden by Lemma 4.8(iii).

Case 2: $\mathcal{R}(\Gamma^*) = B_1(g,3)$. Since $Z_{3,2,2}$, $U_1^4 \cup P_2$ and U_1^6 are forbidden (by Lemmas 4.3(i) and 4.5(ii)), we have $g = 5$. Since $U_2^3(1) \cup 2P_2 \cup K_{1,3}$ is forbidden (by Lemma 4.8(iv)), we have $\varepsilon(F) = 3 = \eta(\overline{\Gamma}) - 1$ by Claim A. Then

$$k = |E(F)| + |E(\Gamma^*)| \geq 4 + 9 = 13.$$

By (24), $q(\Gamma^*) \leq 1$, where $q(\Gamma^*) = 1$ implies that Γ^* is obtained from $B_1(5,3)$ by attaching a path P_t to a 2-vertex of $B_1(5,3)$ (by Corollary 5.11). Since $U_3^3 \cup 2P_2 \cup P_3 \cup P_4$ and $U_1^3 \cup 2P_2 \cup P_5$ are forbidden (by Lemma 4.8(iii)–(iv)) and $\varepsilon(F) = 3$, we have $0 \leq t \leq 4$ and $s \leq 4$ by Lemma 6.6.

Since $k \geq 13$ and $\varepsilon(F) = 3$, we have

$$\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{13}\right) < -1.94 \text{ if } k \text{ is odd}, \quad (27)$$

by Lemma 6.7. Besides, since $s \leq 4 < \frac{k}{2} - 1$,

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{7}\right) < -1.8 \text{ if } k \text{ is even}, \quad (28)$$

by Lemma 6.8.

Combining this with $\lambda_6\big(B_1(5,3)\big) = -1 > \lambda_{n-2}(\overline{\Gamma})$ and $\lambda_7\big(B_1(5,3)\big) > -1.62 > \lambda_{|V(\Gamma^*)|-1}(\Gamma^*)$ (by direct computation and (27)–(28)), it follows that $q(\Gamma^*) = 1$ by (24). Let u_0 be the initial vertex of P_t. Since $Z_{3,2,2}$, $U_5^3(1)$, $U_{3;3,3}(1) \cup 2P_2$ are forbidden (by Lemma 4.3(i) and (iii)), we have $t \leq 1$ if $u_0 \in C_5$ and $t \leq 2$ if $u_0 \in C_3$. In both cases, Γ^* is an induced subgraph of L_6. By Corollary 3.6, we have $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_{11}(L_6) > -1.87$ and $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_{10}(L_6) > -1.63$, which contradicts (27) and (28).

Case 3: $\mathcal{R}(\Gamma^*) = B_2(g,3)$. Since $U_{3,2}^3 \cup 3P_2, U_1^4 \cup P_2, U_1^6$ are forbidden by (Lemmas 4.3(iii) and 4.5(ii)), we have $g = 5$, by Claim A. Using Corollary 5.11 under the assumption that $\varepsilon(F) \leq 3$, we get $q(\Gamma^*) = 0$ and thus $\Gamma^* = B_2(5,3)$. Moreover, from (3) and $\tau(\Gamma^*) = 1$, we get $\varepsilon(F) = 3$. Combining this with Claim A, we obtain $\Delta(F) = 2$. Since $U_{1,1}^3 \cup P_2 \cup P_4, U_{1,1}^3 \cup 2P_3 \cup P_2$ are forbidden (by Lemma 4.8(iii)), there must be $F = 2P_2 \cup P_3$, and thus $k = |E(\Gamma^*)| + |E(F)| = 12$. Since $s = 3 < \frac{k}{2} - 1$, from Lemma 6.8, we get

$$-1 = \lambda_5\big(B_2(5,3)\big) = \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{6}\right) < -1.73,$$

a final contradiction. □

• **Lemmas from Section 9.**

Proof of Lemma 9.2. Assume that $5 \le d \le 7$. By (2), either $\Delta(F) = 3$ or $\Delta(F) = 2$.

Claim A. $\Delta(F) \neq 3$.

Proof of Claim A. Let $\Delta(F) = 3$. Since $U_1^3 \cup Z_{2,1,1}$, $U_1^3 \cup K_{1,3} \cup P_2 \cup P_3$, $U_1^3 \cup K_{1,3} \cup P_4$ are forbidden (by Lemma 4.8(iii)), we have $\Gamma^* = U_5^3$ and $F = K_{1,3}$ by (18), which implies that $k = |E(U_5^3)| + |E(F)| = 11$. By using Lemmas 4.4(iii), and 5.3(ii) we compute

$$-1.74 < \lambda_{11}\big(U_5^3 \cup K_{1,3}\big) = \lambda_{n-1}\big(\overline{\Gamma}\big) = -2\cos\left(\frac{\pi}{k}\right) = -2\cos\left(\frac{\pi}{11}\right) < -1.91,$$

a contradiction. This completes the proof of Claim A.

Claim B. $q(\Gamma^*) \neq 1$.

Proof of Claim B. Let $q(\Gamma^*) = 1$. By (3), we have

$$\varepsilon(F) = \frac{1}{2}(\Delta - 2)(\Delta - 1) - 1, \text{ where } \Delta = \Delta(\Gamma^*). \tag{29}$$

If $\Delta \ge 5$, then $\varepsilon(F) \ge 5$ by (29). Since C_3 is a pendant triangle of Γ^*, we get that $P_2 \cup 3P_3 \cup P_4$ is an induced subgraph of F by Lemmas 6.4, 6.6 and 6.9, but this contradicts the fact that $U_3^3 \cup 2P_2 \cup P_3 \cup P_4$ is forbidden by Lemma 4.8(iv). Thus, we have $\Delta = 4$ and $\varepsilon(F) = 2$ by (29), as $\Delta = 3$ implies $\varepsilon(F) = 0$, contrary to Lemma 6.2 and Claim A. Since C_3 is a pendant triangle of Γ^*, using Lemmas 6.4 and 9.1 we get that $U_{5,1}^3 \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, but this contradicts the fact that $U_{1,1}^3 \cup P_2 \cup 2P_3$ is forbidden by Lemma 4.8(iii). This completes the proof of Claim B.

From (18) and $q(\Gamma^*) \ge 2$ by Claim B we get $\varepsilon(F) \ge 1$. Combining this with $q(\Gamma^*) \ge 2$ and Lemma 6.3, we deduce that

$$k = |E(\overline{\Gamma})| = |E(\Gamma^*)| + |E(F)| \ge 11.$$

Claim C. $d \notin \{6, 7\}$.

Proof of Claim C. Let $d \in \{6, 7\}$. Since $U_{3;6,1} \cup P_2$ is forbidden (by Lemma 4.8(iv)) and $\varepsilon(F) \ge 1$, we have $d_{\Gamma^*}(w_2) = 2$, and then C_3 is a pendant triangle of Γ^*.

If $\Delta \ge 4$, then $\varepsilon(F) \ge q(\Gamma^*) \ge 2$ by (18) and Claim B. This implies that $P_2 \cup P_3$ is an induced subgraph of F by Lemma 6.4. From Lemma 9.1 we get $d_{\Gamma^*}(w_2) = 2$ and that $U_{6,1}^3 \cup P_3 \cup P_2$ is an induced subgraph of $\Gamma^* \cup F$, but this contradicts the fact that $U_{1,1}^3 \cup 2P_3 \cup P_2$ is forbidden by Lemma 4.8(iii). Hence, $\Delta = 3$, and then (18) implies that $\varepsilon(F) = q(\Gamma^*) - 1$. Taking into account that $q(\Gamma^*) \ge 2$ (by Claim B), $d_{\Gamma^*}(w_2) = 2$ and that $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)), we deduce that $U_d^3(j)$ is an induced subgraph of Γ^*, where $1 \le j \le d - 1$. Since $U_1^3 \cup Z_{2,1,1}$ is forbidden (by Lemma 4.8(iii)), we have $1 \le j \le 3$. On the other hand, $U_6^3(3), U_6^3(2) \cup P_2, U_5^3(1)$ are forbidden by Lemma 4.3(iii), contrary to the previous conclusion on j. This completes the proof of Claim C.

Since $W_{5,1,1} \cup 2P_2$ is forbidden (by Lemma 4.8(v)), we have $d_{\Gamma^*}(w_3) = 2$ by (18).

Case 1: $d_{\Gamma^*}(w_2) \ge 3$. In this case, Γ^* contains $U_{3;5,1}$ as its induced subgraph. Since $U_{3;1,1} \cup 2P_2 \cup 2P_3$ is forbidden (by Lemma 4.8(iii)), Lemma 6.6 and (18) lead to $2 \le q(\Gamma^*) \le 3$.

Subcase 1.1: $q(\Gamma^*) = 3$. By (18) and Lemma 6.3, we have $\varepsilon(F) \geq 2$, and thus $k = |E(\Gamma^*)| + |E(F)| \geq 12$. Since $U_{3;1,1} \cup 2P_2 \cup 2P_3$ is forbidden, by Lemma 6.6 and (18), we have $\varepsilon(F) = 2$ and $\Delta(\Gamma^*) = 3$. Since $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)), Γ^* is a unicyclic graph obtained from $U_{3;5,p}$ by attaching exactly one isolated vertex to a 2-vertex of a pendant path of $U_{3;5,p}$, where $1 \leq p \leq 5$. Since $U_5^3(1), U_{3;5,1}(2) \cup 2P_2, U_1^3 \cup Z_{2,1,1}$ are forbidden (by Lemmas 4.3(iii) and 4.8(iii)) and Γ^* contains $U_{3;5,1}$ as an induced subgraph, this isolated vertex is adjacent to some 2-vertex of the pendant path P_p of $U_{3;5,p}$ and $1 \leq p \leq 4$. Combining this with the fact that $U_{3;1,1} \cup 2P_3 \cup 2P_2, Z_{7,2,1} \cup P_2$ are forbidden (by Lemmas 4.3(i) and 4.8(iii)), we get $1 \leq p \leq 3$. Now, since $1 \leq p \leq 3$, Γ^* is an induced subgraph of L_{11}. If k is odd, by Corollary 3.6, we get

$$\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_{12}(L_{11}) > -1.85 > -1.91 > -2\cos\left(\frac{\pi}{11}\right) \geq -2\cos\left(\frac{\pi}{k}\right) = \lambda_{n-1}(\overline{\Gamma}),$$

contrary to Lemma 6.7 and Claim A. If k is even, by the same corollary, we get

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_{11}(L_{11}) > -1.45 > -1.61 > -2\cos\left(\frac{\pi}{6}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma}),$$

and thus $s \geq 5$ by Lemma 6.8 and Claim A. However, $U_{3;1,1} \cup P_5$ is forbidden by Lemma 4.8(iii).

Subcase 1.2: $q(\Gamma^*) = 2$. If $\Delta \geq 4$, then $\varepsilon(F) \geq 2$ by (18). Combining this with $d = 5$ and Lemma 9.1, we get that $\overline{\Gamma}$ contains either $U_{1,1}^3 \cup P_2 \cup P_4$ or $U_{3;1,1} \cup 2P_2 \cup P_4$ as an induced subgraph, contrary to Lemma 4.8(iii). Hence, $\Delta = 3$, and then $\Gamma^* = U_{3;5,p}$ with $1 \leq p \leq 5$. This implies that $k = |E(\Gamma^*)| + |E(F)| \geq 10$ and $F = P_s$ by (18) and Claim A. If k is odd, then $-1.81 < \lambda_{12}(U_{3;5,5}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) < -1.91$ by Corollary 3.6 and Lemma 6.7, a contradiction. If k is even, then $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_{11}(U_{3;5,5}) > -1.50 > -2\cos(\frac{\pi}{5}) \geq -2\cos(\frac{2\pi}{k}) = \lambda_{n-2}(\overline{\Gamma})$ by Lemma 5.3(iii). Combining this with $\Delta(F) = 2$ and Lemma 6.8, we have $s \geq 4$, and then $U_{3;1,1} \cup P_4 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, which contradicts Lemma 4.8(iii).

Case 2: $d_{\Gamma^*}(w_2) = 2$. If $\Delta \geq 4$, then w_1 is the unique vertex of Γ^* with degree at least four by Lemma 9.1. Since C_3 is a pendant triangle and $q(\Gamma^*) \geq 2$ (by Claim B), $U_{1,1}^3 \cup P_2 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 6.4 and (18), but this contradicts Lemma 4.8(iii). Hence, $\Delta = 3$, and thus Γ^* is an induced subgraph of L_{12}, as $Z_{3,2,2}$ is forbidden by Lemma 4.3(i). In this case, $k = |E(\Gamma^*)| + |E(F)| \geq 9$. If k is odd, then $\lambda_{|V(\Gamma^*)|-1}(\Gamma^*) \geq \lambda_{11}(L_{12}) > -1.77 > -2\cos(\frac{\pi}{9}) \geq -2\cos(\frac{\pi}{k}) = \lambda_{n-1}(\overline{\Gamma})$, but this contradicts Lemma 6.7 and Claim A. If k is even, since $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_{10}(L_{12}) > -1.15 > -2\cos(\frac{\pi}{5}) \geq -2\cos(\frac{2\pi}{k}) = \lambda_{n-2}(\overline{\Gamma})$ and $\Delta(F) = 2$, we have $s \geq \frac{k}{2} - 1$ by Lemma 6.8. Combining this with $k \geq |E(U_5^3)| + |E(F)| \geq s + 7 \geq \frac{k}{2} + 6$, we obtain $k \geq 12$. This implies that $s \geq 5$. However, $U_1^3 \cup P_5 \cup P_3$ is forbidden by Lemma 4.8(iii), a contradiction. □

Proof of Lemma 9.3. Let $d_{\overline{\Gamma}}(w_1) \geq 4$. Then $U^3_{1,1}$ is an induced subgraph of $\overline{\Gamma}$ and $d_{\Gamma^*}(w_1) = \Delta \geq 4$ by Lemma 9.1. Since $U^3_{1,1} \cup K_{1,3}$ is forbidden (by Lemma 4.8(iii)), we have $\Delta(F) = 2$, and thus $\varepsilon(F) = \eta(\overline{\Gamma}) - 1$.

Claim A. *If $d_{\overline{\Gamma}}(w_1) \geq 4$, then $q(\Gamma^*) \geq 3$.*

Proof of Claim A. We first suppose that $q(\Gamma^*) = 1$. By Lemma 9.1, w_1 is the unique vertex with degree at least 3. If $\Delta \geq 5$, then $\varepsilon(F) \geq 5$ by (3). From Lemma 6.6 we have that $U^3_{1,1} \cup 2P_3 \cup P_2$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.8(iii). Thus, $\Delta = 4$ and $\varepsilon(F) = 2$ by (3). Combining $\Delta = 4$ and $d \leq 4$ taking into account Lemma 9.2 and (18), we conclude that Γ^* is an induced subgraph of $U^3_{4,4}$. If k is odd, then $-1.62 < \lambda_{10}(U^3_{4,4}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{7}\right) < -1.80$ by Corollary 3.6 and Lemma 6.7, a contradiction. If k is even, since $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \geq \lambda_9(U^3_{4,4}) > -1.34 > -2\cos\left(\frac{\pi}{4}\right) \geq -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$ by virtue of Corollary 3.6, we have $s \geq \frac{k}{2} - 1$ by Lemma 6.8. Since $U^3_{1,1} \cup P_4 \cup P_2$ is forbidden (by Lemma 4.8(iii)), we have $\frac{k}{2} - 1 \leq s \leq 3$, and thus $k = 8$. This implies that $\Gamma^* \cup F = U^3_{1,1} \cup P_2 \cup P_3$, which contradicts Lemma 6.3.

Suppose now that $q(\Gamma^*) = 2$, and let $d_{\Gamma^*}(u) \geq 3$ and $u \neq w_1$. By Lemma 9.1, $d_{\Gamma^*}(u) = 3$ and we have that either $u = w_2$ or $d_{\Gamma^*}(w_2) = 2$ and Γ^* is obtained from $U^3_{s_1,s_2,\ldots,s_{\Delta-2}}$ by attaching an isolated vertex to a 2-vertex of a pendant path of $U^3_{s_1,s_2,\ldots,s_{\Delta-2}}$, as $d \leq 4$ and $Z_{3,2,2}$, H_{13} are forbidden by Lemma 4.3 (i) and (iii). In both cases, from (3) we have

$$\varepsilon(F) = \frac{1}{2}(\Delta - 1)(\Delta - 2).$$

If $\Delta \geq 5$, then $\varepsilon(F) \geq 6$ and thus $U^3_{1,1} \cup P_2 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 6.6, but this contradicts Lemma 4.8(iii). Hence, $\Delta = 4$ and $\varepsilon(F) = 3$.

If $d_{\Gamma^*}(w_2) = 2$, then C_3 is a pendant cycle of Γ^*, and thus $U^3_{1,1} \cup P_2 \cup 2P_3$ is also an induced subgraph of $\overline{\Gamma}$ by Lemma 6.4, but this contradicts Lemma 4.8(iii). Hence, $d_{\Gamma^*}(w_2) = 3$. Since $2P_2 \cup P_3$ is an induced subgraph (by Lemma 6.6) and $U_{3;1,1} \cup 2P_2 \cup 2P_3$, $U^3_{1,1} \cup P_2 \cup 2P_3$ are forbidden by (Lemma 4.8(iii)), we conclude that Γ^* is an induced subgraph of L_{13}, (as $d \leq 4$ by Lemma 9.2, $\Delta = 4$ and $q(\Gamma^*) = 2$). It is easily checked that $k = |E(\Gamma^*)| + |E(F)| \geq 10$.

If k is odd, then $-1.71 < \lambda_{11}(L_{13}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{11}\right) \leq -1.91$ by Corollary 3.6 and Lemma 6.7, a contradiction (as $\Delta(F) = 2$).

If k is even, since $\lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{5}\right) < -1.61 < -1.42 < \lambda_{10}(L_{13}) \leq \lambda_{|V(\Gamma^*)|-2}(\Gamma^*)$ (by Corollary 3.6), we have $s \geq \frac{k}{2} - 1 \geq 4$ by Lemma 6.8 with $\Delta(F) = 2$. However, $U^3_{1,1} \cup P_4 \cup P_2$ is forbidden by Lemma 4.8(iii), a contradiction. This completes the proof of Claim A.

Since $U^3_{1,1} \cup P_2 \cup P_4$, $U^3_{1,1} \cup P_2 \cup 2P_3$ are forbidden (by Lemma 4.8(iii)), $\varepsilon(F) \geq q(\Gamma^*) \geq 3$ (by Claim A and (18)), by taking into account Lemma 6.6, we conclude that $F = 2P_2 \cup P_3$. Hence, $\varepsilon(F) = 3$, and thus $d_{\Gamma^*}(w_2) = 3$ by Lemmas 6.4 and 9.1. Combining this with $\Delta \geq 4$ and the fact that $U^3_{1,1,1} \cup 2P_2 \cup P_3$, $U^3_{1,1} \cup P_2 \cup 2P_3$ are forbidden (by Lemma 4.8(iii)), we obtain $\Delta = 4$ and $q(\Gamma^*) = 3$, as $\varepsilon(F) \geq q(\Gamma^*)$ by (18). From Lemma 9.1 we deduce

that Γ^* contains exactly one 4-vertex, two 3-vertices, four 1-vertices and $|V(\Gamma^*)|-7$ 2-vertices. From (3) we have $\varepsilon(F)=4$, contrary to $F=2P_2\cup P_3$. □

Proof of Lemma 9.4. Assume by way of contradiction that $d_{\overline{\Gamma}}(w_2)\geq 3$, i.e., by taking into account Lemma 9.1, that $d_{\overline{\Gamma}}(w_2)=3$. From Lemmas 9.1 and 9.3 we have $\Delta=3$, and thus $\varepsilon(F)=q(\Gamma^*)-1$ by (18). In this case, $U_{3;1,1}$ is an induced subgraph of $\overline{\Gamma}$. Note that $U_{3;1,1}\cup P_5$, $U_{3;1,1}\cup K_{1,3}$ are forbidden by Lemma 4.8(iii), and then

$$\Delta(F)=2 \text{ and } s\leq 4, \text{ where } P_s \text{ is a longest path of } F.$$

Since $U_{3;1,1}\cup 2P_2\cup 2P_3$ is forbidden (by Lemma 4.8(iii)) and $\varepsilon(F)=q(\Gamma^*)-1$, we also have $2\leq q(\Gamma^*)\leq 4$ by Lemma 6.6.

Claim A. $q(\Gamma^*)\neq 2$.

Proof of Claim A. Assume that $q(\Gamma^*)=2$. By Lemma 9.2 and (18), we have $\Gamma^*=U_{3;t,d}$ with $1\leq t\leq d\leq 4$. If k is odd, by Corollary 3.6 and Lemma 6.7 with $\Delta(F)=2$, we have $-1.75<\lambda_{10}(U_{3;4,4})\leq\lambda_{|V(\Gamma^*)|-1}(\Gamma^*)=\lambda_{n-1}(\overline{\Gamma})=-2\cos\left(\frac{\pi}{k}\right)\leq -2\cos\left(\frac{\pi}{7}\right)<-1.80$, a contradiction.

Let k be even. By Lemma 5.3(iii) and Corollary 3.6, we have

$$\lambda_{|V(\Gamma^*)|-2}(\Gamma^*)\geq\lambda_9(U_{3;4,4})>-1.31>-2\cos\left(\frac{\pi}{4}\right)\geq -2\cos\left(\frac{2\pi}{k}\right)=\lambda_{n-2}(\overline{\Gamma}).$$

Hence,

$$\frac{k}{2}-1\leq s\leq 4 \tag{30}$$

by Lemma 6.8 with $\Delta(F)=2$. This implies that $k\in\{8,10\}$ and $F=P_s$, as $\varepsilon(F)=q(\Gamma^*)-1=1$.

If $k=10$, then $s=4$ by (30). Combining this with $10=k=|E(\Gamma^*)|+|E(F)|$, we get $t\leq 2$. If $t=2$, then $\Gamma^*=U_{3;2,2}$. If $t=1$, then $\Gamma^*=U_{3;3,1}$. Combining this with $F=P_4$, we get $\lambda_{n-2}(\overline{\Gamma})\geq\lambda_9(U_{3;2,2}\cup P_4)>-1.51>-2\cos\left(\frac{\pi}{5}\right)$, contrary to Lemma 5.3(iii).

If $k=8$, then $3\leq s\leq 4$ by (30). Combining this with $8=k=|E(\Gamma^*)|+|E(F)|$, we get $t=1$. If $s=3$, then $\Gamma^*=U_{3;2,1}$. If $s=4$, then $\Gamma^*=U_{3;1,1}$. This implies that $\lambda_{n-2}(\overline{\Gamma})\geq\lambda_7(U_{3;2,1}\cup P_3)>-1.38>-2\cos\left(\frac{\pi}{4}\right)$, contrary to Lemma 5.3(iii). This completes the proof of Claim A.

By Claim A, we have $3\leq q(\Gamma^*)\leq 4$, and thus $2\leq\varepsilon(F)\leq 3$ by (18) with $\Delta=3$.

Case 1: $d_{\overline{\Gamma}}(w_3)=2$.

Subcase 1.1: $q(\Gamma^*)=4$. Then also $\varepsilon(F)=3$ by (18). Since $d_{\overline{\Gamma}}(w_3)=2$, we get $|E(\Gamma^*)|\geq 9$, and so $k=|E(\Gamma^*)|+|E(F)|\geq 13$ by Lemma 6.6. Since $q(\Gamma^*)=4$, we may suppose that $U_{3;p,q}(p-1)$ is an induced subgraph of Γ^* such that $1\leq q\leq p\leq 4$ and p the largest possible. Since $U_{3;1,1}\cup 2P_2\cup 2P_3$ is forbidden (by

Lemma 4.8(iii)), we have $2 \le p \le 3$. If $p = 3$, since $Z_{3,2,2}, Z_{2,2,1}(1)$ are forbidden (by Lemma 4.3(i)–(ii)) and $q(\Gamma^*) = 4$, we conclude that Γ^* is an induced subgraph of L_{14} or L_{15} by the choice of p. If $p = 2$, in exactly the same way we conclude that Γ^* is an induced subgraph of L_{16}. If k is odd, by Corollary 3.6 and Lemma 6.7, we have $-1.934 < \lambda_{12}(L_{15}) = \min\{\lambda_{12}(L_{16}), \lambda_{12}(L_{15}), \lambda_{12}(L_{14})\} \le \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \le -2\cos\left(\frac{\pi}{13}\right) < -1.941$, a contradiction. If k is even, since $s \le 4 < \frac{k}{2} - 1$ and $\Delta(F) = 2$, by Lemma 6.8 and Corollary 3.6, we have $-1.39 < \lambda_{11}(L_{15}) = \min\{\lambda_{11}(L_{16}), \lambda_{11}(L_{15}), \lambda_{11}(L_{14})\} \le \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) = \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \le -2\cos\left(\frac{\pi}{7}\right) < -1.80$, a contradiction.

Subcase 1.2: $q(\Gamma^*) = 3$. Then also $\varepsilon(F) = 2$ by (18). In this case, we have $|E(\Gamma^*)| \ge 7$ by $d_{\overline{\Gamma}}(w_3) = 2$, and so $k = |E(\Gamma^*)| + |E(F)| \ge 9$. Further, since $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)), $q(\Gamma^*) = 3$, and $d \le 4$, we can conclude that Γ^* is an induced subgraph of $\{U_{3;4,4}(3), U_{3;4,4}(2), U_{3;4,4}(1)\}$. If k is odd, by Corollary 3.6 and Lemma 6.7 with $\Delta(F) = 2$, we have

$$-1.82 < \lambda_{11}\big(U_{3;4,4}(3)\big) \le \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \le -2\cos\left(\frac{\pi}{9}\right) < -1.87,$$

a contradiction. If k is even, since $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \ge \lambda_{10}(U_{3;4,4}(3)) > -1.45 > -2\cos\left(\frac{\pi}{5}\right) \ge -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$ (by Corollary 3.6 and Lemma 5.3(iii)), we have $\frac{k}{2} - 1 \le s \le 4$ by Lemma 6.8. This implies that $k = 10$ and $s = 4$, but then $|E(F)| \ge 4$, and so $k = |E(\Gamma^*)| + |E(F)| \ge 11$, a contradiction.

Case 2: $d_{\overline{\Gamma}}(w_3) = 3$. Then also $\varepsilon(F) = q(\Gamma^*) - 1 \ge 2$. Since $W_{1,1,1} \cup P_2 \cup P_4$ is forbidden (by Lemma 4.8(v)), we have $s \le 3$.

Subcase 2.1: $q(\Gamma^*) = 4$. Then $\varepsilon(F) = 3$ and Γ^* is obtained by attaching an isolated vertex to a 2-vertex of a pendant path of W_{s_1,s_2,s_3}, as $Z_{3,2,2}$ is forbidden (by Lemma 4.3(i)). We assume that $s_1 \ge s_2 \ge s_3$. In this case, $k = |E(\Gamma^*)| + |E(F)| \ge 12$. Since $W_{4,1,1} \cup 2P_2 \cup P_3$ is forbidden (by Lemma 4.8(v)), we have $s_1 \le 3$ by Lemma 6.6. Combining this with the fact that $U_{3;1,1} \cup 2P_2 \cup 2P_3$ and $Z_{3,2,2}$ are forbidden (by Lemma 4.8 (iii)), we get that Γ^* is an induced subgraph of $W_{3,3,3}(1)$ by Lemma 6.6. If k is odd, then $-1.88 < \lambda_{12}\big(W_{3,3,3}(1)\big) \le \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right) \le -2\cos\left(\frac{\pi}{13}\right) < -1.94$ (by Corollary 3.6 and Lemma 6.7), a contradiction. If k is even, since $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \ge \lambda_{11}(W_{3,3,3}(1)) > -1.56 > -2\cos\left(\frac{\pi}{6}\right) \ge -2\cos\left(\frac{2\pi}{k}\right) = \lambda_{n-2}(\overline{\Gamma})$ (by Corollary 3.6), we have $s \ge \frac{k}{2} - 1 \ge 5$ by Lemma 6.8, a contradiction.

Subcase 2.2: $q(\Gamma^*) = 3$. Then also $\varepsilon(F) = 2$ and $\Gamma^* = W_{s_1,s_2,s_3}$. In this case, $k = |E(\Gamma^*)| + |E(F)| \ge 8$, and Γ^* is an induced subgraph of $W_{4,4,4}$, as $d \le 4$ (by Lemma 9.2 and (18)).

If k is odd, by Lemma 6.7 and Corollary 3.6, we have

$$-1.919 < \lambda_{14}(W_{4,4,4}) \le \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = \lambda_{n-1}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{k}\right),$$

and thus $k \in \{9, 11\}$. If $k = 11$, then $P_2 \notin F$ by Lemma 6.3. Combining this with $s \leq 3$, we get $F = 2P_3$ and $\Gamma^* = W_{2,1,1}$. If $k = 9$, then Γ^* is an induced subgraph of $W_{2,1,1}$, as $\varepsilon(F) \geq 2$. By Corollary 3.6, we have $-1.62 < \lambda_6(W_{2,1,1}) \leq \lambda_{|V(\Gamma^*)|-1}(\Gamma^*) = -2\cos\left(\frac{\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{9}\right) < -1.87$, a contradiction.

For k even, we claim that $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \leq \lambda_{n-2}(\overline{\Gamma})$. If not, then $\frac{k}{2} - 1 \leq s \leq 3$ by Lemma 6.8, which implies that $k = 8$ and $s = 3$. However, since $\varepsilon(F) = 2$, we have $k = |E(\Gamma^*)| + |E(F)| \geq 6 + s = 9$, a contradiction. Thus $\lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \leq \lambda_{n-2}(\overline{\Gamma})$.

If $k \geq 12$, since Γ^* is an induced subgraph of $W_{4,4,4}$, by Corollary 3.6, we have $-1.67 < \lambda_{13}(W_{4,4,4}) \leq \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \leq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{2\pi}{k}\right) \leq -2\cos\left(\frac{\pi}{6}\right) < -1.73$, a contradiction. If $k \in \{8, 10\}$, then $P_2 \notin F$ by Lemma 6.3. Combining this with $s \leq 3$, we get $F = 2P_3$, and thus $\Gamma^* = W_{1,1,1}$ and $k = 10$. Since Γ^* is an induced subgraph of $W_{2,1,1}$, by Corollary 3.6, we further have $-1 < \lambda_5(W_{2,1,1}) \leq \lambda_{|V(\Gamma^*)|-2}(\Gamma^*) \leq \lambda_{n-2}(\overline{\Gamma}) = -2\cos\left(\frac{\pi}{5}\right) < -1.61$, a contradiction. □

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Connected $(K_4 - e)$-free graphs whose second largest eigenvalue does not exceed 1



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ABSTRACT

Connected graphs whose second largest eigenvalue λ_2 does not exceed 1 have been investigated in the last four decades. Over the years only few particular classes with this spectral property are completely determined. For example, they include bipartite graphs, line graphs and threshold graphs. In this paper we determine all connected $(K_4 - e)$-free graphs, i.e., the graphs that do not contain an induced subgraph isomorphic to the graph obtained by removing an edge from the complete graph of order 4; such graphs are also called diamond-free graphs. Since every triangle-free graph is automatically diamond-free, our results includes all triangle-free graphs with $\lambda_2 \leq 1$. Moreover, it includes all connected bipartite graphs with the same spectral property, and therefore strengthens the result of Petrović (J. Combin. Theory B, 1991).

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1. Introduction

In this paper we deal with finite undirected graphs without loops or multiple edges. For such a graph G we denote its vertex set by $V(G)$ and edge set by $E(G)$. The number of vertices $|V(G)|$ is called the *order* of G. The second largest eigenvalue of the adjacency matrix of G is denoted by λ_2. We say that G is *H-free* if it does not contain the graph H as an induced subgraph.

The problem of characterizing graphs whose second largest eigenvalue does not exceed a comparatively small real constant has attracted a notable attention in the past [20]. According to our knowledge, the first paper that concerns graphs with $\lambda_2 \leq 1$ was Cvetković's [6] published

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in 1982. By the same reference, the problem of characterizing such graphs was posed by Hoffman somewhat earlier. In [6] one can find a partial characterization by means of complementary graphs as well as some particular initial results cited in many forthcoming papers. We mention that all bipartite graphs with $\lambda_2 \leq 1$ are determined by Petrović [13], and all line graphs and generalized line graphs with the same spectral property are determined by Petrović and Milekić [14,15]. These results were pretty elegant and, in contrast to them, a full determination of graphs in question requires intensive technical considerations and a multiple case analysis. More results on this topic can be found in [4,8,11,17–19].

Recently, we have started an ambitious project with the idea to conclude the topic by determining all connected graphs with $\lambda_2 \leq 1$. In the previous work [10], we have determined all connected $\{K_{1,3}, K_5 - e\}$-free graphs with $\lambda_2 \leq 1$, i.e. connected graphs that do not contain an induced subgraph isomorphic to either the star of order 4 or the graph obtained by removing an edge from the complete graph of order 5. This result covers the aforementioned result concerning line graphs, since a graph is a line graph if and only if it does not contain any of $K_{1,3}, K_5 - e$ and the additional seven graphs (not listed here) as an induced subgraph [1,7].

In this paper we determine all connected triangle-free graphs with $\lambda_2 \leq 1$. Concerning connected graphs that contain at least one triangle, we determine all that are diamond-free and have the same spectral property, where a diamond (graph) is the graph $K_4 - e$ obtained by removing an edge of the complete graph of order 4. Since every triangle-free graph is simultaneously diamond-free, in this way we determine all connected diamond-free graphs (with or without triangles) with $\lambda_2 \leq 1$. Since every diamond-free graph is simultaneously $(K_5 - e)$-free, this result adds to that of [10]. After this paper, to conclude the four decades long investigations it remains to determine those which have $\lambda_2 \leq 1$ and contain a diamond as an induced subgraph. We will see in the next section that the result of this paper covers the result concerning bipartite graphs with $\lambda_2 \leq 1$.

We proceed with some related works. It occurs that many diamond-free graphs with $\lambda_2 \leq 1$ are induced subgraphs of a unique strongly regular graph of order 27 and vertex degree 10, in this paper denoted by D_7 and illustrated in the forthcoming Fig. 1. Its spectrum consists of 10, 1 with multiplicity 20 and -5 with multiplicity 6; its complement is known as the *Schläfli graph*. This relates the results of this paper to [17] where Stanić has investigated graphs which contain particular induced subgraphs and have $\lambda_2 = 1$, and [4] where Cheng, Greaves and Koolen have identified all graphs which have exactly three distinct eigenvalues along with $\lambda_2 \leq 1$. In both references, D_7 plays a significant role. Another graph that frequently appears in this paper is the so-called friendship graph, defined in Section 2. This graph plays a crucial role in [5] where Cioabă et al. have determined all connected graphs with all but two eigenvalues equal to ± 1; it occurs that second largest eigenvalue of these graphs is necessarily equal to 1. Our particular result concerning triangle-free graphs with $\lambda_2 \leq 1$ is related to many results concerning triangle-free graphs in various contexts, see for example [2,9,12,16] and the references therein. For example, we know from the work of Lin, Ning and Wu [9] that the sum of squares of two largest eigenvalues of a connected triangle-free graph does not exceed the number of edges, which gives an upper bound for the largest eigenvalue of triangle-free graphs considered in this paper.

The remaining sections are organized in the following way. Our results are formulated in Section 2. Section 3 contains additional terminology, notation, definitions of several classes of graphs and a particular convention related to figures depicted in the paper. The proofs are given in Section 4 (where we consider triangle-free graphs) and Section 5 (where we deal with diamond-free graphs that contain at least one triangle). Section 5 contains a difficult discussion with several long and technical proofs. To make the reading easier, we separate some of them in the Appendix of the paper.

2. Results

To formulate our results we need to introduce some graphs.

We write $K_{s,t}$ for the complete bipartite graph with s vertices in one colour class and t vertices in the other, and K_r^s for the graph obtained by attaching r pendant vertices at a fixed vertex of the complete graph K_s.

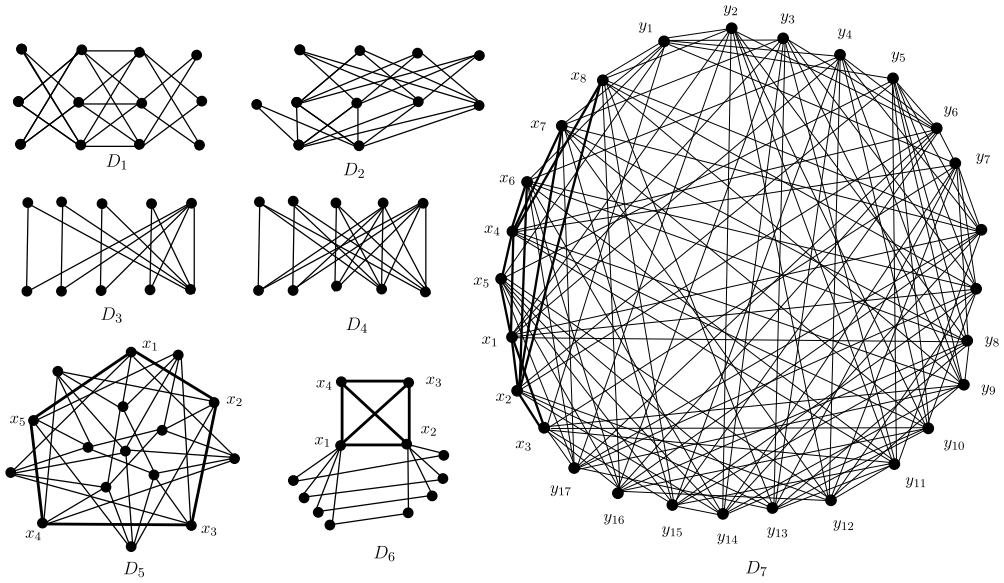


Fig. 1. The graphs $D_1, D_2, \ldots, D_7$.

Let $\mathcal{F}_1$ be the class of bipartite graphs obtained from $K_{2s,2s}$ ($s \geq 1$) in the following way. We first delete s independent edges, i.e. the edges that does not share a common vertex. (Observe that this operation results in a graph with exactly $2s$ vertices of degree $2s$.) Then we attach a pendant vertex at each vertex of degree $2s$.

Let $\mathcal{F}_2$ be the class of bipartite graphs obtained from $K_{s+3,3}$ ($s \geq 1$) in the following way. We first delete three independent edges, which results in a graph with exactly s vertices, say $u_1, u_2, \ldots, u_s$, of degree three. In the next step, we attach a pendant vertex at each of $u_1, u_2, \ldots, u_s$, and then insert a single vertex and join it to each of $u_1, u_2, \ldots, u_s$.

Let $\mathcal{F}_3$ be the class of bipartite graphs obtained from $K_{3,s}$ ($s \geq 1$) in the following way. We attach a pendant vertex at each vertex of $K_{3,s}$ and we add a new vertex and join it to each vertex of the second colour class of $K_{3,s}$ (the one with s vertices) and to all pendant vertices attached at vertices of the first colour class.

Let $D_1, D_2, \ldots, D_7$ be the graphs illustrated in Fig. 1. Let $W_1, W_2, \ldots, W_{14}$ be the graphs illustrated in Fig. 2.

Let $\mathcal{F}_4$ be the class of graphs obtained from W_1 by inserting s independent edges (say, $u_1v_1, u_2v_2, \ldots, u_sv_s$) and adding s edges between w_i and $u_1, u_2, \ldots, u_s$, for $1 \leq i \leq 4$.

Let $\mathcal{F}_5$ be the class of graphs obtained from $K_{s,s}$ by taking a set of s independent edges and inserting a vertex into each of them. In other words, we subdivide each of the mentioned edges. Let $\mathcal{F}_6$ be the class of graphs obtained from K_s ($s \geq 2$) by attaching two pendant vertices at each vertex of K_s.

A *friendship graph* F_s is the graph consisting of s triangles sharing exactly one vertex. Let $\mathcal{F}_7$ be the class of graphs obtained from F_s by inserting s independent edges (say, $u_1v_1, u_2v_2, \ldots, u_sv_s$) and adding s edges $uu_1, uu_2, \ldots, uu_s$, where u is the unique vertex of degree $2s$ in F_s.

Our main results read as follows. The first one treats connected triangle-free graphs.

Theorem 2.1. *The second largest eigenvalue of a connected triangle-free graph G does not exceed* 1 *if and only if G is an induced subgraph of some graph belonging to*

$$\left(\bigcup_{i=1}^{5} \mathcal{F}_i\right) \cup \{D_5, D_7\}.$$

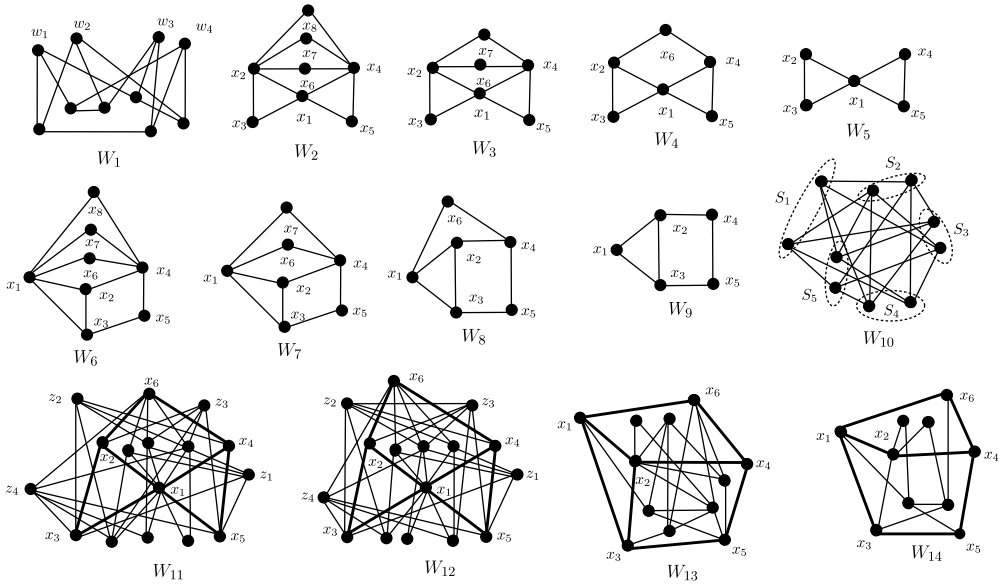


Fig. 2. The graphs $W_1, W_2, \ldots, W_{14}$.

Next, we deal with connected diamond-free graphs that are not triangle-free.

Theorem 2.2. *The second largest eigenvalue of a connected diamond-free graph G that contains at least one triangle does not exceed* 1 *if and only if G is an induced subgraph of some graph belonging to* $\mathcal{F}_6 \cup \mathcal{F}_7 \cup \{D_6, D_7, K_3^5\}$.

Since every triangle-free graph is also diamond-free, by combining the previous two theorems, we obtain the following result.

Theorem 2.3. *The second largest eigenvalue of a connected diamond-free graph G does not exceed* 1 *if and only if G is an induced subgraph of some graph belonging to*

$$\left(\bigcup_{i=1}^{7} \mathcal{F}_i\right) \cup \{D_5, D_6, D_7, K_3^5\}.$$

Therefore, it remains to prove Theorems 2.1 and 2.2. This is performed in the following sections. The following result obtained by Petrović determines all connected bipartite graphs with $\lambda_2 \leq 1$ and allows us to reduce our considerations to the non-bipartite case.

Proposition 2.4 (*[13]*)**.** *The second largest eigenvalue of a connected bipartite graph G does not exceed* 1 *if and only if G is an induced subgraph of some graph belonging to*

$$\left(\bigcup_{i=1}^{3} \mathcal{F}_i\right) \cup \{D_1, D_2, D_3, D_4\}.$$

It is not difficult to see that D_1 is a subgraph of D_7 induced by the vertices x_1, x_2, x_4, x_6–$x_8, y_1, y_5, y_7, y_{15}$–$y_{17}$ (observe Fig. 1). We express these facts by writing $D_1 \subset D_7$ and $D_1 \cong D_7\big[x_1, x_2, x_4, x_6$–$x_8, y_1, y_5, y_7, y_{15}$–$y_{17}\big]$. Similarly, $D_2 \cong D_7\big[x_1, x_2, x_4, x_6$–$x_8, y_1, y_5, y_7, y_8, y_{17}\big]$, $D_3 \cong D_7\big[x_1, x_2, x_4, x_6, y_1, y_5, y_{12}, y_{13}, y_{16}, y_{17}\big]$ and $D_4 \cong D_7\big[x_1, x_2, x_4, x_6$–$x_8, y_1, y_6, y_8, y_{17}\big]$. These observations allow us to exclude D_1, D_2, D_3 and D_4 in the formulations of Theorems 2.1–2.3.

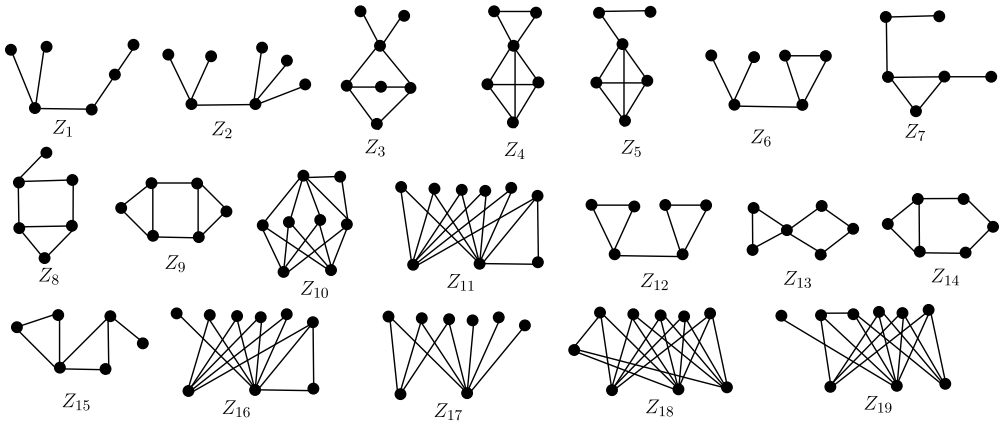


Fig. 3. The graphs $Z_1, Z_2, \ldots, Z_{19}$.

3. Preliminaries

Following [3,7,20], for the graphs G and H, we write $G \cup H$ to denote their disjoint union. For a positive integer k, kG denotes a disjoint union of k copies of G. For $u \in V(G), S \subseteq V(G)$, we write $N_S(u)$ for the set of neighbours of u located in S. We also write $d_S(u)$ for $|N_S(u)|$ (the degree of u in S). We use the same notation when S is an induced subgraph of G. We write $G - S$ (in particular, $G-u$) to denote the graph obtained by removing all vertices of S (in particular, the vertex u) from G.

Note that $\lambda_2 \leq 1$ is a hereditary property in the sense that if it holds for G then it holds for every induced subgraph of G. We say that H is *forbidden* for $\lambda_2 \leq 1$ if H is not an induced subgraph of any graph with second largest eigenvalue being at most 1.

We proceed with more graphs. Let $U^s_{s_1,s_2,\ldots,s_t}$ be a graph obtained from a cycle C_s by attaching t paths $P_{s_1}, P_{s_2}, \ldots, P_{s_t}$ at a fixed vertex of C_s. (Hereafter, when we say that a path is attached at a vertex, we mean that an additional edge is inserted between an endvertex of the path and the vertex in question; this approach does not deviate from the previous one related to attaching of pendant vertices.)

Let $K^s_{s_1;s_2;\ldots;s_r}$ be the graph obtained from a complete graph K_s with vertex set $\{v_1, v_2, \ldots, v_r\}$ by attaching s_i pendant vertices at the vertex v_i, for $1 \leq i \leq r$. This definition covers the particular case concerning the graph K^s_r defined in the previous section.

Let $Z_1, Z_2, \ldots, Z_{19}$ be the graphs illustrated in Fig. 3 and $H_1, H_2, \ldots, H_{13}$ the graphs illustrated in Fig. 4.

Now we give some lemmas. The first one follows by a direct computation.

Lemma 3.1. *If* $G \in \{P_6, U^4_2, U^3_3, U^4_{1,1,1,1}, K^5_4, K^6_3, K^5_{3;1}, K^4_{3;1;1}, K^4_{4;1}, K^3_{4;1;1}, K^4_5, K^3_{3;2}, K^3_{5;1}, 2P_3, Z_1, Z_2, \ldots, Z_{19}\}$, *then* $\lambda_2(G) > 1$.

We recall from the previous section that the definition of every class $\mathcal{F}_i$ $(4 \leq i \leq 7)$ depends on the parameter s.

Lemma 3.2. *For $s \geq 2$, if G is an induced subgraph of a graph of $\mathcal{F}_4 \cup \mathcal{F}_5 \cup \mathcal{F}_6 \cup \mathcal{F}_7$, then $\lambda_2(G) \leq 1$.*

Proof. If $G \in \mathcal{F}_4$, then its spectrum consists of three copies of -2, $s-1$ copies of -1, $s+5$ copies of 1 and the roots of $f_1(x) = x^3 - (4s+7)x - 6$. Since $f_1(-\infty) < 0, f_1(-1) = 4s > 0, f_1(1) = -4(s+3) < 0$, and $f_1(+\infty) > 0$, we have $\lambda_2(G) = 1$.

If $G \in \mathcal{F}_5$, then its spectrum consists of $2(s-1)$ copies of 1, $s-1$ copies of -2, the number $1-s$, and the roots of $x^2 - (s-1)x - 2$. This implies that each graph of $\mathcal{F}_5$ has second largest eigenvalue equal to 1.

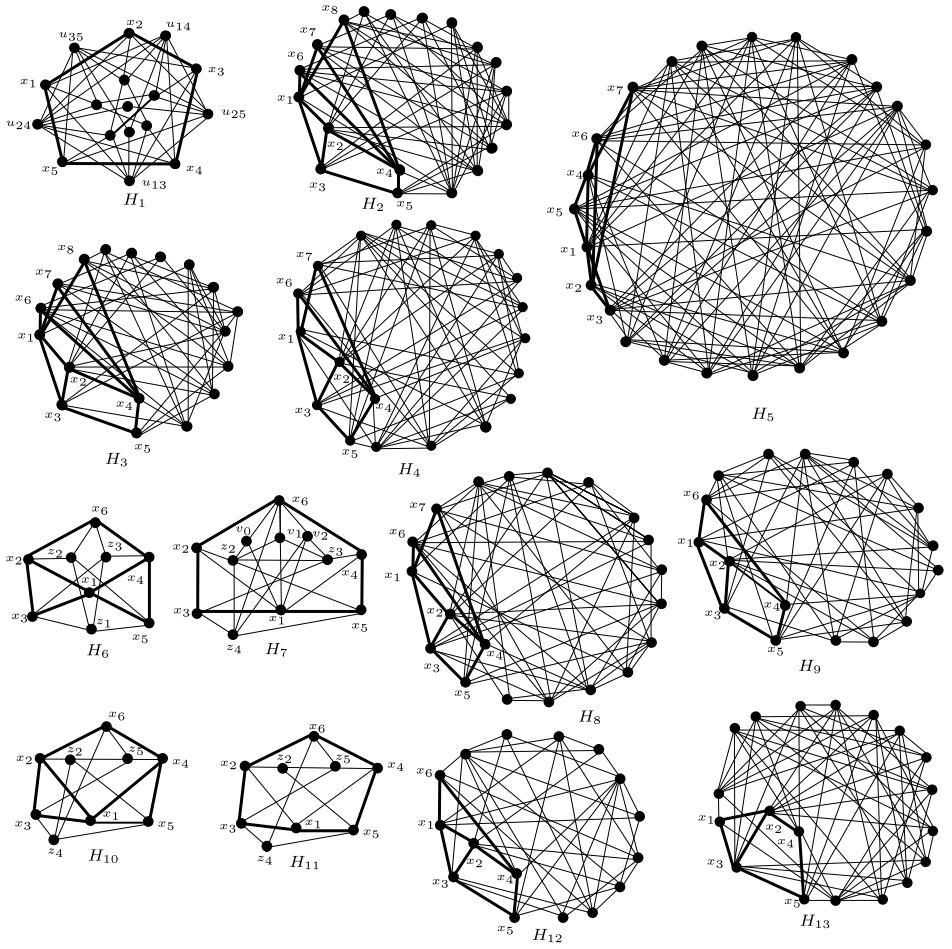


Fig. 4. The graphs $H_1, H_2, \ldots, H_{13}$.

The spectrum of a graph of $\mathcal{F}_6$ consists of $s-1$ copies of -2, $s-1$ copies of 1, s copies of 0, and the roots of $x^2-(s-1)x-2$. Thus, $\lambda_2(G)=1$.

Finally, the spectrum of a graph of $\mathcal{F}_7$ consists of $2s-1$ copies of 1, $2s-1$ copies of -1 and the roots of $f_2(x)=x^3-(3s+1)x-2s$, see [5]. Since $f_2(-\infty)<0$, $f_2(-1)=s>0$, $f_2(1)=-5s<0$ and $f(+\infty)>0$, we have $\lambda_2(G)=1$. ■

The following setting is frequently used in the forthcoming sections. Let H be an induced subgraph of G, $T=V(G)\setminus V(H)$ and $S\subseteq V(H)$. Then $T_S=\{x: x\in T \text{ with } N(x)\cap H=S\}$, and T_i denotes the set of vertices of T which are adjacent to exactly i vertices of H. From the previous definitions, we have $T_1=\bigcup_{x\in V(H)} T_x$. Similarly, T_0 consists of the vertices non-adjacent to any vertex of H. In this context, H is referred to as a *base graph* of G.

We conclude this section with a convention related to the figures. First, in what follows we always use vertex labellings given in the corresponding figure. For example, some vertices of D_5 are labelled in Fig. 1 and, say, x_1 always refers to the vertex specified in this figure. Secondly, we will deal with particular base graphs. To make the reading easier, we use bold lines to specify the edges of such graphs. For instance, the base graph of D_5 (see again Fig. 1) is the cycle C_5 with the vertex set $\{x_1, x_2, \ldots, x_5\}$.

4. Proof of Theorem 2.1

Throughout this and the next section we use the notation of Theorems 2.1–2.3, and so we denote by G a graph under consideration. In this section G is triangle-free and non-bipartite. Since every non-bipartite graph contains at least one odd cycle, we may say that C_g is a shortest odd cycle of G. Since $P_6 \not\subset G$ (otherwise, $\lambda_2(G) \geq \lambda_2(P_6) > 1$), we have $g = 5$. In this section, we use C_5 as the base graph, denote its vertex set by $\{x_1, x_2, \ldots, x_5\}$ and assume that the vertices are labelled in the natural order. Since C_3 is forbidden for G, every vertex of $T = V(G) \setminus V(C_5)$ is adjacent to at most two vertices of C_5, and thus $T = T_0 \cup T_1 \cup T_2$.

We proceed with a sequence of claims. Since G is triangle-free, the first one is a direct consequence of the fact that $Z_1 \not\subset G$ (mentioned in Lemma 3.1).

Claim 4.1. *For distinct i, j, k, s, it holds that T_{x_i} and $T_{\{x_i,x_j\}}$ are independent sets of G. Every vertex of $T_{\{x_i,x_j\}}$ is adjacent to at least $|T_{\{x_s,x_k\}}| - 1$ vertices of $T_{\{x_s,x_k\}}$. Moreover, if $|T_{\{x_i,x_j\}}| \geq 1$, then $x_ix_j \notin E(G)$.*

Claim 4.2. *Every vertex of T_2 is adjacent to at most one vertex of T_0, the neighbours of every vertex of T_0 belong to T_2 and T_0 is an independent set of G.*

Proof. Since $Z_1 \not\subset G$, a vertex of T_2 is adjacent to at most one vertex of T_0. Since $P_6 \not\subset G$, every vertex of T_0 has no neighbours in T_1. Suppose that $|T_0| \geq 1$. If T_0 contains a vertex u such that u is not adjacent to any vertex of T_2, then u must be adjacent to a vertex of T_0, which implies that $P_6 \subset G$, and we have established a contradiction. Thus, every vertex of T_0 has a neighbour in T_2.

Next, assume that there exist vertices u, v of T_0 such that $uv \in E(G)$. Suppose that $uu_1 \in E(G)$ and $vv_1 \in E(G)$ with $u_1 \in T_{\{x_i,x_j\}}$ and $v_1 \in T_{\{x_s,x_k\}}$. Since each vertex of T_2 is adjacent to at most one vertex of T_0, we have $u_1 \neq v_1$, $uv_1 \notin E(G)$ and $vu_1 \notin E(G)$. Since $0 \leq |\{i, j\} \cap \{s, k\}| \leq 2$, we obtain $P_6 \subset G$, which is impossible. Hence, T_0 is an independent set of G. ■

Claim 4.3. *Let i, j, k be distinct integers of $\{1, 2, \ldots, 5\}$ such that $T_{\{x_i,x_j\}} \neq \emptyset$, with $x_ix_k \in E(G)$ and $x_jx_k \in E(G)$. If $u \in T_{x_s}$, then $N_{T_{\{x_i,x_j\}}}(u) = \emptyset$ for $s \in \{i, j, k\}$ and $N_{T_{\{x_i,x_j\}}}(u) = T_{\{x_i,x_j\}}$ for $s \notin \{i, j, k\}$.*

Proof. Since $U_2^4 \not\subset G$, we have $N_{T_{\{x_i,x_j\}}}(u) = \emptyset$ for $s \in \{i, j, k\}$, and $N_{T_{\{x_i,x_j\}}}(u) = T_{\{x_i,x_j\}}$ for $s \notin \{i, j, k\}$. ■

Since $Z_1, U_2^4 \not\subset G$, we immediately arrive at the following one.

Claim 4.4. *For distinct i, j with $u \in T_{x_i}$ and $v \in T_{x_j}$, we have $uv \notin E(G)$ for $x_ix_j \in E(G)$, and $uv \in E(G)$ for $x_ix_j \notin E(G)$. Moreover, $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$.*

Claim 4.5. *Let $u \in T_{\{x_i,x_j\}}$ and $v \in T_{\{x_s,x_k\}}$. If $|\{x_i, x_j\} \cap \{x_s, x_k\}| \leq 1$ and $w \in N_{T_0}(u) \setminus N_{T_0}(v)$, then $uv \in E(G)$.*

Proof. Under the assumption that $uv \notin E(G)$, we have $Z_1 \subset G$ because $|\{x_i, x_j\} \cap \{x_s, x_k\}| \leq 1$. ■

Claim 4.6. *Let $u_1 \in T_{\{x_i,x_j\}}$, $u_2 \in T_{\{x_s,x_k\}}$ and $u_3 \in T_{\{x_s,x_t\}}$. If i, j, k, s, t are distinct and $X = \{u_1, u_2, u_3\}$, then either $G[X] \cong 3K_1$ or $G[X] \cong P_3$ with u_1 being the vertex of degree 2 in P_3.*

Proof. Since G is triangle-free, $u_2u_3 \notin E(G)$. Combining this with $Z_1 \not\subset G$, we obtain either $G[\{u_1, u_2, u_3\}] \cong 3K_1$ or $G[\{u_1, u_2, u_3\}] \cong P_3$ with u_1 in the required role. ■

In what follows, since G is triangle-free, we always suppose that $|T_{\{x_1,x_3\}}| = \max\{|T_{\{x_i,x_j\}}|\}$.

In the remainder of this section we prove a sequence of claims and lemmas. We distinguish two cases depending on $|T_{\{x_1,x_3\}}|$. They are separated into subsections.

4.1. Case: $|T_{\{x_1,x_3\}}| \geq 2$

Since $|T_{\{x_1,x_3\}}| \geq 2$, the following claim implies that under the assumption that $T_{\{x_i,x_j\}} \neq \emptyset$, we have $\{i,j\} \in \big\{\{1,3\},\{2,4\},\{2,5\}\big\}$.

Claim 4.7. *If* $|T_{\{x_i,x_j\}}| \geq 2$, *then* $|T_{\{x_i,x_k\}}| = 0$ *holds for* $k \neq j$.

Proof. Without loss of generality, let $\{i,j\} = \{1,3\}$ and assume that $|T_{\{x_1,x_k\}}| \geq 1$ for $k \neq 3$. Then, $k = 4$ (since G is triangle-free). In this case, $T_{\{x_1,x_4\}} \cup T_{\{x_1,x_3\}}$ is an independent set of G and thus $Z_2 \subset G$, which is contrary to Lemma 3.1. ■

Since $U_2^4 \not\subset G$, we have the following consequence:

$$\text{If } u \in T_0, \text{ then } |N_G(u) \cap T_{\{x_i,x_j\}}| \leq 1 \text{ for } \{i,j\} \in \{\{1,3\},\{2,4\},\{2,5\}\}. \tag{4.1}$$

Claim 4.8. *If* $|T_{\{x_2,x_i\}}| \geq 1$, *then* $T_{x_j} = \emptyset$, *where* $\{i,j\} = \{4,5\}$.

Proof. By symmetry, assume that $u \in T_{x_5}$ and $|T_{\{x_2,x_4\}}| \geq 1$. From Claim 4.3, we have $N_{T_{\{x_1,x_3\}}}(u) = T_{\{x_1,x_3\}}$ and $N_{T_{\{x_2,x_4\}}}(u) = T_{\{x_2,x_4\}}$. Suppose that $v \in T_{\{x_2,x_4\}}$. By Claim 4.1, $|N_{T_{\{x_1,x_3\}}}(v)| \geq |T_{\{x_1,x_3\}}| - 1 \geq 1$, and thus $C_3 \subset G$, which is a contradiction. ■

Lemma 4.9. *If* $d_G(u_0) \geq 3$ *and* $u_0 \in T_0$, *then* G *is an induced subgraph of some graph of* $\mathcal{F}_4$.

Proof. By way of contradiction, assume that G is not an induced subgraph of any graph of $\mathcal{F}_4$.

By Claim 4.2, any neighbour of u_0 belongs to T_2. Since $|N_G(u_0) \cap T_{\{x_i,x_j\}}| \leq 1$ for $\{i,j\} \in \{\{1,3\},\{2,4\},\{2,5\}\}$ (by (4.1)), from Claim 4.7 and the assumption that $d_G(u_0) \geq 3$, we conclude that $|N_G(u_0) \cap T_{\{x_i,x_j\}}| = 1$ holds for $\{i,j\} \in \{\{1,3\},\{2,4\},\{2,5\}\}$ along with $d_G(u_0) = 3$. Suppose that $N_G(u_0) \cap T_{\{x_1,x_3\}} = \{u_1\}$, $N_G(u_0) \cap T_{\{x_2,x_4\}} = \{u_2\}$ and $N_G(u_0) \cap T_{\{x_2,x_5\}} = \{u_3\}$. Due to Claim 4.7, we have $T_{\{x_2,x_4\}} = \{u_2\}$ and $T_{\{x_2,x_5\}} = \{u_3\}$. Since G is triangle-free and $N_G(u_0) = \{u_1,u_2,u_3\}$, it follows that u_1, u_2 and u_3 induce an independent set of G. Combining $u_1 \notin N_G(u_2) \cup N_G(u_3)$ with Claim 4.1, we obtain that every vertex of $\{u_2,u_3\}$ is adjacent to all vertices of $T_{\{x_1,x_3\}} \setminus \{u_1\}$. This leads to the conclusion that $G[V(C_5 \cup T_2 \cup \{u_0\})] \cong J_1 \subset \mathcal{F}_4$, where J_1 is the first graph of Fig. 5 in which the vertices $v_1, v_2, \ldots, v_t$ induce $T_{\{x_1,x_3\}} \setminus \{u_1\}$.

The assumption on G formulated in our statement rejects the possibility that $G \cong G[V(C_5 \cup T_2 \cup \{u_0\})]$, and thus $\big(T_0 \setminus \{u_0\}\big) \cup T_1 \neq \emptyset$.

If $T_1 = \emptyset$, then $T_0 \setminus \{u_0\} \neq \emptyset$. By Claim 4.2, every vertex of T_2 is adjacent to at most one vertex of T_0. Combining this with (4.1), we deduce that every vertex $v \in T_0 \setminus \{u_0\}$ is a pendant vertex of G adjacent to some vertex of $T_{x_1x_3} \setminus \{u_1\}$. In other words, v is adjacent to exactly one vertex of $\{v_1, v_2, \ldots, v_t\}$. Therefore, G is obtained from J_1 by attaching some pendant vertices at some of $\{v_1, v_2, \ldots, v_t\}$, which implies that $G \subset J_2 \subset \mathcal{F}_4$, a contradiction. Thus, $T_1 \neq \emptyset$.

By Claim 4.8, we have $|T_{x_4}| = |T_{x_5}| = 0$ and thus $T_1 = T_{x_1} \cup T_{x_2} \cup T_{x_3} \neq \emptyset$. Moreover, by Claim 4.4, we have $\max\{|T_{x_1}|, |T_{x_2}|, |T_{x_3}|\} \leq 1$ and so $1 \leq |T_1| \leq 3$. We will show that $G \subset J_3 \subset \mathcal{F}_4$.

First, if $z \in T_{x_2} \neq \emptyset$, then $N_G(z) \cap \big(T_0 \cup T_2\big) = \emptyset$ by Claims 4.2 and 4.3. From $|T_{x_4}| = |T_{x_5}| = 0$ and Claim 4.4, we obtain $N_G(z) = \{x_2\}$, that is, z is a pendant vertex of G.

Secondly, if $y \in T_{x_1} \neq \emptyset$, then $N_G(y) \cap \{u_1,u_2,u_3\} = \{u_2\}$ by Claim 4.3. Combining this with Claim 4.4, we deduce that $2 \leq d_G(y) \leq 3$, where $d_G(y) = 3$ if and only if the third neighbour of y is the unique vertex of T_{x_3}. Similarly, we also have $2 \leq d_G(w) \leq 3$ for $w \in T_{x_3} \neq \emptyset$, where $d_G(w) = 3$ if and only if the third neighbour of w is the unique vertex of T_{x_1}.

Now, the conclusions on w, y, z lead to $G \subset J_3 \subset \mathcal{F}_4$. This completes the proof. ■

Lemma 4.10. *If there exists* $u_0 \in T_0$ *with* $d_G(u_0) = 2$ *and* $N_G(u_0) \cap T_{\{x_1,x_3\}} = \emptyset$, *then* G *is an induced subgraph of some graph of* $\mathcal{F}_4$.

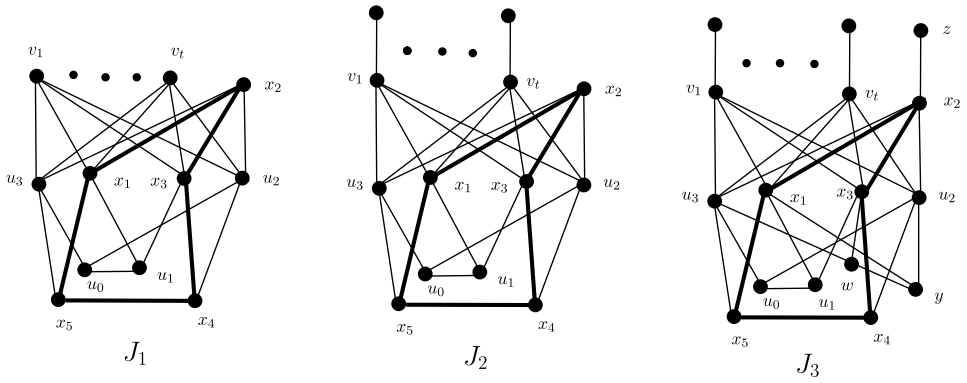


Fig. 5. The graphs J_1, J_2 and J_3 for the proofs of Lemmas 4.9 and 4.10.

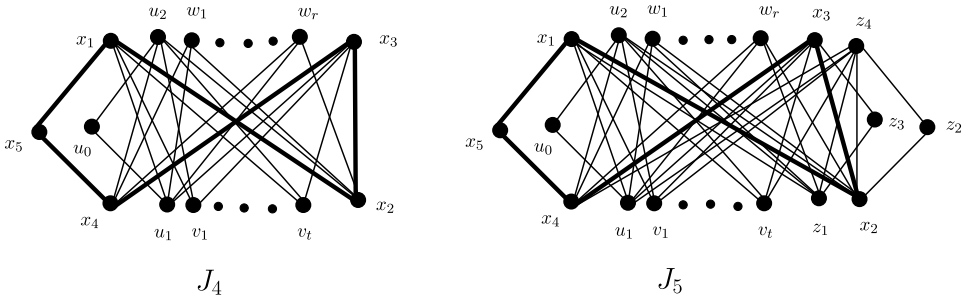


Fig. 6. The graphs J_4, J_5 for the proof of Lemma 4.11.

Proof. By Claim 4.2, every neighbour of u_0 belongs to T_2. Since $|N_G(u_0) \cap T_{\{x_i,x_j\}}| \leq 1$ for $\{i,j\} \in \{\{2,4\},\{2,5\}\}$ (by (4.1)) and $|N_G(u_0) \cap T_{\{x_1,x_3\}}| = 0$, we have $|N_G(u_0) \cap T_{\{x_2,x_4\}}| = 1 = |N_G(u_0) \cap T_{\{x_2,x_5\}}|$. By Claim 4.7, we have $1 = |T_{\{x_2,x_4\}}| = |T_{\{x_2,x_5\}}|$ and thus we may suppose that $T_{\{x_2,x_i\}} = \{u_{i-2}\}$ for $i \in \{4,5\}$. If $v \in \{u_2,u_3\}$, then v must be adjacent to every vertex of $T_{\{x_1,x_3\}}$, provided by $|N_G(u_0) \cap T_{\{x_1,x_3\}}| = 0$ and Claim 4.5. It follows that $G[V(C_5 \cup T_2 \cup \{u_0\})] \cong J_1 - u_1 \subset \mathcal{F}_4$.

The remainder of the proof is similar to that of Lemma 4.9. We again assume that $(T_0 \setminus \{u_0\}) \cup T_1 \neq \emptyset$.

First, if $T_1 = \emptyset$, then $T_0 \setminus \{u_0\} \neq \emptyset$. By Claim 4.2, every vertex of T_2 is adjacent to at most one vertex of T_0. Combining this with (4.1) and $1 = |T_{\{x_2,x_i\}}| = |N_G(u_0) \cap T_{\{x_2,x_i\}}|$ for $4 \leq i \leq 5$, we deduce that every vertex of $T_0 \setminus \{u_0\}$ is a pendant vertex of G adjacent to some vertex of $T_{\{x_1,x_3\}}$. This leads to $G \subset J_2 - u_1 \subset \mathcal{F}_4$. Hence, $T_1 \neq \emptyset$.

We will show that $G \subset J_3 - u_1$ to obtain a contradiction, as $J_3 - u_1 \subset \mathcal{F}_4$. From Claims 4.4 and 4.8, we have $|T_{x_4}| = |T_{x_5}| = 0 \leq \max\{|T_{x_1}|, |T_{x_2}|, |T_{x_3}|\} \leq 1$. Combining this with $T_1 \neq \emptyset$, we arrive at $1 \leq |T_1| \leq 3$.

For $z \in T_{x_2} \neq \emptyset$, we obtain $N_G(z) \cap \big(T_0 \cup T_2\big) = \emptyset$ and $N_G(z) = \{x_2\}$ by Claims 4.2–4.4. From Claims 4.3 and 4.4, if $y \in T_{x_1}$, then $N_G(y) \cap \{u_2,u_3\} = \{u_2\}$ and $N_{T_{\{x_1,x_3\}}}(y) = \emptyset$, and thus $2 \leq d_G(y) \leq 3$, where $d_G(y) = 3$ if and only if the third neighbour of y is the unique vertex of T_{x_3}. Similarly, $2 \leq d_G(w) \leq 3$ for $w \in T_{x_3}$, where $d_G(w) = 3$ if and only if the third neighbour of w is the unique vertex of T_{x_1}.

As before, the conclusions on w, y, z lead to the desired result. ■

Lemma 4.11. *Let T_0 contain a vertex u_0 with $d_G(u_0) = 2$. If $N_G(u) \cap T_{\{x_1,x_3\}} \neq \emptyset$ holds for every vertex u of T_0 with $d_G(u) = 2$, then G is an induced subgraph of some graph of $\mathcal{F}_5$.*

Proof. From (4.1), we have $|N_G(u_0) \cap T_{\{x_i,x_j\}}| \leq 1$ for $\{i,j\} \in \{\{1,3\},\{2,4\},\{2,5\}\}$. Combining this with $d_G(u_0) = 2$, we arrive at $|N_G(u_0) \cap T_{\{x_1,x_3\}}| = |N_G(u_0) \cap T_{\{x_2,x_4\}}| = 1$. Let $N_G(u_0) \cap T_{\{x_1,x_3\}} = \{u_1\}$ and $N_G(u_0) \cap T_{\{x_2,x_4\}} = \{u_2\}$. Since $C_3 \not\subset G$, we have $u_1u_2 \notin E(G)$. Combining this with Claim 4.1, we obtain $N_{T_{\{x_1,x_3\}}}(u_2) = T_{\{x_1,x_3\}} \setminus \{u_1\}$ and $N_{T_{\{x_2,x_4\}}}(u_1) = T_{\{x_2,x_4\}} \setminus \{u_2\}$.

We claim that $|T_{\{x_2,x_5\}}| = 0$. Indeed, if $|T_{\{x_2,x_5\}}| \geq 1$, then we first have $|T_{\{x_2,x_4\}}| = |T_{\{x_2,x_5\}}| = 1$ by Claim 4.7, so let $T_{\{x_2,x_5\}} = \{u_3\}$. Since $u_0u_3 \notin E(G)$, we have $u_2u_3 \in E(G)$ by Claim 4.5, but this implies that $C_3 \subset G$, which is a contradiction.

Now, $|T_{\{x_2,x_5\}}| = 0$ implies that J_4 of Fig. 6 is an induced subgraph of G, where the vertices $v_1, v_2, \ldots, v_s$ induce $T_{\{x_1,x_3\}} \setminus \{u_1\}$ and the vertices $w_1, w_2, \ldots, w_r$ induce $T_{\{x_2,x_4\}} \setminus \{u_2\}$. By Claim 4.1, a vertex $w \in \{w_1, w_2, \ldots, w_r\}$ is adjacent to either $t-1$ or t vertices of $\{v_1, v_2, \ldots, v_t\}$, a vertex $v \in \{v_1, v_2, \ldots, v_t\}$ is adjacent to either $r-1$ or r vertices of $\{w_1, w_2, \ldots, w_r\}$. This implies that $G[V(C_5) \cup \{u_0\} \cup T_2] \subset \mathcal{F}_5$.

As in the previous proofs, we now assume that $(T_0 \setminus \{u_0\}) \cup T_1 \neq \emptyset$. If $T_1 = \emptyset$, then $T_0 \setminus \{u_0\} \neq \emptyset$. Let y be a vertex of $T_0 \setminus \{u_0\}$. From Claim 4.2 and (4.1), either $N_G(y) = \{u_3, u_4\}$ or $N_G(y) = \{u_5\}$ such that $u_3 \in \{v_1, v_2, \ldots, v_t\}$, $u_4 \in \{w_1, w_2, \ldots, w_r\}$ and $u_5 \in \{w_1, w_2, \ldots, w_r, v_1, v_2, \ldots, v_t\} \setminus \{u_3, u_4\}$. In the former case we have $u_3u_4 \notin E(G)$ (as $C_3 \not\subset G$), and thus u_3 is adjacent to every vertex of $\{w_1, w_2, \ldots, w_r\} \setminus \{u_4\}$ and u_4 is adjacent to every vertex of $\{v_1, v_2, \ldots, v_t\} \setminus \{u_3\}$ by Claim 4.1. In the latter case u_5 must be adjacent to every vertex of $\{w_1, w_2, \ldots, w_r\}$ if $u_5 \in T_{x_1x_3}$, and u_5 must be adjacent to every vertex of $\{v_1, v_2, \ldots, v_t\}$ if $u_5 \in T_{\{x_2,x_4\}}$, both by Claim 4.5. These conclusions lead to the desired result that G is an induced subgraph of some graph of $\mathcal{F}_5$.

It remains to consider the case in which $T_1 \neq \emptyset$. Under the latter assumption, from Claims 4.4 and 4.8, we have $|T_{x_5}| = 0 \leq \max\{|T_{x_i}| : 1 \leq i \leq 4\} \leq 1$, and thus $1 \leq |T_1| \leq 4$. Next, suppose that $z_i \in T_{x_i}$ for $1 \leq i \leq 4$. By virtue of Claims 4.2 and 4.3, we deduce that $N_G(z_1) \cap \left(T_{\{x_1,x_3\}} \cup T_0\right) = \emptyset$, $N_G(z_1) \cap T_{\{x_2,x_4\}} = T_{\{x_2,x_4\}}$, $N_G(z_i) \cap \left(T_{\{x_1,x_3\}} \cup T_{\{x_2,x_4\}} \cup T_0\right) = \emptyset$ for $i \in \{2,3\}$, $N_G(z_4) \cap \left(T_{\{x_2,x_4\}} \cup T_0\right) = \emptyset$ and $N_G(z_4) \cap T_{\{x_1,x_3\}} = T_{\{x_1,x_3\}}$. Further, by Claim 4.4, we have $N_G(z_2) \cap \{z_1, z_3\} = \emptyset$, $z_2z_4 \in E(G)$, $z_4z_1 \in E(G)$, $z_3z_4 \notin E(G)$ and $z_1z_3 \in E(G)$. Altogether, the adjacency relations of T_1 are as in J_5. Now, following the case $T_1 = \emptyset, T_0 \setminus \{u_0\} \neq \emptyset$ and using Claims 4.1 and 4.5, we arrive at the conclusion that G is an induced subgraph of $\mathcal{F}_5$. ■

Lemma 4.12. *If $\min\{|T_{\{x_2,x_4\}}|, |T_{\{x_2,x_5\}}|\} \geq 1$ and $d_G(u) = 1$ holds for every vertex $u \in T_0$, then G is an induced subgraph of some graph of $\mathcal{F}_4$.*

Proof. From Claim 4.7, we have $|T_{\{x_2,x_4\}}| = |T_{\{x_2,x_5\}}| = 1$, and thus $T_{x_4} = T_{x_5} = \emptyset$ by Claim 4.8.

Suppose that $T_{\{x_2,x_i\}} = \{u_{i-3}\}$ for $i \in \{4,5\}$. By virtue of Claim 4.5, if $u \in T_0$ and $uu_0 \in E(G)$, then $u_0 \in T_{\{x_1,x_3\}}$ and $u_0u_{i-3} \in E(G)$ for $i \in \{4,5\}$. Since $|T_{\{x_1,x_3\}}| - 1 \leq |N_{T_{\{x_1,x_3\}}}(u_{i-3})| \leq |T_{\{x_1,x_3\}}|$ (by Claim 4.1), by employing Claim 4.6 we conclude that, apart from at most one vertex say u_3 of $T_{\{x_1,x_3\}}$, every vertex of $T_{\{x_1,x_3\}} \setminus \{u_3\}$ is adjacent to both $\{u_1, u_2\}$ (and u_3 is not adjacent to any vertex of $\{u_1, u_2\}$). Since $\max\{|T_{x_1}|, |T_{x_2}|, |T_{x_3}|\} \leq 1$, the last conclusion together with Claims 4.3–4.5, leads to the desired result. ■

Lemma 4.13. *If $\min\{|T_{\{x_2,x_4\}}|, |T_{\{x_2,x_5\}}|\} = 0$ and $d_G(u) = 1$ holds for every vertex $u \in T_0$, then G is an induced subgraph of some graph of $\mathcal{F}_4 \cup \mathcal{F}_5$.*

Proof. If $|T_{\{x_2,x_4\}}| = |T_{\{x_2,x_5\}}| = 0$, then G is an induced subgraph of some graph of $\mathcal{F}_4$ by Claims 4.3 and 4.4, as $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$.

Suppose next that $|T_{\{x_2,x_4\}}| \geq 1$ and $|T_{\{x_2,x_5\}}| = 0$. From Claims 4.4 and 4.8, we have $|T_{x_5}| = 0 \leq \max\{|T_{x_i}| : 1 \leq i \leq 4\} \leq 1$. Suppose that v is adjacent to $u \in T_0$. From Claim 4.5, v is adjacent to every vertex of $T_{\{x_2,x_4\}}$ if $v \in T_{\{x_1,x_3\}}$, and v is adjacent to every vertex of $T_{\{x_1,x_3\}}$ if $v \in T_{\{x_2,x_4\}}$. Combining this with Claims 4.1, 4.3 and 4.4, we obtain that G is an induced subgraph of some graph of $\mathcal{F}_5$. ■

4.2. Case: $|T_{\{x_1,x_3\}}| \leq 1$

By the choice of $T_{\{x_1,x_3\}}$, we have $|T_2| \leq 5$. Denote by u_{ij} the vertex (if any) of $T_{\{x_i,x_j\}}$ for $1 \leq i < j \leq 5$.

Lemma 4.14. *If T_2 is an independent set of G, then $G \subset D_5$.*

Proof. If $T_2 = \emptyset$, then $T_0 = \emptyset$ and $|T_1| \leq 5$ by Claims 4.2 and 4.4, and thus $G \subset D_5$ by Claim 4.4. Next, suppose that $T_2 \neq \emptyset$. Using the assumption that T_2 is an independent set of G and Claim 4.5, we deduce that every vertex of T_0 is adjacent to every vertex of T_2. Combining this with the fact that every vertex of T_2 is adjacent to at most one vertex of T_0 (this one follows from Claim 4.2), we obtain $|T_0| \leq 1$. Now, $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$ together with Claims 4.3 and 4.4, leads to the conclusion that $G \subset D_5$. ■

Lemma 4.15. *If T_2 is not an independent set of G, then $G \subset H_1 \subset D_7$.*

Proof. From the assumption of the statement, we have $|T_2| \geq 2$, while $|T_{\{x_1,x_3\}}| = 1$ holds by the choice of $T_{\{x_1,x_3\}}$. One can easily check that $H_1 \cong D_7 - \{y_2\text{–}y_5, y_7, y_{11}, y_{14}\text{–}y_{17}\}$, so it suffices to show that $G \subset H_1$.

Case 1: $4 \leq |T_2| \leq 5$. For $|T_2| = 5$, since T_2 is not an independent set of G, we may suppose that $u_{25}u_{13} \in E(G)$. By Claim 4.6, $G[T_2] \cong C_5 : u_{25}u_{13}u_{24}u_{35}u_{14}u_{25}$, which implies an impossible scenario: $Z_3 \subset G$. For $|T_2| = 4$, without loss of generality we may suppose that $T_{x_1x_4} = \emptyset$. Again, since T_2 is not an independent set, we have $G[T_2] \cong P_4$ with $E(G[T_2]) = \{u_{25}u_{13}, u_{24}u_{35}, u_{24}u_{13}\}$ (by Claim 4.6), which as before leads to $Z_3 \subset G$.

Case 2: $|T_2| = 3$. Using $|T_{x_1x_3}| = 1$, by symmetry we may suppose that either $T_{x_1x_4} = \emptyset = T_{x_3x_5}$ or $T_{x_1x_4} = \emptyset = T_{x_2x_4}$. In fact, we can deduce that the unique possibility is $T_{x_1x_4} = \emptyset = T_{x_3x_5}$. To see this, we assume that $T_{x_1x_4} = \emptyset = T_{x_2x_4}$. Then $|T_{x_3x_5}| = |T_{x_2x_5}| = 1$, as $|T_2| = 3$ and $|T_{x_1x_3}| = 1$. Note that $G[T_2]$ is not an independent set of G and G is triangle-free. Thus, $u_{13}u_{25} \in E(G)$, $u_{35}u_{13} \notin E(G)$ and $u_{25}u_{35} \notin E(G)$, which implies that $Z_3 \subset G$, contradicting Lemma 3.1. Hence, $T_{x_1x_4} = \emptyset = T_{x_3x_5}$. Combining this with Claim 4.6 and $|T_3| = 3$, we obtain $T_2 = \{u_{13}, u_{24}, u_{25}\}$ and $G[T_2] = P_3$ with u_{13} in the role of the vertex of degree 2 in P_3.

Since $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$, for $|T_0| = 0$, we obtain $G \subset H_1 - \{u_{14}, u_{35}\}$ by Claims 4.3 and 4.4. Suppose now that $|T_0| \geq 1$, and let $u_0 \in T_0$.

If $N_G(u_0) \cap \{u_{24}, u_{25}\} = \emptyset$, then u_0 is a pendant vertex adjacent to u_{13}, by Claim 4.2. Otherwise, $N_G(u_0) \cap \{u_{24}, u_{25}\} \neq \emptyset$, and thus $|N_G(u_0) \cap \{u_{24}, u_{25}\}| = 2$ by Claim 4.5. By Claim 4.2, we have $|T_0 \setminus \{u_0\}| \leq 1$, where the equality case implies that the unique vertex of $T_0 \setminus \{u_0\}$ is a pendant vertex adjacent to u_{13}. In both cases, the inequality $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$, together with Claims 4.3 and 4.4, leads to $G \subset H_1 - \{u_{14}, u_{35}\}$.

Case 3: $|T_2| = 2$. Since T_2 is not an independent set of G, we have $G[T_2] \cong K_2$. By symmetry, we suppose that $T_2 = \{u_{13}, u_{24}\}$.

By Claim 4.2, we have $|T_0| \leq 2$ and each vertex of T_0 is a pendant vertex of G adjacent to either u_{13} or u_{24}. Moreover, Claim 4.2 also implies that either u_{13} or u_{24} is adjacent to at most one vertex of T_0. This fact, together with $\max\{|T_{x_i}| : 1 \leq i \leq 5\} \leq 1$ and Claims 4.3 and 4.4, leads to $G \subset H_1 - \{u_{14}, u_{25}, u_{35}\}$. ■

4.3. The final step

If G is bipartite, then the desired result follows from Proposition 2.4. In what follows we assume that G is non-bipartite and collect the results formulated in lemmas of the previous two subsections. We use C_5 with $V(C_5) = \{x_1, x_2, \ldots, x_5\}$ as the base graph, along with the notation introduced in Section 3.

For $|T_{\{x_1,x_3\}}| \geq 2$. If T_0 contains a vertex whose degree in G is at least 3, then G is an induced subgraph of some graph of $\mathcal{F}_4$, by Lemma 4.9. Otherwise, if T_0 contains a vertex whose degree in G is 2, then G is an induced subgraph of some graph of $\mathcal{F}_4 \cup \mathcal{F}_5$, as follows by Lemmas 4.10 and 4.11. Finally, if every vertex of T_0 is a pendant vertex in G, then we again have that G is an induced subgraph of some graph of $\mathcal{F}_4 \cup \mathcal{F}_5$, as follows by Lemmas 4.12 and 4.13.

For $|T_{\{x_1,x_3\}}| \leq 1$, G is an induced subgraph of D_5 or D_7 depending on whether T_2 is an independent set in G or not, as follows by Lemmas 4.14 and 4.15, and the proof is completed.

5. Proof of Theorem 2.2

Throughout this section, let K_q be a fixed maximal clique of G. We divide our considerations into two cases depending on q. They are separated into subsections.

5.1. Case: $q \geq 4$

Here, we always use K_q as the base graph. Since the diamond is forbidden, every vertex outside K_q is adjacent to at most one vertex of K_q. In other words, $T = T_0 \cup T_1$.

Claim 5.1. *If $q \geq 4$, then $T = T_1$ and T_{x_i} is an independent set of G.*

Proof. Since $q \geq 4$ and $Z_4 \not\subset G$, T_{x_i} is an independent set of G. Assume that $T_0 \neq \emptyset$. Since every vertex of T is adjacent to at most one vertex of K_q, one vertex of T_0 is adjacent to a vertex of T_1, which implies that $Z_5 \subset G$, but this is impossible by Lemma 3.1. Hence, $T = T_1$. ■

Lemma 5.2. *If $q \geq 5$, then G is an induced subgraph of some graph of $\mathcal{F}_6 \cup K_3^5$.*

Proof. By Claim 5.1, we have $T_0 = \emptyset$ and T_{x_i} is an independent set of G. Suppose that $u \in T_{x_i}$ and $v \in T_{x_j}$ for $i \neq j$. Since $Z_5 \not\subset G$, $uv \notin E(G)$. Let $|T_{x_1}| = \max\{|T_{x_i}| : 1 \leq i \leq q\}$. Next, we assume that G is not an induced subgraph of any graph of $\mathcal{F}_6$. Then, $|T_{x_1}| \geq 3$. Combining this with $K_4^5, K_3^6 \not\subset G$, we obtain $|T_{x_1}| = 3$ and $q = 5$. Since $K_{3;1}^5 \not\subset G$, we have $T_1 = T_{x_1}$, and so $G \cong K_3^5$. ■

Lemma 5.3. *If $q = 4$, then G is an induced subgraph of some graph of $\mathcal{F}_6 \cup D_6$.*

Proof. Let $|T_{x_i}| = s_i$ for $1 \leq i \leq 4$. Without loss of generality, we may suppose that $s_4 \leq s_3 \leq s_2 \leq s_1$. Since $K_5^4 \not\subset G$, we have $s_1 \leq 4$.

Case 1: $s_3 \geq 1$. We show that $G \cong K_{s_1;s_2;s_3;s_4}^4$. From Claim 5.1, we have $T = T_1$ and T_{x_i} is an independent set of G. Therefore, to show that $G \cong K_{s_1;s_2;s_3;s_4}^4$, it suffices to prove the following: If $u \in T_{x_i}$, $v \in T_{x_j}$ and $w \in T_{x_k}$, then u, v, w induce an independent set of G. Indeed, if we assume that $uv \in E(G)$, then, since $Z_7 \not\subset G$, either $wu \in E(G)$ or $vw \in E(G)$. This implies $Z_8 \subset G$ or $Z_9 \subset G$, but both are impossible by Lemma 3.1.

Hence, $G \cong K_{s_1;s_2;s_3;s_4}^4$. Since $K_{3;1;1}^4 \not\subset G$ and $s_3 \geq 1$, we have $s_1 \leq 2$, which implies that G is an induced subgraph of some graph of $\mathcal{F}_6$.

Case 2: $s_3 = 0$. We will show that $G \subset D_6$. Assume, by way of contradiction, that $G \not\subset D_6$. Since $Z_6 \not\subset G$, every vertex of T_{x_i} is adjacent to at most one vertex of T_{x_j} for $\{i, j\} = \{1, 2\}$. Combining this with $K_{3;2}^3, K_{4;1}^4 \not\subset G$, we obtain $3 \leq s_2 \leq 4$, because $G \subset D_6$ for $s_2 \leq 2$.

If $s_1 = 3$, then $s_2 = 3$. By employing $K_{3;2}^3 \not\subset G$, we obtain $G[T_{x_1} \cup T_{x_2}] \in \{3K_2,\ 2K_2 \cup 2K_1\}$. The latter implies $G \subset D_6$, and so there must be $s_1 = 4$. But in this case from $K_{4;1}^4 \not\subset G$, we deduce that $G[T_{x_1} \cup T_{x_2}] \cong 4K_2$ for $|T_{x_2}| = 4$, and $G[T_{x_1} \cup T_{x_2}] \cong 3K_2 \cup K_1$ for $|T_{x_2}| = 3$. In both cases, we also have $G \subset D_6$, which is the final contradiction. ■

5.2. Case: $q = 3$

Since $q = 3$, we have $K_4 \not\subset G$. In this subsection we use different base graphs tailored for every particular situation. We start with the following result.

Lemma 5.4. *If $W_2 \subset G$, then $G \subset D_7$.*

Proof. Since this is a considerably long proof, we start with a short concept; the same concept is used in several forthcoming proofs. In the first part, we give some initial results concerning the

structure of G; in particular, we will see that $T_i = \emptyset$ for $i = 1$ or $i \geq 6$. In the next step, we consider the sets T_5–T_2. Then we proceed with a list of 12 facts, where each of them is a simple consequence of the previous results. Finally, we consider the structure of T_0 and conclude the proof.

We use W_2 as the base graph of G. Let $X_1 = \{x_1, x_2, \ldots, x_5\}$ and $X_2 = \{x_6, x_7, x_8\}$, where the vertex labellings correspond Fig. 2. For every $u \in T$, since the diamond is forbidden and $q = 3$, we have

$$|N_{X_1}(u)| \leq 2, \text{ where the equality case implies } ux_1 \notin E(G). \tag{5.1}$$

Since $Z_1, Z_7, K^3_{3;2} \not\subset G$, we have $T_1 = \emptyset$. Combining this with (5.1), we arrive at the following setting

$$T = T_0 \cup T_2 \cup T_3 \cup T_4 \cup T_5.$$

Bearing in mind that the diamond is forbidden and taking into account (5.1), we deduce that a vertex of T_5 must be adjacent to each of $\{x_3\} \cup \{x_i \mid 5 \leq i \leq 8\}$, and so $T_5 = T_{\{x_3, x_5 - x_8\}}$. Together with, $Z_{10} \not\subset G$, this gives $0 \leq |T_5| \leq 1$.

Suppose that $u \in T_4$. If $N_{X_2}(u) = X_2$, then u is adjacent to exactly one of x_1, x_3, x_5. This leads to the impossible scenario $Z_1 \subset G$ or $Z_2 \subset G$. Thus, $|N_{X_2}(u)| = 2$ by (5.1). Moreover, by the same fact, we have that u must be adjacent to x_3 and x_5. Combining this with $K_4 - e, Z_1 \not\subset G$, we arrive at $T_4 = T_{\{x_3, x_5 x_6, x_7\}} \cup T_{\{x_3, x_5, x_6, x_8\}} \cup T_{\{x_3, x_5, x_7, x_8\}}$ and $|T_{\{x_3, x_5, x_i, x_j\}}| \leq 1$ for $\{i, j\} \in \{\{6, 7\}, \{6, 8\}, \{7, 8\}\}$. This implies that $|T_4| \leq 3$ and T_4 is an independent set of G.

Consider now a vertex of T_3, denoted again by u. From $2P_3 \not\subset G$ and (5.1), we obtain $1 \leq |N_{X_2}(u)| \leq 2$. If $|N_{X_2}(u)| = 1$, then either u is adjacent to x_2, x_5 or u is adjacent to x_3, x_4 by (5.1), as $K_4 - e, Z_1 \not\subset G$. Next, for $i \in \{6, 7, 8\}$, we have $\max\{|T_{\{x_i, x_2, x_5\}}|, |T_{\{x_i, x_3, x_4\}}|\} \leq 1$, as the diamond is forbidden. Similarly, if $|N_{X_2}(u)| = 2$, then u must be adjacent to x_1, as $K_4 - e, Z_1 \not\subset G$. Combining this with $Z_3 \not\subset G$, we obtain $|T_{\{x_i, x_j, x_1\}}| \leq 1$ for $\{i, j\} \in \{\{6, 7\}, \{6, 8\}, \{7, 8\}\}$. Amalgamating the previous results, we arrive at $T_3 = \bigcup_{i=6}^{8} \big(T_{\{x_i, x_2, x_5\}} \cup T_{\{x_i, x_3, x_4\}}\big) \cup T_{\{x_6, x_7, x_1\}} \cup T_{\{x_6, x_8, x_1\}} \cup T_{\{x_7, x_8, x_1\}}$ and $|T_{\{x_i, x_j, x_k\}}| \leq 1$ for $T_{\{x_i, x_j, x_k\}} \subseteq T_3$. Finally, the assumption that the diamond is forbidden, ensures that $\bigcup_{i=6}^{8} T_{\{x_i, x_2, x_5\}}$, $\bigcup_{i=6}^{8} T_{\{x_i, x_3, x_4\}}$ and $T_{\{x_6, x_7, x_1\}} \cup T_{\{x_6, x_8, x_1\}} \cup T_{\{x_7, x_8, x_1\}}$ are independent sets of G.

In a similar way, we consider T_2 by taking $u \in T_2$. From $2P_3 \not\subset G$, we have $|N_{X_2}(u)| \leq 1$. If $|N_{X_2}(u)| = 1$, then u must be adjacent to x_1, as $Z_1, Z_7 \not\subset G$. If $|N_{X_2}(u)| = 0$, then $ux_1 \notin E(G)$ by (5.1). Combining this with $Z_1, K_4 - e \not\subset G$, we arrive at $T_2 = T_{\{x_2, x_4\}} \cup T_{\{x_2, x_5\}} \cup T_{\{x_3, x_4\}} \cup T_{\{x_1, x_6\}} \cup T_{\{x_1, x_7\}} \cup T_{\{x_1, x_8\}}$. Since $K^3_{3;2}, K^3_{5;1}, Z_1, K_4 - e \not\subset G$, we also have that $|T_{\{x_i, x_j\}}| \leq 1$ and $T_{\{x_1, x_6\}} \cup T_{\{x_1, x_7\}} \cup T_{\{x_1, x_8\}}$ is an independent set of G.

We proceed with the following facts. Observe that they give a structure of a subgraph of D_7 having W_2 as the base graph along with $T_0 = \emptyset$.

(**F1**) If $u \in T_5$, then $uv \notin E(G)$ for $v \in T_3 \cup T_4 \cup T_{\{x_2, x_4\}}$, $uv \in E(G)$ for $v \in T_{\{x_1, x_i\}}$ with $i \in \{6, 7, 8\}$ or $v \in T_{\{x_2, x_5\}} \cup T_{\{x_3, x_4\}}$, all these since $K_4 - e, Z_1, Z_2, U^4_{1,1,1,1} \not\subset G$;

(**F2**) If $u \in T_{\{x_3, x_5, x_i, x_j\}}$ and $v \in T_{\{x_s, x_t, x_k\}}$ for $\{t, k\} \in \{\{2, 5\}, \{3, 4\}\}$, then $uv \notin E(G)$ for $s \in \{i, j\}$ and $uv \in E(G)$ for $s \notin \{i, j\}$, as $Z_1 \not\subset G$;

(**F3**) If $u \in T_{\{x_3, x_5, x_i, x_j\}}$ and $v \in T_{\{x_1, x_s, x_t\}}$, then $uv \notin E(G)$ for $\{i, j\} = \{s, t\}$ and $uv \in E(G)$ for $\{i, j\} \neq \{s, t\}$, as $K_4 - e, Z_1 \not\subset G$;

(**F4**) If $u \in T_{\{x_3, x_5, x_i, x_j\}} \cup T_{\{x_1, x_i, x_j\}}$ and $v \in T_{\{x_1, x_s\}}$, then $uv \notin E(G)$ for $s \in \{i, j\}$ and $uv \in E(G)$ for $s \notin \{i, j\}$, as $Z_1 \not\subset G$;

(**F5**) If $u \in T_{\{x_3, x_5, x_i, x_j\}}$ and $v \in T_{\{x_s, x_t\}}$, then $uv \in E(G)$ for $\{s, t\} = \{2, 4\}$ and $uv \notin E(G)$ for $\{s, t\} \in \{\{2, 5\}, \{3, 4\}\}$, as $Z_1 \not\subset G$;

(**F6**) If $u \in T_{\{x_1, x_i, x_j\}}$ and $v \in \bigcup_{s=6}^{8} \big(T_{\{x_s, x_2, x_5\}} \cup T_{\{x_s, x_3, x_4\}}\big)$, then $uv \in E(G)$ for $s \notin \{i, j\}$ and $uv \notin E(G)$ for $s \in \{i, j\}$, as $K_4 - e, Z_1 \not\subset G$;

(**F7**) If $u \in T_{\{x_i, x_2, x_5\}}$ and $v \in T_{\{x_s, x_3, x_4\}}$, then $uv \notin E(G)$ for $i = s$ and $uv \in E(G)$ for $i \neq s$, as $K_4 - e, U^4_2 \not\subset G$;

(**F8**) If $u \in T_{\{x_1, x_i, x_j\}}$ and $v \in T_{\{x_s, x_t\}}$, then $uv \notin E(G)$ for $\{s, t\} = \{2, 4\}$ and $uv \in E(G)$ for $\{s, t\} \in \{\{2, 5\}, \{3, 4\}\}$, as $Z_1, Z_2 \not\subset G$;

(**F9**) If $u \in T_{\{x_i, x_2, x_5\}} \cup T_{\{x_i, x_3, x_4\}}$ and $v \in T_{\{x_1, x_s\}}$, then $uv \notin E(G)$ for $i = s$ and $uv \in E(G)$ for $i \neq s$, as $Z_1 \not\subset G$;

(**F10**) If $u \in T_{\{x_i,x_j,x_k\}}$ and $v \in T_{\{x_s,x_t\}}$ for $\min\{i,j,k,s,t\} \geq 2$, then $uv \notin E(G)$ for $|\{i,j,k\} \cap \{s,t\}| \geq 1$ and $uv \in E(G)$ for $|\{i,j,k\} \cap \{s,t\}| = 0$, as $Z_1, U_2^4 \not\subset G$;
(**F11**) If $u \in T_{\{x_i,x_j\}}$ and $v \in T_{\{x_1,x_k\}}$ for $\min\{i,j,k\} \geq 2$, then $uv \in E(G)$ for $\{i,j\} = \{2,4\}$ and $uv \notin E(G)$ for $\{i,j\} \in \{\{2,5\},\{3,4\}\}$, as $Z_2 \not\subset G$;
(**F12**) If $u \in T_{\{x_2,x_i\}}$ and $v \in T_{\{x_j,x_k\}}$ for $\min\{i,j,k\} \geq 2$, then $uv \notin E(G)$ for $(i,j,k) = (5,3,4)$, $uv \in E(G)$ for $(i,j,k) = (4,3,4)$ or $(i,j,k) = (5,2,4)$, as $Z_2, K_{4;1;1}^3 \not\subset G$.

Now, we consider T_0. If $u \in T_0$, then clearly u must be adjacent to some vertex v of $T_2 \cup T_3 \cup T_4 \cup T_5$. Now, the case $v \in T_5$ is eliminated by $U_{1,1,1,1}^4 \subset G$, $v \in T_4$ is eliminated by $Z_1 \subset G$, $v \in T_3$ is eliminated by $Z_2 \subset G$ and $v \in T_2$ is eliminated by $Z_1, Z_7 \subset G$. This contradiction leads to $T_0 = \emptyset$. Now, by combining $(F1)$–$(F12)$, we arrive at $G \subset D_7$. ■

We quote the following two lemmas. Their proofs follow the idea of the proof of Lemma 5.4. For the sake of completeness, they are given in the Appendix in full details.

Lemma 5.5. *If $W_3 \subset G$ and $W_2 \not\subset G$, then $G \subset H_5 \subset D_7$.*

Lemma 5.6. *If $W_4 \subset G$ and $W_3 \not\subset G$, then $G \subset D_7$.*

We continue by lemmas concerning the remaining possibilities for G.

Lemma 5.7. *If $W_5 \subset G$ and $W_4 \not\subset G$, then $G \subset \mathcal{F}_7$.*

Proof. Here, we use W_5 as the base graph with $V(W_5) = \{x_1, x_2, \ldots, x_5\}$ (see Fig. 2). From $K_4 - e, W_4 \not\subset G$, we have $T = T_0 \cup T_1$. From $Z_{15} \not\subset G$, we also have $T_1 = T_{x_1}$. If $T_0 = \emptyset$, then G is an induced subgraph of some graph of $\mathcal{F}_7$, as the diamond is forbidden. Therefore, let $u_0 \in T_0$ with $u_0v_0 \in E(G)$. Since G is connected, we have $v_0 \in T_1$.

We claim that the neighbours of every vertex of T_0 belong to T_1. Otherwise, since G is connected, we assume that $w_0 \in T_0$ such that $w_0u_0 \in E(G)$, and then $N_{W_5}(u_0) \cup N_{W_5}(w_0) = \emptyset$. Since $U_3^3 \not\subset G$, we also have $v_0w_0 \in E(G)$ (where v_0 is specified before), and so $Z_{12} \subset G$, which is impossible.

Actually, we can require that each vertex of T_0 is a pendant vertex. To see this, assume that u_0 itself is not a pendant vertex and hence it is adjacent to at least two vertices of T_1. Since the diamond is forbidden, we have $Z_{13} \subset G$.

Moreover, since $Z_6 \not\subset G$ and the neighbours of every vertex of T_0 belong to T_1, if $v \in T_1$ is a neighbour of some vertex of T_0, then it is adjacent to exactly one vertex of T_0. Together with $Z_{15} \not\subset G$, this implies that v has degree 2 in G. Combining this with the structure of T_0, we arrive at the desired conclusion. ■

Lemma 5.8. *If $W_6 \subset G$ and $W_5 \not\subset G$, then $G \subset H_2 \subset D_7$ or $G \subset H_3 \subset D_7$.*

Proof. Since $H_2 \cong D_7 - \{y_8, y_9, y_{11}, y_{13}\text{–}y_{17}\}$ and $H_3 \cong D_7 - \{y_5, y_7, y_8, y_{12}\text{–}y_{17}\}$, it suffices to show that $G \subset H_2$ or $G \subset H_3$. We use W_6 as the base graph. Let $u \in T$. Since $K_4 - e, K_4 \not\subset G$, u is adjacent to at most one vertex of the unique triangle and u cannot be adjacent to all vertices outside the triangle of W_6, which yields $|N_G(u) \cap V(W_6)| \leq 5$.

As in the proof of Lemma 5.4, we proceed with some initial settings. Since $Z_{10}, W_5, K_4 - e \not\subset G$, the equality $|N_G(u) \cap V(W_6)| = 5$ is impossible. From $Z_1, Z_2, U_2^4, U_{1,1,1,1}^4, W_5 \not\subset G$, we deduce that $T_1 = T_{x_1}$ and $|T_1| \leq 1$. Since $Z_1, Z_2, Z_7, K_4 - e, U_{1,1,1,1}^4, U_2^4, W_5 \not\subset G$, we also have $T_2 = \bigcup_{i=6}^{8} T_{x_2x_i}$, where $|T_{\{x_2,x_i\}}| \leq 1$ and T_2 is an independent set of G.

Now we consider the structure of T_4, T_3 and T_0. Suppose that $u \in T_4$. Since $Z_1, Z_2, K_4 - e \not\subset G$, we have $ux_2 \in E(G)$, $ux_5 \in E(G)$ and $|N_G(u) \cap \{x_6, x_7, x_8\}| = 2$, that is $T_4 = T_{\{x_2,x_5,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6,x_8\}} \cup T_{\{x_2,x_5,x_7,x_8\}}$. Since $Z_1, K_4 - e \not\subset G$, $|T_{\{x_2,x_5,x_i,x_j\}}| \leq 1$ and T_4 is an independent set of G.

Suppose that $u \in T_3$. Since $U_2^4, K_4 - e \not\subset G$, we have $|N_G(u) \cap \{x_1, x_2, x_3\}| = 1$. If $ux_1 \in E(G)$, then $u \in T_{\{x_1,x_4,x_5\}}$ and $|T_{\{x_1,x_4,x_5\}}| \leq 1$, as $W_5, K_4 - e \not\subset G$. Next, $ux_2 \in E(G)$ does not hold because $Z_1 \subset G$

or $K_4 - e \subset G$. If $ux_3 \in E(G)$, then $u \in \left(\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}}\right) \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_7,x_8\}}$, as $W_5 \not\subset G$. This leads to

$$T_3 = \left(\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}}\right) \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_7,x_8\}} \cup T_{\{x_1,x_4,x_5\}}.$$

Since $Z_2, K_4 - e \not\subset G$, we also have $|T_{\{x_i,x_j,x_k\}}| \leq 1$.

If $u \in T_0$ with $uv \in E(G)$, then $v \notin T_1 \cup T_2 \cup T_3 \cup T_4$, as $U_2^4, Z_2 \not\subset G$, which means that $T_0 = \emptyset$.

Now, we proceed with the following facts.

(**F32**) If $u \in T_1$, then $uv \notin E(G)$ for $v \in T_2 \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_7,x_8\}}$ and $uv \in E(G)$ for $v \in \left(\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}}\right) \cup T_4 \cup T_{\{x_1,x_4,x_5\}}$, as $Z_1, Z_8 \not\subset G$.

(**F33**) Let $u \in T_{\{x_2,x_i\}}$. Since $Z_1, W_5 \not\subset G$, if $v \in T_{\{x_2,x_5,x_s,x_t\}} \cup T_{\{x_3,x_s,x_t\}}$ with $6 \leq s < t \leq 8$, then $uv \notin E(G)$ for $i \in \{s,t\}$ and $uv \in E(G)$ for $i \notin \{s,t\}$; if $v \in T_{\{x_3,x_4,x_j\}}$, then $uv \in E(G)$ for $i \neq j$ and $uv \notin E(G)$ for $i = j$.

(**F34**) Let $u \in T_{\{x_2,x_5,x_s,x_t\}}$. Since $Z_1, K_4 - e \not\subset G$, if $v \in T_{\{x_3,x_i,x_j\}}$ for $6 \leq i < j \leq 8$, then $uv \notin E(G)$ for $|\{s,t\} \cap \{i,j\}| = 2$ and $uv \in E(G)$ for $|\{s,t\} \cap \{i,j\}| = 1$; if $v \in T_{\{x_3,x_4,x_i\}}$, then $uv \notin E(G)$ for $i \in \{s,t\}$ and $uv \in E(G)$ for $i \notin \{s,t\}$.

Finally, we distinguish two cases depending on $\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}}$.

Case 1: $\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}} = \emptyset$. Let $T_{\{x_1,x_4,x_5\}} = \{u_0\}$. Since $Z_1, K_4 - e \not\subset G$, u_0 is adjacent to each vertex of $T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_7,x_8\}}$ and $T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_7,x_8\}}$ is an independent set of G.

Since $Z_2, K_4 - e \not\subset G$, we have $u_0 v \in E(G)$ for every $v \in T_2$, and also u_0 is not adjacent to any vertex of T_4. Combining this with (F32)–(F34), we arrive at $G \subset H_2$.

Case 2: $\bigcup_{i=6}^{8} T_{\{x_3,x_4,x_i\}} \neq \emptyset$. By symmetry, suppose that $u_0 \in T_{\{x_3,x_4,x_6\}} \neq \emptyset$. Since $W_5, Z_1, K_4 - e \not\subset G$, we have $T_{\{x_1,x_4,x_5\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_3,x_4,x_8\}} \cup T_{\{x_3,x_7,x_8\}} = \emptyset$ and $T_3 \subset T_{\{x_3,x_6,x_8\}} \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_4,x_6\}}$. Combining this with the assumption that the diamond is forbidden, we conclude that T_3 is an independent set of G. Now, taking into consideration (F32)–(F34), we deduce that $G \subset H_3$. ■

The proofs of the following three lemmas are given in Appendix.

Lemma 5.9. *If $W_7 \subset G$ and $W_5, W_6 \not\subset G$, then $G \subset H_4 \subset D_7$ or $G \subset H_8 \subset D_7$.*

Lemma 5.10. *If $W_8 \subset G$ and $W_5, W_7 \not\subset G$, then $G \subset H_9 \subset D_7$ or $G \subset H_{12} \subset D_7$.*

Lemma 5.11. *If $W_9 \subset G$ and $W_5, W_8 \not\subset G$, then $G \subset H_{13} \subset D_7$.*

We conclude our considerations with the following result.

Lemma 5.12. *If $W_5, W_9 \not\subset G$, then G is an induced subgraph of some graph of $\mathcal{F}_7 \cup D_7$.*

Proof. Here we use C_3 as the base graph with $V(C_3) = \{x_1, x_2, x_3\}$. Since $K_4 - e, K_4 \not\subset G$, we have $T = T_0 \cup T_1$, where $T_1 = T_{x_3} \cup T_{x_2} \cup T_{x_1}$. Since $W_5, W_9 \not\subset G$, T_1 is an independent set of G.

We claim that if $T_0 \neq \emptyset$, then G is an induced subgraph of some graph of $\mathcal{F}_7$. To see this, we let $u_0 \in T_0$ and $v_0 \in T_1$ with $u_0 v_0 \in E(G)$, as G is connected. Since $U_3^3, Z_{12} \not\subset G$, u_0 is not adjacent to any other vertex of T_0. If $d_G(v_0) \geq 3$, then G contains Z_6 as an induced subgraph, as T_1 is an independent set of G. Thus, $d_G(v_0) = 2$. Combining this with $Z_{13}, Z_{14} \not\subset G$, we deduce that $d_G(u_0) = 1$. By the choice of u_0 and v_0, we conclude that each vertex of T_0 is a pendant vertex adjacent to a vertex of T_1, and this vertex of T_1 has degree 2 in G.

Suppose that $v_0 \in T_{x_1}$. Since $Z_7 \not\subset G$ and $d_G(v_0) = 2 > 1 = d_G(u_0)$, we have $|T_{x_2}| = |T_{x_3}| = 0$. Combining this with the established fact that T_{x_1} is an independent set of G, we conclude that G is an induced subgraph of some graph of $\mathcal{F}_7$, which proves our claim.

Accordingly, we may suppose that $T_0 = \emptyset$, and so $T = T_{x_1} \cup T_{x_2} \cup T_{x_3}$. Next, assume that G is not an induced subgraph of any graph of $\mathcal{F}_7$. By symmetry, suppose that $|T_{x_1}| \geq |T_{x_2}| \geq |T_{x_3}|$. By the assumption on G, we have that T_1 is an independent set of G with $|T_{x_2}| \geq 1$, and so $|T_{x_1}| \leq 4$, as

$K^3_{5;1} \not\subset G$.

If $|T_{x_1}| = 4$, then $|T_{x_3}| = 0 < 1 = |T_{x_2}|$ (as $K^3_{4;1;1}, K^3_{3;2} \not\subset G$), and thus $G = K^3_{4;1} \subset H_5 \subset D_7$.

If $|T_{x_1}| = 3$, then $|T_{x_2}| = 1$ (as $K^3_{3;2} \not\subset G$), and thus $G \subset H_5$, as $0 \leq |T_{x_3}| \leq 1$.

If $|T_{x_1}| \leq 2$, then $G \subset D_7$ (as $|T_{x_3}| \leq |T_{x_2}| \leq 2$), and we are done. ■

5.3. The final step

If the size q of a maximal induced clique is at least 5, then G is an induced subgraph of some graph of $\mathcal{F}_6 \cup K^5_3$, by Lemma 5.2. If $q = 4$, then G is an induced subgraph of some graph of $\mathcal{F}_6 \cup D_6$, by Lemma 5.3. Finally, for $q = 3$, G is an induced subgraph of some graph of $\mathcal{F}_7 \cup D_7$, as follows by Lemmas 5.4–5.12.

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Appendix

Here we give the proofs of five lemmas from Section 5.2. As we have pointed out, the concept of every proof is similar to that of Lemma 5.4 (outlined at its beginning).

Proof of Lemma 5.5. Here, we use W_3 as the base graph. In what follows, we partition its vertices as: $X_1 = \{x_1, x_2, \ldots, x_5\}$, $X_2 = \{x_6, x_7\}$. For every $u \in T$, since the diamond is forbidden, (5.1) remains valid. Thus, $T = T_0 \cup T_1 \cup T_2 \cup T_3 \cup T_4$. Since $H_5 \cong D_7 - \{y_{16}, y_{17}\}$, it suffices to show that $G \subset H_5$.

From $K_4 - e, W_2 \not\subset G$ and (5.1), we have that $T_4 = T_{\{x_3,x_5,x_6,x_7\}}$ is an independent set of G and $|T_4| \leq 2$. Since $Z_1, Z_6, Z_8, U^3_{3;2} \not\subset G$, we have $T_1 = T_{x_1}$ and $|T_1| \leq 1$.

Suppose that $u \in T_3$. If $N_{X_2}(u) = X_2$, then $N_{X_1}(u) = \{x_1\}$, as $Z_1, K_4 - e \not\subset G$. If $N_{X_2}(u) \neq X_2$, then $|N_{X_2}(u)| = 1$ by (5.1). From the assumption on the diamond and (5.1), we have $N_{X_1}(u) = \{x_2, x_5\}$, or $N_{X_1}(u) = \{x_3, x_4\}$, or $N_{X_1}(u) = \{x_3, x_5\}$. Thus, $T_3 = \bigcup_{i=6}^{7}\big(T_{\{x_3,x_5,x_i\}} \cup T_{\{x_2,x_5,x_i\}} \cup T_{\{x_3,x_4,x_i\}}\big) \cup T_{\{x_1,x_6,x_7\}}$. Since $K_4 - e, Z_1, Z_3 \not\subset G$, we have $|T_{\{x_i,x_j,x_k\}}| \leq 1$, and thus $|T_3| \leq 7$.

Suppose that $u \in T_2$. From $2P_3 \not\subset G$, we have $|N_{X_2}(u)| \leq 1$. If $|N_{X_2}(u)| = 1$, then u must be adjacent to x_1, as $Z_1 \not\subset G$. If $|N_{X_2}(u)| = 0$, then $N_{X_2}(u) = \{x_2, x_5\}$ or $N_{X_2}(u) = \{x_3, x_4\}$, as $Z_1, W_2, K_4 - e \not\subset G$. Hence, $T_2 = T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}} \cup T_{\{x_1,x_6\}} \cup T_{\{x_1,x_7\}}$. Since $Z_2, K_4 - e \not\subset G$, we deduce that $T_{\{x_i,x_j\}}$ is an independent set of G and $|T_{\{x_i,x_j\}}| \leq 2$.

If $u \in T_0 \neq \emptyset$, then u must be adjacent to some vertex v of T. On the other hand, we have $v \notin T_1 \cup T_2$ (as $Z_1 \not\subset G$), $v \notin T_3$ (as $Z_1, Z_2 \not\subset G$), and $v \notin T_4$ (as $U^4_2 \not\subset G$), and thus $T_0 = \emptyset$.

We now prove the following claim.

Claim A. $G[T_4 \cup T_2] \subset W_{10}$.

Proof. Denote $S_1 = T_{\{x_3,x_5,x_6,x_7\}}$, $S_2 = T_{\{x_2,x_5\}}$, $S_3 = T_{\{x_3,x_4\}}$, $S_4 = T_{\{x_1,x_6\}}$, and $S_5 = T_{\{x_1,x_7\}}$. Next, suppose that $\{i, j, k, s, t\} = \{1, 2, \ldots, 5\}$. Since $Z_1, Z_2, Z_3, Z_8, K_4 - e \not\subset G$, we have:

(**F13**) If $|S_i| = 2$, then each vertex of S_j is adjacent to exactly one vertex of S_i, and $N_{S_j}(u) \neq N_{S_j}(v)$ for $u, v \in S_i$; If $u \in S_i$, $v \in S_j$ and $w \in S_k$, then $G[\{u, v, w\}] \cong 3K_1$ or $G[\{u, v, w\}] \cong P_3$.

From (F13) and the fact that $G[S_i]$ is an independent set of G for $1 \leq i \leq 5$, we deduce that $G[T_4 \cup T_2]$ is triangle-free. Next, we will show that $G[T_4 \cup T_2] \subset W_{10}$. Observing Fig. 2, we have that

two vertices in each dotted area are in the same S_i for $1 \le i \le 5$. For a contradiction, assume that $G[T_4 \cup T_2] \not\subset W_{10}$, and thus $|S_r| = \max\{|S_i| : 1 \le i \le 5\} \ge 1$. By the former arguments for T_4 and T_2, we have $|T_4| \le 2$ and $|T_{\{x_i,x_j\}}| \le 2$, which indicates $|S_r| \le 2$.

If $|S_r| = 2$, from $(F13)$, we have $|N_{S_r}(u)| = 1$ for every $u \in S_j$, $N_{S_j}(u) \ne N_{S_j}(v)$ for $u, v \in S_r$, and $G[S_r \cup S_j] \cong 2K_2$ for $|S_j| = 2$. For $u \in S_j$ and $v \in S_k$, from $(F13)$, we see that $uv \in E(G)$ for $N_{S_r}(u) \ne N_{S_r}(v)$ and $uv \notin E(G)$ for $N_{S_r}(u) = N_{S_r}(v)$. This implies that $G[T_4 \cup T_2] \subset W_{10}$, which is impossible. Hence, $|S_r| = 1$.

If $|S_r| = 1$, from $(F13)$, for $u \in S_i$, $v \in S_j$ and $w \in S_k$, we have $G[\{u, v, w\}] \cong 3K_1$ or $G[\{u, v, w\}] \cong P_3$. Thus, $G[T_4 \cup T_2] \subset K_{1,4}$, or $G[T_4 \cup T_2] \subset K_{2,3}$, or $G[T_4 \cup T_2] \subset 5K_1$. The latter implies $G[T_4 \cup T_2] \subset W_{10}$. $\diamond$

We proceed with the following facts. (As in the previous proofs, they give the structure of a desired induced subgraph, in this case an induced subgraph of H_5.)

(**F14**) If $u \in T_4$, then $uv \in E(G)$ for $v \in T_1$ and $uv \notin E(G)$ for $v \in T_3$, as $Z_1, K_4 - e \not\subset G$;

(**F15**) If $u \in T_{\{x_1,x_6,x_7\}}$, then $uv \in E(G)$ for $v \in T_{\{x_3,x_5,x_6\}} \cup T_{\{x_3,x_5,x_7\}} \cup T_1 \cup T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}$ and $uv \notin E(G)$ for $v \in \bigcup_{i=6}^{7} \big(T_{\{x_2,x_5,x_i\}} \cup T_{\{x_3,x_4,x_i\}} \cup T_{\{x_1,x_i\}}\big)$, as $Z_1, Z_2, K_4 - e \not\subset G$;

(**F16**) If $u \in T_{\{x_3,x_5,x_i\}}$ for $i \in \{6, 7\}$ and $j \ne i$, then $uv \in E(G)$ for $v \in T_{\{x_2,x_5,x_j\}} \cup T_{\{x_3,x_4,x_j\}} \cup T_{\{x_1,x_j\}}$ and $uv \notin E(G)$ for $v \in T_{\{x_3,x_5,x_j\}} \cup T_{\{x_3,x_4,x_i\}} \cup T_{\{x_2,x_5,x_i\}} \cup T_{\{x_1,x_i\}} \cup T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}} \cup T_1$, as $Z_1, K_4 - e \not\subset G$;

(**F17**) If $u \in T_{\{x_3,x_4,x_i\}}$ for $i \in \{6, 7\}$ and $j \ne i$, then $uv \in E(G)$ for $v \in T_{\{x_2,x_5\}} \cup T_{\{x_2,x_5,x_j\}} \cup T_{\{x_1,x_j\}} \cup T_1$ and $uv \notin E(G)$ for $v \in T_{\{x_3,x_4,x_j\}} \cup T_{\{x_2,x_5,x_i\}} \cup T_{\{x_1,x_i\}} \cup T_{\{x_3,x_4\}}$, as $Z_1, U_2^4, K_4 - e \not\subset G$;

(**F18**) If $u \in T_{\{x_2,x_5,x_i\}}$ for $i \in \{6, 7\}$ and $j \ne i$, then $uv \in E(G)$ for $v \in T_{\{x_3,x_4\}} \cup T_{\{x_1,x_j\}} \cup T_1$ and $uv \notin E(G)$ for $v \in T_{\{x_2,x_5,x_j\}} \cup T_{\{x_2,x_5\}} \cup T_{\{x_1,x_i\}}$, as $Z_1, U_2^4, K_4 - e \not\subset G$;

(**F19**) If $u \in T_2$ and $v \in T_1$, then $uv \notin E(G)$, as $Z_1 \not\subset G$.

Combining the previous facts with Claim A, we arrive at $G \subset H_5$. ■

Proof of Lemma 5.6. This is the longest proof in the paper. After the initial settings we combine claims and simple facts, and at some points deal with case analysis.

We use W_4 as the base graph of G with vertices labelled as in Fig. 2. Since the diamond is forbidden, the inequality (5.1) remains valid, and so $T = T_0 \cup T_1 \cup T_2 \cup T_3$. Since $Z_1, Z_7, Z_{15}, K_{5;1}^3 \not\subset G$, it follows that $T_1 = T_{x_1}$ with $|T_1| \le 3$, and T_1 is an independent set of G.

From (5.1) and and the assumption on the diamond, we have $T_3 = T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_5,x_6\}}$. Since $W_3, K_4 - e \not\subset G$, we have $|T_{\{x_i,x_j,x_k\}}| \le 1$ and T_3 is an independent set of G.

Since $Z_7, Z_{11}, U_2^4, W_3, K_4 - e \not\subset G$, we have $T_2 = T_{\{x_1,x_6\}} \cup T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}} \cup T_{\{x_3,x_5\}}$, where $|T_{\{x_1,x_6\}}| \le 3$, $T_{\{x_1,x_6\}}$ is an independent set of G and $|T_{\{x_i,x_j\}}| \le 1$ for $\{i, j\} \in \{\{2, 5\}, \{3, 4\}, \{3, 5\}\}$.

If $u \in T_0 \ne \emptyset$ with $uv \in E(G)$, then $v \notin T_1$ (as $Z_7 \not\subset G$), $v \notin T_2$ (as $Z_7, Z_8 \not\subset G$) and $v \notin T_3$ (as $Z_8 \not\subset G$). In other words, $T_0 = \emptyset$ and $T = T_1 \cup T_2 \cup T_3$.

Here are some facts useful to determine the structure of G.

(**F20**) Since $U_{1,1,1,1}^4, Z_1, Z_2, K_4 - e, Z_{10}, Z_{17} \not\subset G$, we have $|T_1| - 2 \le |N_{T_1}(u)| \le 1$ for $u \in T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}} \cup T_{\{x_1,x_6\}}$, $|T_1| - 1 \le |N_{T_1}(u)| \le 2$ for $u \in T_{\{x_3,x_5,x_6\}}$, $|T_{\{x_1,x_6\}}| - 2 \le |T_{\{x_1,x_6\}}(u)| \le 1$ for $u \in T_1 \cup T_{\{x_3,x_5,x_6\}}$, and $|T_{\{x_1,x_6\}}| - 1 \le |T_{\{x_1,x_6\}}(u)| \le 2$ for $u \in T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}$;

(**F21**) If $u \in T_{\{x_3,x_5\}}$, then $uv \in E(G)$ for $v \in T_{\{x_1,x_6\}}$ and $uv \notin E(G)$ for $v \in T_1$, as $P_6 \not\subset G$;

(**F22**) Let $u \in T_1$, $v \in T_{\{x_1,x_6\}}$ and $z \in T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}}$. Since $K_4 - e, W_3, Z_1 \not\subset G$, if $uv \in E(G)$, then $zv \notin E(G)$ and $zu \in E(G)$; if $uz \in E(G)$ and $uv \notin E(G)$, then $vz \in E(G)$. Moreover, if $z_1 \in T_{\{x_3,x_4\}}$ and $z_2 \in T_{\{x_2,x_5\}}$ with $G[\{v, z_1, z_2\}] = C_3$, then $uv \notin E(G)$ and $|N_G(u) \cap \{z_1, z_2\}| = 1$, as $Z_8, W_3, K_4 - e \not\subset G$;

(**F23**) Let $v \in T_{x_3x_4}$, $w \in T_{x_2x_5}$ and $vw \in E(G)$. Since $Z_8 \not\subset G$, we have $N_{T_1}(w) \cap N_{T_1}(v) = \emptyset$;

(**F24**) Let $v \in T_{x_3x_4}$, $w \in T_{x_2x_5}$ and $vw \notin E(G)$. Since $Z_1 \not\subset G$, we have $N_{T_{x_1x_6}}(v) = N_{T_{\{x_1,x_6\}}}(w)$ and $N_{T_1}(w) = N_{T_1}(v)$;

(**F25**) Let $v \in T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}}$ and $w \in T_{\{x_3,x_5,x_6\}}$. Since $U_2^4, Z_8, W_3, K_4 - e \not\subset G$, we have the following: If $vw \in E(G)$, then $T_1 = T_{\{x_1,x_6\}} = \emptyset$; if $vw \notin E(G)$, then $N_{T_1}(v) \subseteq N_{T_1}(w)$ and $N_{T_{\{x_1,x_6\}}}(w) \subseteq N_{T_{\{x_1,x_6\}}}(v)$;

(**F26**) Let $S \subseteq T_1 \cup T_{\{x_1,x_6\}}$ such that S is an independent set of G and let $z \in T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}$. Since $U_{1,1,1,1}^4, Z_{17} \not\subset G$, $|S| \le 3$. If $|T_{\{x_1,x_6\}} \cap S| = 2$ and $|T_1 \cap S| = 1$, then $T_1 \cap S \subseteq N_G(z)$ for

$|N_{T_{\{x_1,x_6\}}\cap S}(z)| = 2$ and $N_{T_1\cap S}(z) = \emptyset$ for $|N_{T_{\{x_1,x_6\}}\cap S}(z)| = 1$; if $|T_1 \cap S| = 2$ and $|T_{\{x_1,x_6\}} \cap S| = 1$, then $G[T_1 \cup T_{\{x_1,x_6\}} \cup \{z\}] \cong 4K_1$ or $G[T_1 \cup T_{\{x_1,x_6\}} \cup \{z\}] \cong P_3 \cup K_1$ with $|N_{T_1}(z)| = |N_{T_{\{x_1,x_6\}}}(z)| = 1$, as $Z_1, Z_3 \not\subset G$.

Throughout the proof, we suppose that $T_1 \subseteq \{u_0, u_1, \ldots, u_{i-1}\}$ for $|T_1| = i$, $T_{\{x_1,x_6\}} \subseteq \{v_0, v_1, \ldots, v_{j-1}\}$ for $|T_{\{x_1,x_6\}}| = j$, $z_1 \in T_{\{x_3,x_5\}}$, $z_2 \in T_{\{x_2,x_5\}}$, $z_3 \in T_{\{x_3,x_4\}}$, $z_4 \in T_{\{x_3,x_5,x_6\}}$ and $z_5 \in T_{\{x_3,x_4,x_6\}} \cup T_{\{x_2,x_5,x_6\}}$.

In what follows, we show that $G \subset D_7$. Actually, we will see that all graphs involved in this lemma have at most 16 vertices. One can easily check that $W_{11} \cong D_7 - \{y_1, y_7, y_9\text{–}y_{17}\}$, $W_{12} \cong D_7 - \{y_1, y_5\text{–}y_7, y_{11}\text{–}y_{17}\}$, $H_6 \cong D_7\big[\{x_1\text{–}x_6, y_{11}, y_{14}, y_{15}\}\big]$ and $H_7 \cong D_7\big[\{x_1\text{–}x_8, y_1, y_2, y_5, y_{10}\}\big]$. Therefore, to complete the proof, it suffices to show that $G \subset W_{11}\cup W_{12}\cup H_6\cup H_7$. We first show that $G \subset W_{11}\cup W_{12}$ for $T_3 = \emptyset$ in Claim B. Secondly, we show that $G \subset H_6\cup H_7$ for $T_{\{x_2,x_5,x_6\}}\cup T_{\{x_3,x_4,x_6\}} \neq \emptyset$ in Claim C. Finally, we show that $G \subset W_{11} \cup W_{12} \cup H_7$ for $T_{\{x_3,x_5,x_6\}} \neq \emptyset = T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_4,x_6\}}$ in Claim D.

Claim B. *If $T_3 = \emptyset$, then $G \subset W_{11} \cup W_{12}$.*

Proof. Denote $X_0 = V(W_4)\cup T_1\cup T_{\{x_1,x_6\}}\cup T_{\{x_3,x_4\}}\cup T_{\{x_2,x_5\}}$. Since $U_2^4 \not\subset G$, we have $N_G(z_1)\cap\{z_2, z_3\} = \emptyset$. By $(F21)$, $N_{T_1}(z_1) = \emptyset$ and $N_{T_{\{x_1,x_6\}}}(z_1) = T_{\{x_1,x_6\}}$. From this we see that we can ignore the existence of z_1 when consider the structure of G. Next, we only need to show that $G[X_0] \subset W_{11} - \{z_1, z_4\}$ for $z_2z_3 \notin E(G)$ and $G[X_0] \subset W_{12} - \{z_1, z_4\}$ for $z_2z_3 \in E(G)$.

By way of contradiction, we assume that the latter does not hold. If $T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}} = \emptyset$, then $G[X_0] \subset W_{11} - \{z_1\text{–}z_4\}$ by $(F20)$ and $(F26)$, which is impossible. Hence, $1 \leq |T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}}| \leq 2$, and so $2K_2 \not\subset G[T_1 \cup T_{\{x_1,x_6\}}]$ by $(F20)$ and $(F22)$. From $2K_2 \not\subset G[T_1 \cup T_{\{x_1,x_6\}}]$, $(F20)$, $(F22)$ and $(F26)$, we obtain $G[X_0] \subset W_{11} - \{z_1, z_3, z_4\}$ for $|T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}}| = 1$. This yields $|T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5\}}| = 2$.

Now we distinguish two cases.

Case B1: $z_2z_3 \notin E(G)$. By $(F20)$ and $(F24)$, we have $G[X_0] \subset W_{11}-\{z_1, z_4\}$ whenever $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} = 0$. Hence, $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} \geq 1$.

If either $|T_{\{x_1,x_6\}}| = 3$ or $|T_1| = 3$, then $|T_1 \cup T_{\{x_1,x_6\}}| = 4$ by $(F20)$, as $2K_2 \not\subset G[T_1 \cup T_{\{x_1,x_6\}}]$ and $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} \geq 1$. Since $N_{T_1}(z_2) = N_{T_1}(z_3)$ and $N_{T_{\{x_1,x_6\}}}(z_2) = N_{T_{\{x_1,x_6\}}}(z_3)$ by $(F24)$, we have $G[X_0] \subset W_{11} - \{z_1, z_4\}$ by $(F20)$ and $(F22)$, which is a contradiction.

If $|T_{\{x_1,x_6\}}| = 2$ and $|T_1| = 2$, then $G[T_1 \cup T_{\{x_1,x_6\}}] \cong K_2 \cup 2K_1$ by $(F20)$ and $(F26)$, as $2K_2 \not\subset G[T_1 \cup T_{\{x_1,x_6\}}]$. Suppose that $u_0v_0 \in E(G)$. From $(F20)$ and $(F22)$, we have $N_{T_1}(z_2) = \{u_0\}$ and $N_{T_{\{x_1,x_6\}}}(z_2) = \{v_1\}$. From $(F24)$, we also have $G[X_0] \subset W_{11} - \{z_1, z_4\}$, again a contradiction.

If $|T_{\{x_1,x_6\}}| = 2$ and $|T_1| = 1$, then $G[T_1 \cup T_{\{x_1,x_6\}}] \cong K_2 \cup K_1$ by $(F20)$, $(F24)$ and $(F26)$, as $G[X_0] \not\subset W_{11} - \{z_1, z_4\}$. Suppose that $u_0v_0 \in E(G)$. From $(F20)$ and $(F22)$, we have $N_{T_1}(z_2) = \{u_0\}$ and $N_{T_{\{x_1,x_6\}}}(z_2) = \{v_1\}$. From $(F24)$, we also have $G[X_0] \subset W_{11} - \{z_1, z_4\}$, which is a contradiction, as before.

If $|T_{\{x_1,x_6\}}| = 1$ and $|T_1| = 2$, then $G[T_1\cup T_{x_1x_6}] \cong K_2\cup K_1$ by $(F20)$, $(F26)$ and $G[X_0] \not\subset W_{11}-\{z_1, z_4\}$. From $(F20)$, $(F22)$ and $(F24)$, we also have $G[X_0] \subset W_{11} - \{z_1, z_4\}$, and we are done.

Finally, if $|T_{\{x_1,x_6\}}| = 1 = |T_1|$, then $G[X_0] \subset W_{11} - \{z_1, z_4\}$ by $(F22)$ and $(F24)$, and the case is closed.

Case B2: $z_2z_3 \in E(G)$. From $(F23)$ and and the assumption on the diamond, we have $|N_{T_{\{x_1,x_6\}}}(z_2) \cap N_{T_{\{x_1,x_6\}}}(z_3)| \leq 1$ and $N_{T_1}(z_2) \cap N_{T_1}(z_3) = \emptyset$ implying that $G[T_1 \cup T_{\{x_1,x_6\}}]$ is an independent set of G by $(F22)$. Since $z_2z_3 \in E(G)$ and $Z_1 \not\subset G$, we have $|N_G(v) \cap \{z_2, z_3\}| \geq 1$ for $v \in T_{\{x_1,x_6\}}$ and $|N_{T_1}(z_2) \cup N_{T_1}(z_3)| \geq 1$ for $|T_1| \geq 2$. From these arguments and $(F20)$, we have $G[X_0] \subset W_{12}-\{z_1, z_4\}$ for $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} = 0$, which is a contradiction. From $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} \geq 1$ and the fact that $G[T_1 \cup T_{\{x_1,x_6\}}]$ is an independent set of G, we have $\max\{|T_{\{x_1,x_6\}}|, |T_1|\} \leq 2$ by $(F26)$.

If $|T_{\{x_1,x_6\}}| = 2$, then $|T_1| = 1$ by $(F26)$. For $N_G(u_0) \cap \{z_2, z_3\} \neq \emptyset$, we have $|N_G(u_0) \cap \{z_2, z_3\}| = 1$. By symmetry, suppose that $z_2u_0 \in E(G)$. From $(F20)$ and $(F22)$, we have $|N_{T_{\{x_1,x_6\}}}(z_2)| = 2$ and $|N_{T_{\{x_1,x_6\}}}(z_3)| = 1$. This implies $G[X_0] \subset W_{12} - \{z_1, z_4\}$. Otherwise, $N_G(u_0) \cap \{z_2, z_3\} = \emptyset$. Then, $|N_{T_{\{x_1,x_6\}}}(z_2)| = 1 = |N_{T_{\{x_1,x_6\}}}(z_3)|$ by $(F20)$ and $(F26)$. From $(F22)$, we have $N_{T_{\{x_1,x_6\}}}(z_2) \neq N_{T_{\{x_1,x_6\}}}(z_3)$ and so $G[X_0] \subset W_{12} - \{z_1, z_4\}$, and we are done.

If $|T_{\{x_1,x_6\}}| = 1$ and $1 \le |T_1| \le 2$, then $|N_G(v_0) \cap \{z_2, z_3\}| \ge 1$. For $|N_G(v_0) \cap \{z_2, z_3\}| = 2$, we have $G[X_0] \subset W_{12} - \{z_1, z_4\}$ by $(F22)$ and $N_{T_1}(z_2) \cap N_{T_1}(z_3) = \emptyset$. Otherwise, $|N_G(v_0) \cap \{z_2, z_3\}| = 1$. By symmetry, suppose that $|N_{T_{\{x_1,x_6\}}}(z_2)| = 1$. From $(F22)$, we have $N_{T_1}(z_3) = \emptyset = N_{T_{\{x_1,x_6\}}}(z_3)$. Similarly, from $(F26)$ and $G[X_0] \not\subset W_{12} - \{z_1, z_4\}$, we have $|T_1| = 1$. Finally, for $0 \le |N_{T_1}(z_2)| \le 1$, we have $G[X_0] \subset W_{12} - \{z_1, z_4\}$, and the claim is proved. $\diamond$

Claim C. *If $T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_4,x_6\}} \neq \emptyset$, then $G \subset H_6 \cup H_7$.*

Proof. Since $Z_1, W_3, K_4 - e \not\subset G$, we have $T_{x_1x_6} \cup T_1 = \emptyset$. Since $U_2^4 \not\subset G$, we also have $z_1z_5 \in E(G)$ if z_1 exists. By symmetry, suppose that $T_{\{x_3,x_4,x_6\}} \neq \emptyset$. Then $T_{\{x_3,x_4\}} = \emptyset$, as $W_3, K_4 - e \not\subset G$. The same argument leads to $|T_{\{x_3,x_5\}} \cup T_{\{x_3,x_5,x_6\}}| \le 1$.

If $T_{\{x_2,x_5,x_6\}} \neq \emptyset$, then $T_{\{x_2,x_5\}} = \emptyset = T_{\{x_3,x_5,x_6\}}$, since $W_3, K_4 - e \not\subset G$ and T_3 is an independent set of G. Since z_1 must be adjacent to all vertices of $T_{\{x_3,x_4,x_6\}} \cup T_{\{x_2,x_5,x_6\}}$, we have $G \subset H_6$.

If $T_{\{x_2,x_5\}} \neq \emptyset$ and $T_{\{x_2,x_5,x_6\}} = \emptyset$, then $z_2z_5 \in E(G)$, as $U_2^4 \not\subset G$. We claim that $T_{\{x_3,x_5\}} = \emptyset$. Indeed, since $z_1z_5 \in E(G)$ and the diamond is forbidden, we have $z_1z_2 \notin E(G)$, and so $W_3 \subset G$, which is impossible. Now, $T_{\{x_3,x_5\}} = \emptyset$ and the fact that T_3 is an independent set imply that $G \subset H_{10} \subset H_7$ for $z_2z_4 \in E(G)$ or $G \subset H_{11} \subset H_7$ for $z_2z_4 \notin E(G)$, as $H_{10} \cong H_7 - \{x_2, x_3, v_0\}$ and $H_{11} \cong H_7 - \{v_0, v_1, v_2\}$.

If $T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5\}} = \emptyset$, then $G \subset H_{11} \subset H_7$ for $T_{\{x_3,x_5,x_6\}} \neq \emptyset$ or $G \subset H_6$ for $T_{\{x_3,x_5\}} \neq \emptyset$, as $z_1z_5 \in E(G)$ and $|T_{\{x_3,x_5\}} \cup T_{\{x_3,x_5,x_6\}}| \le 1$. $\diamond$

Claim D. *If $T_{\{x_3,x_5,x_6\}} \neq \emptyset = T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_4,x_6\}}$, then $G \subset W_{11} \cup W_{12} \cup H_7$.*

Proof. Since $W_3, K_4 - e \not\subset G$, it holds $T_{\{x_3,x_5\}} = \emptyset$. We will show that $G \subset H_{11} \subset H_7$ for $N_G(z_4) \cap \{z_2, z_3\} \neq \emptyset$ and $G \subset W_{11} \cup W_{12}$ for $N_G(z_4) \cap \{z_2, z_3\} = \emptyset$.

First, suppose that $N_G(z_4) \cap \{z_2, z_3\} \neq \emptyset$. By symmetry, we may suppose that $z_2z_4 \in E(G)$. From $(F25)$ and $z_2z_4 \in E(G)$, we have $T_1 = T_{\{x_1,x_6\}} = \emptyset$. Hence, $G \subset H_{11} \subset H_7$ for $T_{\{x_3,x_4\}} = \emptyset$. For $T_{\{x_3,x_4\}} \neq \emptyset$, we have $|N_G(z_4) \cap \{z_2, z_3\}| = 1$, and so $z_4z_3 \notin E(G)$, as $W_3, K_4 - e \not\subset G$. Since $Z_1 \not\subset G$, we also have $z_2z_3 \in E(G)$, and so $G \cong H_{11} \subset H_7$.

Next, we suppose that $N_G(z_4) \cap \{z_2, z_3\} = \emptyset$ in order to show that $G \subset W_{11} \cup W_{12}$. From $(F25)$, we have:

$$N_{T_{\{x_1,x_6\}}}(z_4) \subseteq N_{T_{\{x_1,x_6\}}}(z_2) \cap N_{T_{\{x_1,x_6\}}}(z_3) \text{ and } N_{T_1}(z_2) \cup N_{T_1}(z_3) \subseteq N_{T_1}(z_4). \tag{A.1}$$

Here are the following facts.

(**F27**) For $0 \le i \le j \le 2$, if $u_iv_j \in E(G)$, then $u_iz_4 \in E(G)$ and $z_4v_j \notin E(G)$; if $u_iv_j \notin E(G)$ and $z_4v_j \in E(G)$, then $z_4u_i \in E(G)$, as $K_4 - e, W_3, U_2^4, Z_8 \not\subset G$;

(**F28**) Suppose that $k \in \{2, 3\}$, $u_iv_j \notin E(G)$, and $z_4z_k \notin E(G)$. If $v_jz_k \in E(G)$, $v_jz_4 \notin E(G)$ and $u_i \in N_{T_1}(z_k) \cup N_{T_1}(z_4)$, then $u_i \in N_{T_1}(z_k) \cap N_{T_1}(z_4)$, as $Z_1 \not\subset G$. If $u_iz_4 \in E(G)$, $u_iz_k \notin E(G)$ and $v_j \in N_{T_{\{x_1,x_6\}}}(z_k) \cup N_{T_{\{x_1,x_6\}}}(z_4)$, then $v_j \in N_{T_{\{x_1,x_6\}}}(z_k) \cap N_{T_{\{x_1,x_6\}}}(z_4)$, as $Z_1 \not\subset G$;

(**F29**) Let $S \subseteq T_1 \cup T_{\{x_1,x_6\}}$ such that S is an independent set of G, with $|S| = 3$. Since $Z_2, K_4 - e \not\subset G$, we have the following: If $|N_{T_1 \cap S}(z_4)| = 2$, then $T_{\{x_1,x_6\}} \cap S \subseteq N_G(z_4)$; If $|N_{T_1 \cap S}(z_4)| = 1$ and $|T_{\{x_1,x_6\}} \cap S| = 2$, then $|N_{T_{\{x_1,x_6\}} \cap S}(z_4)| = 1$;

(**F30**) From $Z_1, K_4 - e \not\subset G$ and $(F20)$, we deduce that if $N_{T_{\{x_1,x_6\}}}(z_i) = \{v_1, v_2\}$ for $i \in \{2, 3\}$, then $|N_G(z_4) \cap \{v_1, v_2\}| = 1$; if $N_{T_1}(z_4) = \{u_1, u_2\}$, then $|N_G(z_i) \cap \{u_1, u_2\}| = 1$ for $i \in \{2, 3\}$.

We claim that $G \subset W_{12} - \{z_1, z_2, z_3\}$ holds whenever $u_iv_j \in E(G)$ holds for some $0 \le i \le j \le 2$. To see this, suppose that $u_0v_0 \in E(G)$ by symmetry, and so $v_0z_4 \notin E(G)$ and $u_0z_4 \in E(G)$ by $(F27)$. First, if $z \in T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}} \neq \emptyset$, then $v_0z \notin E(G)$ and $u_0z \in E(G)$ by $(F22)$, and thus $W_3 \subset G$, which is impossible. Hence, $T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}} = \emptyset$ and so $T_2 = T_{\{x_1,x_6\}}$. Combining this with $(F20)$, $(F26)$, $(F27)$ and $(F29)$, we obtain $G \subset W_{12} - \{z_1, z_2, z_3\}$ and so our claim holds.

In what follows, we suppose that $u_iv_j \notin E(G)$ for $0 \le i \le j \le 2$. In other words, $G[T_1 \cup T_{\{x_1,x_6\}}]$ is an independent set of G. From $(F26)$, we have $|T_1 \cup T_{\{x_1,x_6\}}| \le 3$. We will prove that $G \subset W_{12}$ for $|T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}| \le 1$ and $G \subset W_{11} \cup W_{12}$ for $|T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}| = 2$.

Next, we claim that $G \subset W_{12} - \{z_1\}$ holds for $|T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}| \le 1$. If $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} = 0$, then $G \subset W_{12} - \{z_1\}$ by $(F20)$, $(F30)$ and (A.1). If $|T_{\{x_1,x_6\}}| = 2$, then $|T_1| = 1$. From $(F20)$, $(F26)$, $(F27)$,

($F29$), ($F30$) and (A.1), we have $G \subset W_{12} - \{z_1\}$. If $|T_{\{x_1,x_6\}}| = 1$ and $|T_1| = 2$, then $G \subset W_{12} - \{z_1\}$ by ($F20$), ($F22$), ($F27$)–($F30$) and (A.1). If $|T_{\{x_1,x_6\}}| = 1 = |T_1|$, then $G \subset W_{12} - \{z_1\}$ by ($F22$), ($F27$), ($F28$) and (A.1).

Next, suppose that $|T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}| = 2$. Recall that $|T_1 \cup T_{\{x_1,x_6\}}| \leq 3$. Here are two cases.

Case 1: $z_2z_3 \in E(G)$. From ($F23$) and the assumption on the diamond, we have $N_{T_1}(z_2) \cap N_{T_1}(z_3) = \emptyset$ and $|N_{T_{\{x_1,x_6\}}}(z_2) \cap N_{T_{\{x_1,x_6\}}}(z_3)| \leq 1$. Since $z_2z_3 \in E(G)$ and $Z_1, Z_8 \not\subset G$, we have:

(**F31**) $|N_G(v) \cap \{z_2, z_3\}| \geq 1$ for $v \in T_{\{x_1,x_6\}}$, $|N_{T_1}(z_2) \cup N_{T_1}(z_3)| \geq 1$ for $|T_1| \geq 2$, and $vz_4 \in E(G)$ for $v \in N_{T_{\{x_1,x_6\}}}(z_2) \cap N_{T_{\{x_1,x_6\}}}(z_3)$. If $v \in N_{T_{\{x_1,x_6\}}}(z_i) \setminus N_{T_{\{x_1,x_6\}}}(z_j)$ for $\{i,j\} = \{2,3\}$, then $vz_4 \notin E(G)$. If $v \in N_{T_1}(z_4)$, then $v \in N_{T_1}(z_2) \setminus N_{T_1}(z_3)$ or $v \in N_{T_1}(z_3) \setminus N_{T_1}(z_2)$.

If $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} = 0$, then $G \subset W_{12} - \{z_1\}$ by ($F20$), ($F30$), ($F31$) and (A.1). Next, suppose that $1 \leq \min\{|T_1|, |T_{\{x_1,x_6\}}|\} \leq \max\{|T_1|, |T_{\{x_1,x_6\}}|\} \leq 2$, as $|T_1 \cup T_{\{x_1,x_6\}}| \leq 3$.

If $|T_{\{x_1,x_6\}}| = 2$, then $|T_1| = 1$. By ($F20$), ($F26$), ($F28$), ($F31$) and (A.1), we have $G \subset W_{12} - \{z_1\}$. If $|T_{\{x_1,x_6\}}| = 1$ and $|T_1| = 2$, then $G \subset W_{12} - \{z_1\}$ by ($F20$), ($F22$), ($F27$), ($F30$), ($F31$) and (A.1). If $|T_{\{x_1,x_6\}}| = 1 = |T_1|$, then $G \subset W_{12} - \{z_1\}$ by ($F22$), ($F27$), ($F31$) and (A.1).

Case 2: $z_2z_3 \notin E(G)$. If $\min\{|T_1|, |T_{\{x_1,x_6\}}|\} = 0$, then $G \subset W_{11} - \{z_1\}$ by ($F20$), ($F24$), ($F30$) and (A.1).

Next, suppose that $1 \leq \min\{|T_1|, |T_{\{x_1,x_6\}}|\} \leq \max\{|T_1|, |T_{\{x_1,x_6\}}|\} \leq 2$. If $|T_{\{x_1,x_6\}}| = 2$, then $|T_1| = 1$. By ($F20$), ($F24$), ($F26$)–($F28$), ($F30$) and (A.1), we have $G \subset W_{11} - \{z_1\}$. If $|T_{x_1x_6}| = 1$ and $|T_1| = 2$, then $G \subset W_{11} - \{z_1\}$ by ($F20$), ($F22$), ($F24$), ($F26$), ($F27$)–($F30$) and (A.1). If $|T_{x_1x_6}| = 1 = |T_1|$, then $G \subset W_{11} - \{z_1\}$ by ($F22$), ($F27$), ($F28$) and (A.1). This completes the proof of the last claim, and the proof of the entire lemma. ■

Proof of Lemma 5.9. Since $H_4 \cong D_7 - \{y_{11}\text{–}y_{17}\}$ and $H_8 \cong D_7 - \{y_8, y_{10}\text{–}y_{12}, y_{14}, y_{16}, y_{17}\}$, it suffices to show that $G \subset H_4$ or $G \subset H_8$. Here, we use W_7 as the base graph. Let $u \in T$. Since $K_4 - e, K_4 \not\subset G$, u is adjacent to at most one vertex of the unique triangle and it cannot be adjacent to all vertices outside the triangle of W_7, and thus $|N_G(u) \cap V(W_7)| \leq 4$.

Since $Z_1, Z_2, Z_8, W_5, U_2^4 \not\subset G$, we have that $T_1 = T_{x_1} \cup T_{x_2}$, where $|T_{x_i}| \leq 1$ and T_1 is an independent set of G. Since $Z_1, Z_2, Z_{13}, K_4 - e, U_2^4, W_5, W_6 \not\subset G$, $T_2 = T_{\{x_2,x_6\}} \cup T_{\{x_2,x_7\}} \cup T_{\{x_3,x_6\}} \cup T_{\{x_3,x_7\}} \cup T_{\{x_1,x_5\}} \cup T_{\{x_3,x_4\}}$ and $|T_{\{x_i,x_j\}}| \leq 1$.

Since $Z_{10}, W_5, K_4 - e \not\subset G$, we have $T_4 = T_{\{x_2,x_5,x_6,x_7\}}$ and $|T_{\{x_2,x_5,x_6,x_7\}}| \leq 1$.

Suppose that $u \in T_3$. Since $Z_1, K_4 - e \not\subset G$, we have $|N_G(u) \cap \{x_1, x_2, x_3\}| = 1$. If $ux_1 \in E(G)$, then $u \in T_{\{x_1,x_4,x_5\}}$, as $W_5 \not\subset G$. If $ux_2 \in E(G)$, then $u \in T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}}$, as $Z_1, K_4 - e \not\subset G$. If $ux_3 \in E(G)$, then $u \in T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_3,x_6,x_7\}}$, as $W_5 \not\subset G$. Now, we conclude that

$$T_3 = T_{\{x_1,x_4,x_5\}} \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_3,x_6,x_7\}}.$$

Since $Z_1, Z_3, K_4 - e \not\subset G$, we also have $|T_{\{x_i,x_j,x_k\}}| \leq 1$.

We proceed with the following facts.

(**F35**) If $u \in T_{x_1}$, then $uv \notin E(G)$ for $v \in T_{\{x_2,x_6\}} \cup T_{\{x_2,x_7\}} \cup T_{\{x_3,x_6\}} \cup T_{\{x_3,x_7\}} \cup T_{\{x_1,x_5\}} \cup T_{\{x_3,x_6,x_7\}}$, and $uv \in E(G)$ for $v \in T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_1,x_4,x_5\}}$, as $Z_1, Z_8 \not\subset G$;

(**F36**) If $u \in T_{x_2}$, then $uv \notin E(G)$ for $v \in T_2 \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}}$, and $uv \in E(G)$ for $v \in T_{\{x_3,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6,x_7\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_1,x_4,x_5\}}$, as $Z_1, Z_3, Z_8 \not\subset G$.

(**F37**) If $u \in T_{\{x_2,x_i\}}$ with $i \neq j$ and $\{i,j\} = \{6,7\}$, then $uv \notin E(G)$ for $v \in T_{\{x_2,x_j\}} \cup T_{\{x_3,x_i\}} \cup T_{\{x_2,x_5,x_i\}} \cup T_{\{x_3,x_4,x_i\}} \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6,x_7\}}$, and $uv \in E(G)$ for $v \in T_{\{x_3,x_j\}} \cup T_{\{x_1,x_5\}} \cup T_{\{x_3,x_4\}} \cup T_{\{x_3,x_4,x_j\}} \cup T_{\{x_2,x_5,x_j\}} \cup T_{\{x_1,x_4,x_5\}}$, as $Z_1, Z_8 \not\subset G$;

(**F38**) If $u \in T_{\{x_3,x_i\}}$ with $i \neq j$ and $\{i,j\} = \{6,7\}$, then $uv \notin E(G)$ for $v \in T_{\{x_3,x_j\}} \cup T_{\{x_2,x_5,x_i\}} \cup T_{\{x_1,x_5\}} \cup T_{\{x_3,x_4\}} \cup T_{\{x_3,x_4,x_i\}} \cup T_{\{x_3,x_6,x_7\}}$, and $uv \in E(G)$ for $v \in T_{\{x_2,x_5,x_j\}} \cup T_{\{x_3,x_4,x_j\}} \cup T_{\{x_1,x_4,x_5\}} \cup T_{\{x_2,x_5,x_6,x_7\}}$, as $Z_1, Z_8 \not\subset G$;

(**F39**) If $u \in T_{\{x_1,x_5\}}$, then $uv \notin E(G)$ for $v \in T_{\{x_3,x_4\}} \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}} \cup T_{\{x_1,x_4,x_5\}}$, and $uv \in E(G)$ for $v \in T_{\{x_3,x_6,x_7\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_2,x_5,x_6,x_7\}}$, as $Z_1, Z_3, Z_8, K_4 - e \not\subset G$;

(**F40**) If $u \in T_{\{x_3,x_4\}}$, then $uv \notin E(G)$ for $v \in T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}} \cup T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \cup T_{\{x_1,x_4,x_5\}}$, and $uv \in E(G)$ for $v \in T_{\{x_2,x_5,x_6,x_7\}} \cup T_{\{x_3,x_6,x_7\}}$, as $Z_1, Z_2 \not\subset G$;

(**F41**) If $u \in T_{\{x_2,x_5,x_i\}}$ with $i \neq j$ and $\{i,j\} = \{6,7\}$, then $uv \notin E(G)$ for $v \in T_{\{x_2,x_5,x_j\}} \cup T_{\{x_3,x_4,x_i\}} \cup T_{\{x_1,x_4,x_5\}} \cup T_{\{x_2,x_5,x_6,x_7\}}$, and $uv \in E(G)$ for $v \in T_{\{x_3,x_4,x_j\}} \cup T_{\{x_3,x_6,x_7\}}$, as $U_2^4, K_4 - e \not\subset G$.

If $u \in T_0$ and $uv \in E(G)$, then $v \notin T_1$ (as $U_2^4 \not\subset G$), $v \notin T_2$ (as $U_2^4 \not\subset G$), $v \notin T_3$ (as $Z_1, Z_2 \not\subset G$) and $v \notin T_4$ (as $Z_8 \not\subset G$). Hence, $T_0 = \emptyset$.

Case 1: $T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} = \emptyset$. Let $T_{\{x_1,x_4,x_5\}} = \{u_0\}$. Since $U_2^4, K_4 - e \not\subset G$ and there is no edge between u_0 and the unique vertex of T_4, u_0 must be adjacent to the unique vertex of $T_{\{x_3,x_6,x_7\}}$, while the vertex of T_4 is not adjacent to the unique vertex of $T_{\{x_3,x_6,x_7\}}$. Combining this with (*F*35)–(*F*41), we obtain $G \subset H_4$.

Case 2: $T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \neq \emptyset$. $T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_4,x_7\}} \neq \emptyset$. By symmetry, suppose that $u_0 \in T_{\{x_3,x_4,x_6\}} \neq \emptyset$. Since $W_5, K_4 - e \not\subset G$, we have $T_{\{x_1,x_4,x_5\}} = \emptyset = T_{\{x_3,x_4,x_7\}} = \emptyset$, and thus $T_3 \subset T_{\{x_3,x_4,x_6\}} \cup T_{\{x_3,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_2,x_5,x_7\}}$. Since the diamond is forbidden, u_0 is not adjacent to the vertex of $T_{\{x_3,x_6,x_7\}} \cup T_{\{x_2,x_5,x_6,x_7\}}$. Combining this with (*F*35)–(*F*41), we obtain $G \subset H_8$. ■

Proof of Lemma 5.10. We use W_8 as the base graph. Let $u \in T$. Since $K_4 - e$ and $K_4 \not\subset G$, u is adjacent to at most one vertex of the unique triangle and it cannot be adjacent to all vertices outside the triangle of W_8, and thus $|N_G(u) \cap V(W_8)| \leq 3$.

Since $U_2^4, Z_1, Z_2, Z_8, W_5 \not\subset G$, it holds $T_1 = T_{x_1} \cup T_{x_2} \cup T_{x_3}$, where $\max\{|T_{x_1}|, |T_{x_3}|\} \leq 1$ $|T_{x_2}| \leq 2$, and T_1 is an independent set of G.

Since $Z_1Z_8, K_4 - e, W_5, W_7 \not\subset G$, we have $T_2 = T_{\{x_1,x_5\}} \cup T_{\{x_2,x_5\}} \cup T_{\{x_2,x_6\}} \cup T_{\{x_3,x_6\}}$, where $|T_{\{x_i,x_j\}}| \leq 1$ for $\{i,j\} \in \{\{1,5\}, \{2,5\}, \{2,6\}, \{3,6\}\}$.

Since $Z_{18}, W_5, K_4 - e \not\subset G$, we have

$$T_3 = T_{\{x_1,x_4,x_5\}} \cup T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_4,x_6\}},$$

with $\max\{|T_{\{x_1,x_4,x_5\}}|, |T_{\{x_3,x_4,x_6\}}|\} \leq 1$ and $|T_{\{x_2,x_5,x_6\}}| \leq 2$. Since the diamond is forbidden, T_3 is an independent set of G.

If $u \in T_0$ with $uv \in E(G)$. Then, $v \notin T_1$ (as $U_2^4 \not\subset G$), $v \notin T_2$ (as $U_2^4 \not\subset G$) and $v \notin T_3$ (as $Z_8 \not\subset G$). Hence, $T_0 = \emptyset$.

We deduce the following facts.

(**F42**) If $u \in T_{x_1}$, then $uv \notin E(G)$ for $v \in T_{\{x_1,x_5\}} \cup T_{\{x_2,x_6\}} \cup T_{\{x_3,x_6\}}$ and $uv \in E(G)$ for $v \in T_{\{x_2,x_5\}} \cup T_3$, as $Z_1, Z_8 \not\subset G$;

(**F43**) Let $u \in T_{x_2}$ and $w \in T_{\{x_i,x_j\}} \cup T_{\{x_2,x_5,x_6\}}$, where $\{i,j\} \in \{\{1,5\}, \{3,6\}\}$. Since $Z_1, Z_3, Z_8, Z_{19}, W_5 \not\subset G$, we have the following: If $v \in T_{\{x_2,x_5\}} \cup T_{\{x_2,x_6\}}$, then $uv \notin E(G)$; If $v \in T_{\{x_1,x_4,x_5\}} \cup T_{\{x_3,x_4,x_6\}}$, then $uv \in E(G)$. Moreover, we also have $|T_{x_2}| - 1 \leq |N_{T_{x_2}}(w)| \leq 1$ and $|T_{\{x_2,x_5,x_6\}}| - 1 \leq |N_{T_{\{x_2,x_5,x_6\}}}(u)| \leq 1$;

(**F44**) If $u \in T_{x_3}$, then $uv \notin E(G)$ for $v \in T_{\{x_1,x_5\}} \cup T_{\{x_2,x_5\}} \cup T_{\{x_3,x_6\}}$ and $uv \in E(G)$ for $v \in T_3 \cup T_{\{x_2,x_6\}}$, as $Z_1, Z_8 \not\subset G$;

(**F45**) For $u \in T_{\{x_1,x_5\}}$, taking into account that $K_4 - e, Z_1, Z_2, Z_8 \not\subset G$, we obtain the following: If $v \in T_{\{x_2,x_5\}} \cup T_{\{x_1,x_4,x_5\}}$, then $uv \notin E(G)$; If $v \in T_{\{x_3,x_4,x_6\}} \cup T_{\{x_2,x_6\}}$, then $uv \in E(G)$. Moreover, we also have $|T_{\{x_2,x_5,x_6\}}| - 1 \leq |N_{T_{\{x_2,x_5,x_6\}}}(u)| \leq 1$;

(**F46**) If $u \in T_{\{x_2,x_5\}}$, then $uv \notin E(G)$ for $v \in T_{\{x_1,x_4,x_5\}} \cup T_{\{x_2,x_5,x_6\}}$ and $uv \in E(G)$ for $v \in T_{\{x_2,x_6\}} \cup T_{\{x_3,x_6\}} \cup T_{\{x_3,x_4,x_6\}}$, as $U_2^4, K_4 - e \not\subset G$.

(**F47**) If $u \in T_{\{x_2,x_6\}}$, then $uv \notin E(G)$ for $v \in T_{\{x_2,x_5,x_6\}} \cup T_{\{x_3,x_6\}} \cup T_{\{x_3,x_4,x_6\}}$ and $uv \in E(G)$ for $v \in T_{\{x_1,x_4,x_5\}}$, as $Z_8, U_2^4, K_4 - e \not\subset G$;

(**F48**) If $u \in T_{\{x_3,x_6\}}$, taking into account that $Z_2, Z_8, K_4 - e \not\subset G$, we obtain the following: If $v \in T_{\{x_3,x_4,x_6\}}$, then $uv \notin E(G)$; If $v \in T_{\{x_1,x_4,x_5\}}$, then $uv \in E(G)$. Moreover, we also have $|T_{\{x_2,x_5,x_6\}}| - 1 \leq |N_{T_{\{x_2,x_5,x_6\}}}(u)| \leq 1$;

(**F49**) Since $Z_1, Z_8, K_4 - e \not\subset G$, either $G[\{u,v,w\}] \cong 3K_1$ or $G[\{u,v,w\}] \cong P_3$ holds whenever $u \in T_{\{x_1,x_5\}}$, $v \in T_{x_2} \cup T_{\{x_2,x_5,x_6\}}$ and $w \in T_{\{x_3,x_6\}}$, or $u \in T_{\{x_1,x_5\}}$, $v \in T_{x_2}$ and $w \in T_{\{x_2,x_5,x_6\}}$, or $u \in T_{x_2}$, $v \in T_{\{x_2,x_5,x_6\}}$ and $w \in T_{\{x_3,x_6\}}$.

Since T_1 and T_3 are independent sets, the facts (*F*42)–(*F*48) tell us that the structure of G is determined by the structure of $G[S]$, where $S = T_{x_2} \cup T_{\{x_1,x_5\}} \cup T_{\{x_3,x_6\}} \cup T_{\{x_2,x_5,x_6\}}$.

We claim that $G[S] \subset W_{13} \cong H_9 - \{y_1\text{–}y_6\}$ or $G[S] \subset W_{14} \cong H_{12} - \{y_1\text{–}y_6\}$ (as a consequence, we will have $G \subset H_9 \cong D_7 - \{y_7\text{–}y_{12}, y_{14}\text{–}y_{16}\}$ or $G \subset H_{12} \cong D_7 - \{y_6\text{–}y_9, y_{11}\text{–}y_{17}\}$ as in the statement formulation). To prove this, we consider the following cases.

Case 1: $T_{\{x_2,x_5,x_6\}} \neq \emptyset$. If $u \in T_{\{x_3,x_6\}} \cup T_{\{x_1,x_5\}}$ and $v \in T_{\{x_2,x_5,x_6\}}$, then $uv \in E(G)$, as $W_7 \not\subset G$. Combining this with $(F49)$ and $W_5 \not\subset G$, we obtain $|T_{\{x_3,x_6\}} \cup T_{\{x_1,x_5\}}| \leq 1$. Since $W_5 \not\subset G$, $G[T_{\{x_2,x_5,x_6\}} \cup T_{x_2}]$ is an independent set of G.

If $|T_{\{x_2,x_5,x_6\}}| = 2$, then $T_{x_2} = \emptyset$ by $(F43)$, as $G[T_{\{x_2,x_5,x_6\}} \cup T_{x_2}]$ is an independent set of G. Similarly, we have $T_{\{x_3,x_6\}} \cup T_{\{x_1,x_5\}} = \emptyset$ by $(F45)$ and $(F48)$. Hence, $G[S] \subset W_{13}$.

Next, suppose that $|T_{\{x_2,x_5,x_6\}}| = 1$. Since $G[T_{\{x_2,x_5,x_6\}} \cup T_{x_2}]$ is an independent set of G, we have $|T_{x_2}| \leq 1$ by $(F43)$. Moreover, if $u \in T_{\{x_3,x_6\}} \cup T_{\{x_1,x_5\}} \neq \emptyset$ and $T_{x_2} \neq \emptyset$, then u is adjacent to each vertex of $T_{\{x_2,x_5,x_6\}} \cup T_{x_2}$ by $(F49)$, as $N_{T_{\{x_2,x_5,x_6\}}}(u) = T_{\{x_2,x_5,x_6\}}$. Now, since $|T_{\{x_3,x_6\}} \cup T_{\{x_1,x_5\}}| \leq 1$, we conclude that $G[S] \subset W_{13}$.

Case 2: $T_{\{x_2,x_5,x_6\}} = \emptyset$. If $|T_{\{x_1,x_5\}} \cup T_{\{x_3,x_6\}}| \leq 1$, then $G[S] \subset W_{13}$ by $(F43)$. Next, suppose that $|T_{\{x_1,x_5\}} \cup T_{\{x_3,x_6\}}| = 2$ with $u_0 \in T_{\{x_3,x_6\}}$ and $v_0 \in T_{\{x_1,x_5\}}$. If $u_0v_0 \notin E(G)$, then $G[S] \subset W_{13}$ by $(F49)$. Otherwise, $u_0v_0 \in E(G)$. From $(F43)$ and $(F49)$, we have $|N_G(w) \cap \{u_0, v_0\}| = 1$ for $w \in T_{x_2}$ and $N_{T_{x_2}}(u_0) \cap N_{T_{x_2}}(v_0) = \emptyset$, which implies $G[S] \subset W_{14}$. ■

Proof of Lemma 5.11. Since $H_{13} \cong D_7 - \{y_8, y_9, y_{12}\text{–}y_{17}\}$, it suffices to show that $G \subset H_{13}$. Since the diamond is forbidden, we have $T_3 = T_{\{x_1,x_4,x_5\}}$ and $|T_3| \leq 1$. Since $Z_1, Z_8, W_5, U^4_{1,1,1,1} \not\subset G$, we have $T_1 = T_{x_1} \cup T_{x_2} \cup T_{x_3}$, where $|T_{x_1}| \leq 1$, $\max\{|T_{x_2}|, |T_{x_3}|\} \leq 3$ and T_{x_i} is an independent set of G.

Since $K_4 - e, W_5, W_8, Z_9, Z_{11} \not\subset G$, it follows that $T_2 = T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}$, where $|T_{\{x_i,x_j\}}| \leq 3$ and $T_{\{x_i,x_j\}}$ is an independent set of G for $\{i,j\} \in \{\{3,4\},\{2,5\}\}$. Combining above arguments with $Z_7, Z_8 \not\subset G$, we obtain $T_0 = \emptyset$, and so $T = T_1 \cup T_2 \cup T_3$. If $u \in T_{\{x_1,x_4,x_5\}}$, then $N_{T_1}(u) = T_1$ and $N_{T_2}(u) = \emptyset$, as $Z_8, K_4 - e \not\subset G$. Combining this with $W_5, W_8 \not\subset G$, we obtain that if $T_{\{x_1,x_4,x_5\}} \neq \emptyset$, then $T_2 \cup T_1 = \emptyset$, and hence $G \subset H_{13}$. Thus, we may suppose that $T_{\{x_1,x_4,x_5\}} = \emptyset$.

(**F50**) If $u \in T_{x_1}$, then u is not adjacent to any other vertex of T_1, and u is adjacent to each vertex of T_2, as $U^4_2 \not\subset G$. Combining this with $W_8 \not\subset G$, we conclude that either $T_{x_1} = \emptyset$ or $T_2 = \emptyset$;

(**F51**) Let $u \in T_{\{x_i,x_j\}}$, and $v \in T_{x_k}$ with $i < j$ and $k \in \{2,3\}$. Since $W_5, Z_1, Z_2, Z_3, Z_{10}, Z_{16}, Z_{17}, U^4_{1,1,1,1} \not\subset G$, we have the following: If $k = i$, then $uv \notin E(G)$ and $|T_{\{x_i,x_j\}} \cup T_{x_k}| \leq 3$; If $k \neq i$, then $|T_{\{x_i,x_j\}}| - 1 \leq |N_{T_{\{x_i,x_j\}}}(v)| \leq 2$, $|T_{x_k}| - 1 \leq |N_{T_{x_k}}(u)| \leq 2$ and $G[\{u_1, u_2, v_1, v_2\}] \in \{2K_2, P_4\}$ for $u_1, u_2 \in T_{\{x_i,x_j\}}$, $v_1, v_2 \in T_{x_k}$; If $k \neq i$ and $N_{T_{\{x_i,x_j\}}}(v) = \{u_1, u_2\}$, then $|N_G(w) \cap \{u_1, u_2\}| = 1$ for $w \in T_{\{x_k,x_s\}}$, where $\{\{i,j\},\{k,s\}\} = \{\{2,5\},\{3,4\}\}$; If $k \notin \{i,j\}$ and $N_{T_{x_i}}(w) = \{u_1, u_2\}$, then $N_{T_{\{x_i,x_j\}}}(w) = T_{\{x_i,x_j\}}$ for $w \in T_{\{x_k,x_s\}}$, where $\{\{i,j\},\{k,s\}\} = \{\{2,5\},\{3,4\}\}$;

(**F52**) Since $Z_1, Z_2, Z_3, Z_{10} \not\subset G$, we have: For either $S \subset T_{x_2} \cup T_{x_3}$ or $S \subset T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}$, if $G[S]$ is an independent set of G, then $|S| \leq 3$; For $\{i,j\} = \{2,3\}$, if $u \in T_{x_i}$, then $|N_{T_{x_j}}(u)| \leq 1$; For $\{\{i,j\},\{s,t\}\} = \{\{2,5\},\{3,4\}\}$, if $u \in T_{\{x_i,x_j\}}$, then $|N_{T_{\{x_s,x_t\}}}(u)| \leq 1$; For $\{\{i,j\},\{s,t\}\} = \{\{2,5\},\{3,4\}\}$, if $v \in T_{x_i}$, $u \in T_{\{x_i,x_j\}}$, $w \in T_{\{x_s,x_t\}}$ and $uw \in E(G)$, then $vw \in E(G)$, as $uv \notin E(G)$ by $(F51)$; For $\{\{i,j\},\{s,t\}\} = \{\{2,5\},\{3,4\}\}$, if $2 \leq |T_{\{x_i,x_j\}}| \leq 3$, $u \in T_{\{x_s,x_t\}}$ and $v \in T_{x_i}$ with $uv \in E(G)$, then $|N_{T_{\{x_i,x_j\}}}(u)| = 1$;

(**F53**) Suppose that $u \in T_{x_i}$, $v \in T_{x_j}$, $w \in T_{\{x_i,x_s\}}$, where $(i,j,s) \in \{(2,3,5),(3,2,4)\}$. From $Z_1, Z_2, Z_3 \not\subset G$, $(F51)$ and $(F52)$, we obtain that $uv \in E(G)$ implies $vw \in E(G)$; Similarly, if $uv \notin E(G)$ and $|T_{\{x_i,x_s\}}| \geq 2$, then $|N_{T_{\{x_i,x_s\}}}(v)| = |T_{\{x_i,x_s\}}| - 1 = 1$; If $N_{T_{x_j}}(w) = \{v_1, v_2\}$, then $|N_G(u) \cap \{v_1, v_2\}| = 1$; Finally, if $\{u_1, u_2\} \cap N_G(v) = \emptyset$ for $\{u_1, u_2\} \subseteq T_{x_i}$, then $vw \notin E(G)$;

(**F54**) Suppose that $u \in T_{x_2}$, $v \in T_{x_3}$, $w \in T_{\{x_3,x_4\}}$ and $z \in T_{\{x_2,x_5\}}$. If $uw \in E(G)$ and $vz \in E(G)$, then either $wz \in E(G)$ or $uv \in E(G)$, as $Z_1 \not\subset G$.

By symmetry, we suppose that $|T_{\{x_2,x_5\}}| \geq |T_{\{x_3,x_4\}}|$ and consider the following cases.

Case 1: $|T_{\{x_2,x_5\}}| = 3$. From $(F50)$, $(F51)$ and $|T_{\{x_2,x_5\}} \cup T_{x_2}| \leq 3$, we have $T_{x_2} = T_{x_1} = \emptyset$.

If $|T_{\{x_3,x_4\}}| = 3$, then $T_{x_3} = \emptyset$ by $(F51)$, and so $G \subset H_{13}$ by $(F52)$.

If $|T_{\{x_3,x_4\}}| = 2$, then $|T_{x_3}| \leq 1$ and $T_{\{x_3,x_4\}} \cup T_{x_3}$ is an independent set of G by $(F51)$. By $(F52)$, we have $G[T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}] \cong 2K_2 \cup K_1$, and thus $G \subset H_{13}$ by $(F51)$ and $(F52)$.

If $|T_{\{x_3,x_4\}}| = 1$, then $|T_{x_3}| \leq 2$ and $T_{\{x_3,x_4\}} \cup T_{x_3}$ is an independent set of G by $(F51)$. From $(F52)$, we have $G[T_{\{x_2,x_5\}} \cup T_{\{x_3,x_4\}}] \cong K_2 \cup 2K_1$, and thus $G \subset H_{13}$ by $(F51)$ and $(F52)$.

If $|T_{\{x_3,x_4\}}| = 0$, then $|T_{x_3}| \leq 3$, and thus $G \subset H_{13}$ by $(F51)$.

Case 2: $|T_{\{x_2,x_5\}}| = 2$. From $(F50)$, we have $T_{x_1} = \emptyset$. From $(F51)$, we have $|T_{x_i} \cup T_{\{x_i,x_j\}}| \leq 3$ and $T_{\{x_i,x_j\}} \cup T_{x_i}$ is an independent set of G, where $(i,j) \in \{(3,4),(2,5)\}$.

If $|T_{\{x_3,x_4\}}| = 2$, then $G[T_2] \cong 2K_2$ or $G[T_2] \cong K_2 \cup 2K_1$ by $(F52)$. From $(F51)$, we also have $\max\{|T_{x_2}|, |T_{x_3}|\} \leq 1$. For $G[T_2] \cong 2K_2$, we deduce that $G \subset H_{13}$ by $(F52)$ and $(F53)$. For $G[T_2] \cong K_2 \cup 2K_1$, we deduce that $G \subset H_{13}$ by $(F51)$, $(F52)$ and $(F53)$.

If $|T_{\{x_3,x_4\}}| = 1$, then $G[T_2] \cong 3K_1$ or $G[T_2] \cong K_2 \cup K_1$ by $(F52)$. From $(F51)$, we have $|T_{x_2}| \leq 1$ and $|T_{x_3}| \leq 2$. For $G[T_2] \cong K_2 \cup K_1$, we deduce that $G \subset H_{13}$ by $(F51)$–$(F54)$. For $G[T_2] \cong 3K_1$, we have $|N_{T_{\{x_2,x_5\}}}(u)| = 1$ and $uv \notin E(G)$ whenever $u \in T_{x_3}$ and $v \in T_{x_2}$ by $(F51)$ and $(F53)$. Combining this with $(F54)$, we obtain $vw \notin E(G)$ for $v \in T_{x_2}$ and $w \in T_{\{x_3,x_4\}}$. From $(F51)$ and $(F52)$, we deduce that $G \subset H_{13}$.

If $|T_{\{x_3,x_4\}}| = 0$, then $|T_{x_2}| \leq 1$ and $|T_{x_3}| \leq 3$. If $uv \in E(G)$ for two vertices $u \in T_{x_2}$ and $v \in T_{x_3}$, then we have $N_{T_{\{x_2,x_5\}}}(v) = T_{\{x_2,x_5\}}$ and $N_{T_{x_3}}(u) = \{v\}$ by $(F52)$ and $(F53)$. Combining this with $(F51)$, we obtain $G \subset H_{13}$. If $uv \notin E(G)$ for any two vertices $u \in T_{x_2}$ and $v \in T_{x_3}$, we have $|T_{x_2} \cup T_{x_3}| \leq 3$ by $(F52)$. Taking into account $(F51)$ and $(F53)$, we obtain $G \subset H_{13}$.

Case 3: $|T_{\{x_2,x_5\}}| = 1$. Then $T_{x_1} = \emptyset$ and $|T_{x_2}| \leq 2$.

If $|T_{\{x_3,x_4\}}| = 1$, then $G[T_2] \cong K_2$ or $G[T_2] \cong 2K_1$. From $(F51)$, we have $|T_{x_3}| \leq 2$. If $G[T_2] \cong K_2$, then $N_{T_{x_i}}(u) = T_{x_i}$ for $u \in T_{\{x_j,x_k\}}$ by $(F52)$, where $(i,j,k) \in \{(2,3,5),(3,2,4)\}$. From $(F52)$ and $(F53)$, we have $G \subset H_{13}$. If $G[T_2] \cong 2K_1$ and $uv \in E(G)$ for two vertices $u \in T_{x_2}$ and $v \in T_{x_3}$, then $G \subset H_{13}$ by $(F51)$–$(F54)$. If $G[T_2] \cong 2K_1$ and $uv \notin E(G)$ for any two vertices $u \in T_{x_2}$, $v \in T_{x_3}$, then $\min\{|T_{x_2}|, |T_{x_3}|\} \leq 1$ and $G \subset H_{13}$ by $(F51)$–$(F54)$.

If $|T_{\{x_3,x_4\}}| = 0$, then $|T_{x_3}| \leq 3$. From $(F51)$–$(F53)$, we have $G \subset H_{13}$.

Case 4: $|T_{\{x_2,x_5\}}| = 0$. Then $|T_{\{x_3,x_4\}}| = 0$. Taking into account $(F50)$, we may neglect T_{x_1}. By symmetry, suppose that $|T_{x_2}| \geq |T_{x_3}|$.

If $|T_{x_2}| = 2$ and $|T_{x_3}| = 2$, then $G[T_{x_2} \cup T_{x_3}] \cong 2K_2$ or $G[T_{x_2} \cup T_{x_3}] \cong K_2 \cup 2K_1$ by $(F52)$. This implies $G \subset H_{13}$.

From $(F52)$, we also have $G \subset H_{13}$ whenever $|T_{x_2}| = 3$ or $|T_{x_2}| \leq 2$ and $|T_{x_3}| \leq 1$. This concludes the entire proof. ■

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The A_α-spectral radius of dense graphs

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ABSTRACT

A c-cyclic graph is a connected graph with n vertices and $n+c-1$ edges. In this paper, we consider the problem that: in the class of graphs, each of which is the complement graph of a c-cyclic graph with n vertices, which graph has the largest A_α-spectral radius. We shall show that, for $0 \leq c \leq n-4$, the extremal graph must be a graph with an isolated vertex. This implies that the maximum degree of G is larger, then the A_α-spectral radius of its complement graph is also larger. We also determine the structure of the extremal graph with largest A_α-spectral radius among the class of graphs, each of which is the complement graph of a c-cyclic graph with n vertices and maximum degree $n-1$ for $0 \leq c \leq n-3$ and $n-2$ for $0 \leq c \leq n-4$, respectively.

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1. Introduction

Throughout this paper, we only concern with simple undirected graphs. Let $G = (V, E)$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, and let $N_G(v_i)$ and $d_G(v_i)$ be the neighbour set and degree of vertex v_i of G, respectively. A vertex of degree 1 will be referred as a *pendent vertex* of G. Denote by $\delta(G)$ and $\Delta(G)$ the minimum degree and maximum degree of G, respectively. We use $\overline{G}$ to denote the complement graph of a graph G. Let $A(G)$ and $D(G)$ be the adjacency matrix and diagonal matrix of graph G, respectively. Then, $Q(G) = D(G) + A(G)$ and $L(G) = D(G) - A(G)$ are called the signless Laplacian matrix and Laplacian matrix of G, respectively. In 2017, to merge the A-spectral and Q-spectral theories, Nikiforov [1] put forward the notation of *A_α-matrix* $A_\alpha(G)$ for a graph G, where $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$ and $\alpha \in [0, 1]$. Let $\rho_\alpha(G)$ be the maximum eigenvalue of $A_\alpha(G)$ and we call $\rho_\alpha(G)$ the *A_α-spectral radius* of G. Especially, $\rho(G) = \rho_0(G)$ is equal to the spectral radius (maximum eigenvalue) of $A(G)$. In what follows, if G has the maximum A_α-spectral radius among all graphs of a given graph category $\mathcal{G}$, then we call G as a *ρ_α-maximal graph* of $\mathcal{G}$.

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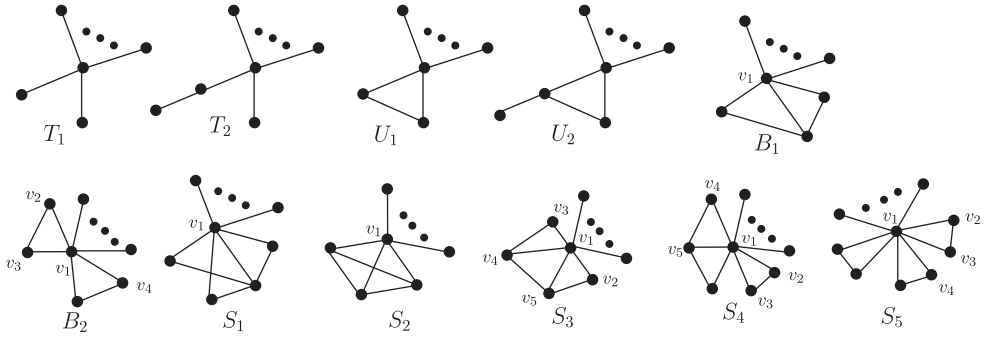


Figure 1. The graphs $T_1, T_2, U_1, U_2, B_1, B_2, S_1, S_2, \ldots, S_5$ with n vertices.

As usual, let K_n, C_n, P_n and $K_{1,n-1}$ be the complete graph, cycle, path and star with n vertices, respectively. Let $G = G_1 \vee G_2$ be the *join graph* of two vertex disjoint graphs G_1 and G_2, that is, $V(G) = V(G_1) \cup V(G_2)$ and $E(G) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1)$ and $v \in V(G_2)\}$. Let $T_1, T_2, U_1, U_2, B_1, B_2, S_1, S_2, \ldots, S_5$ be the 11 graphs with n vertices as shown in Figure 1, and let $\overline{\mathbb{G}}(n; c)$ be the class of graphs, each of which is the complement graph of a c-cyclic graph with n vertices, that is,

$$\overline{\mathbb{G}}(n; c) = \{\overline{G} : G \text{ is a } c-\text{cyclic graph with } n \text{ vertices}\}.$$

Denoted by $\overline{\mathbb{G}}(n, k; c)$ the class of graphs, each of which is the complement graph of a c-cyclic graph with n vertices and maximum degree k, that is,

$$\overline{\mathbb{G}}(n, k; c) = \{\overline{G} : G \text{ is a } c-\text{cyclic graph with } n \text{ vertices and maximum degree } k\}.$$

As early as in 1981, Cvetković [2] indicated 12 directions in further investigations of graph spectra, one of which is 'classifying and ordering graphs'. Hence ordering graphs with various properties by their spectra becomes an attractive topic (see [3–5]). In this direction, scholars mainly study the ordering problem of (signless Laplacian) spectral radius and Laplacian spectral radius of trees, unicyclic graphs, bicyclic graphs and/or tricyclic graphs [3–6]. Later, the Majorization theorem and Scale theorem of (signless Laplacian) spectral radius and Laplacian spectral radius (see the fifth section of [6] and [7–9]) are shown to be two effective tools to deal with the ordering problem of (signless Laplacian) spectral radius and Laplacian spectral radius of trees, unicyclic graphs, bicyclic graphs and/or tricyclic graphs.

Note that trees, unicyclic graphs, bicyclic graphs and tricyclic graphs are sparse graphs. Thus it is natural for us to consider the ordering problem of dense graphs. Recently, motivated from this problem, some scholars pay attention to the ordering problem of the spectral radius of the complement graphs of trees, unicyclic graphs, bicyclic graphs and tricyclic graphs [10–12], their results are as follows:

Theorem 1.1: *Let $\overline{G}$ be a ρ-maximal graph of $\overline{\mathbb{G}}(n; c)$.*

(1) [10] *If $c = 1$, then $G = U_1$;*
(2) [11] *If $c = 2$ and $n \geq 5$, then $G = B_1$;*

(3) [12] *If* $c = 3$ *and* $n \geq 8$, *then* $G = S_1$.

Later, the unique ρ_α-maximal graph in the class of complement graphs of trees, unicyclic graphs and bicyclic graphs is determined respectively, in [13], that is,

Theorem 1.2 ([13]): *Let* $0 \leq \alpha < 1$ *and let* $\overline{G}$ *be a* ρ_α*-maximal graph of* $\overline{\mathbb{G}}(n; c)$.

(1) *If* $c = 0$, *then* $G = K_{1,n-1}$;
(2) *If* $c = 1$, *then* $G = U_1$;
(3) *If* $c = 2$ *and* $n \geq 5$, *then* $G = B_1$.

One can easily see that Theorem 1.2(2)–(3) extend the corresponding results of Theorem 1.1(1)–(2). By Theorem 1.1, for the ρ-maximal graph $\overline{G}$ in the class of complement graphs of trees, unicyclic graphs, bicyclic graphs and tricyclic graphs with n vertices, the maximum degree of G is equal to $n-1$. In this paper, we shall prove the following much more general result:

Theorem 1.3: *Let* $0 \leq \alpha < 1$ *and let* $\overline{G}$ *be a* ρ_α*-maximal graph of* $\overline{\mathbb{G}}(n; c)$. *If* $0 \leq c \leq n - 4$, *then* $\Delta(G) = n - 1$.

Theorem 1.3 implies the close relation between the eigenvalue of graph G and the maximum degree of its complement graph. One can easily check that Theorem 1.3 is a consequence of the following result:

Theorem 1.4: *Let* $0 \leq \alpha < 1$, *and let* $\overline{G_1}$ *and* $\overline{G_2}$ *be a* ρ_α*-maximal graph of* $\overline{\mathbb{G}}(n, s; c)$ *and* $\overline{\mathbb{G}}(n, t; c)$, *respectively. If* $0 \leq c \leq n - 4$ *and* $2 \leq s < t \leq n - 1$, *then* $\rho_\alpha(\overline{G_2}) > \rho_\alpha(\overline{G_1})$.

If G has no $2K_2$, P_4 or C_4 as an induced subgraph, then G is called a *split graph* (see [14]). From Theorem 1.3 (or Theorem 1.4), the ρ_α-maximal graph of $\overline{\mathbb{G}}(n; c)$ must be a graph, whose complement graph is a c-cyclic graph with maximum degree $n-1$. The next theorem will identify the structure of the ρ_α-maximal graph of $\overline{\mathbb{G}}(n, n - 1; c)$.

Theorem 1.5: *Let* $\overline{G}$ *be a* ρ_α*-maximal graph of* $\overline{\mathbb{G}}(n, n - 1; c)$ *with* $d_G(w_0) = n - 1$ *and let* $W_0 = V(G) \setminus \{w_0\}$. *If* $0 \leq c \leq n - 3$ *and* $0 \leq \alpha < 1$, *then* Z_0 *is the unique component of* $G[W_0]$ *containing at least two vertices and* Z_0 *is a split graph with* c *edges. Furthermore,* Z_0 *contains a vertex* y *such that* $d_{Z_0}(y) = |Z_0| - 1$.

By Theorem 1.4, the second ρ_α-maximal graph of $\overline{\mathbb{G}}(n; c)$ is either the ρ_α-maximal graph of $\overline{\mathbb{G}}(n, n - 2; c)$ or a graph of $\overline{\mathbb{G}}(n, n - 1; c)$. Thus it is interesting to determine the structure of the ρ_α-maximal graph of $\overline{\mathbb{G}}(n, n - 2; c)$. For this, we raise the following result:

Theorem 1.6: *Let* $\overline{G}$ *be a* ρ_α*-maximal graph of* $\overline{\mathbb{G}}(n, n - 2; c)$ *with* $d_G(u_0) = n - 2$ *and* $u_0v_0 \notin E(G)$ *and let* $S_0 = V(G) \setminus \{u_0\}$. *If* $0 \leq c \leq n - 4$ *and* $0 \leq \alpha < 1$, *then* H_0 *is the unique component of* $G[S_0]$ *containing at least two vertices and* H_0 *is a split graph with* $c + 1$ *edges. Furthermore, if* $d_{H_0}(v_0) \geq 2$, *then* x *is adjacent to every vertex of* $V(H_0)$ *for each vertex* $x \in N_{H_0}(v_0)$.

Since T_1 and U_1 are, respectively, the unique tree and unicyclic graph with n vertices and maximum degree $n-1$, it is easily checked that (1) and (2) of Theorem 1.2 follow from Theorem 1.3 straightly. Furthermore, since K_2 and P_3 are, respectively, the unique connected graph with one and two edges, from Theorems 1.4 and 1.6, we have

Corollary 1.1: *Let $0 \le \alpha < 1$ and $n \ge 4$.*

(1) *If $\overline{G} \in \overline{\mathbb{G}}(n;0) \setminus \{\overline{T_1}, \overline{T_2}\}$, then $\rho_\alpha(\overline{G}) < \rho_\alpha(\overline{T_2}) < \rho_\alpha(\overline{T_1})$;*
(2) *If $\overline{G} \in \overline{\mathbb{G}}(n;1) \setminus \{\overline{U_1}, \overline{U_2}\}$, then $\rho_\alpha(\overline{G}) < \rho_\alpha(\overline{U_2}) < \rho_\alpha(\overline{U_1})$.*

Note that B_1 and B_2 are all bicyclic graphs with n vertices and maximum degree $n-1$. Thus Theorem 1.2(3) follows from Theorems 1.3 and 1.5. For the case of $c = 3$, we have

Corollary 1.2: *Let $0 \le \alpha < 1$, $n \ge 7$ and let $\overline{G}$ be a ρ_α-maximal graph of $\overline{\mathbb{G}}(n;3)$.*

(1) *If $0 \le \alpha < 0.5$, then $G = S_1$;*
(2) *If $\alpha = 0.5$, then $G \in \{S_1, S_2\}$ and $\rho_{0.5}(\overline{S_1}) = \rho_{0.5}(\overline{S_2})$;*
(3) *If $0.5 < \alpha < 1$, then $G = S_2$.*

2. The proofs of Theorems 1.4 and 1.6

For the maximum eigenvalue of an irreducible nonnegative matrix, it is well known that

Lemma 2.1 ([15]): *Let M be an $n \times n$ irreducible non-negative matrix with maximum eigenvalue $\theta(M)$, and let $R_i(M)$ be the ith row sum of M. Then,*

$$\min\{R_i(M) : 1 \le i \le n\} \le \theta(M) \le \max\{R_i(M) : 1 \le i \le n\},$$

with either equality holding if and only if all row sums of M are equal.

When G is connected, by the Perron–Frobenius Theorem of non-negative matrices, $\rho_\alpha(G)$ has a unique positive unit eigenvector [1,15]. In this paper, we use $\mathbf{f} = (f(v_1), \ldots, f(v_n))^T$ to indicate this special eigenvector corresponding to $\rho_\alpha(G)$, and call $\mathbf{f}$ the *Perron vector* of G.

Lemma 2.2 ([13]): *Let $0 \le \alpha < 1$ and let $\overline{G}$ be the complement graph of a graph G such that $\overline{G}$ is connected and $\{u, v\} \subset V(G)$. Suppose that $vw_i \notin E(G)$ and $uw_i \in E(G)$ for $i \in \{1, 2, \ldots, k\}$ and $\mathbf{f}$ is the Perron vector of $\overline{G}$. Let*

$$G^* = G + vw_1 + vw_2 + \cdots + vw_s - uw_1 - uw_2 - \cdots - uw_s,$$

where $1 \le s \le k$. If $f(u) \ge f(v)$, then $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G})$.

Lemma 2.3: *Let $0 \le \alpha < 1$ and let $\overline{G}$ be a graph of $\overline{\mathbb{G}}(n;c)$. If $0 \le c \le n-4$ and $\Delta(G) \le n-2$, then $\overline{G}$ is connected.*

Proof: By contradiction, we assume that $\overline{G}$ is disconnected, then $G = G_1 \vee G_2$. Since $\Delta(G) \le n-2$, $|V(G_1)| \ge |V(G_2)| \ge 2$. This implies that G contains at least $|V(G_1)| \cdot$

$|V(G_2)| \geq 2(n-2)$ edges, that is, $n+c-1 = |E(G)| \geq 2(n-2)$, contrary with $0 \leq c \leq n-4$. ■

Lemma 2.4: *Let $0 \leq \alpha < 1$ and let $\overline{G}$ be a ρ_α-maximal graph of $\overline{\mathbb{G}}(n,k;c)$, where $0 \leq c \leq n-4$ and $k \leq n-2$. Let u and v be two vertices of G and let $\mathbf{f}$ be the Perron vector of $\overline{G}$. If $d_{\overline{G}}(u) < d_{\overline{G}}(v)$, then $f(u) < f(v)$.*

Proof: By contradiction, assume that $d_{\overline{G}}(u) < d_{\overline{G}}(v)$ and $f(u) \geq f(v)$. Combining $\overline{G} \in \overline{\mathbb{G}}(n,k;c)$ with $k \leq n-2$ and Lemma 2.3, G is a c-cyclic graph and $\overline{G}$ is connected.

Let P be a shortest path of G connected vertices u and v. Since $d_{\overline{G}}(u) < d_{\overline{G}}(v)$, we have $d_G(v) < d_G(u)$. By the choice of P and since $d_G(v) < d_G(u)$, there exists vertex set $\{w_1, w_2, \ldots, w_s\} \subseteq N_G(u) \setminus N_G(v)$ such that $\{w_1, w_2, \ldots, w_s\} \cap V(P) = \emptyset$, where $s = d_G(u) - d_G(v)$. Let $G^* = G + vw_1 + vw_2 + \cdots + vw_s - uw_1 - uw_2 - \cdots - uw_s$. Then, G^* is also a c-cyclic graph. By Lemma 2.2, $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G})$. Furthermore, since the degree sequences of G^* and G are the same, $\Delta(G^*) = \Delta(G) = k \leq n-2$, contrary with the choice of $\overline{G}$. ■

Lemma 2.5: *Let $0 \leq \alpha < 1$ and let $\overline{G}$ be a graph of $\overline{\mathbb{G}}(n,k;c)$, where $0 \leq c \leq n-4$. If $k \leq n-2$, then there exists a graph $\overline{G^*}$ of $\overline{\mathbb{G}}(n,k+1;c)$ such that $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G})$.*

Proof: We may suppose that $\overline{G}$ is a ρ_α-maximal graph of $\overline{\mathbb{G}}(n,k;c)$. Since $k \leq n-2$, $\overline{G}$ is connected by Lemma 2.3. Let $\mathbf{f}$ be the Perron vector of $\overline{G}$, and let $u \in V(\overline{G})$ with $f(u) = \min\{f(x) : x \in V(\overline{G})\}$. By Lemma 2.4, $d_{\overline{G}}(u) = \delta(\overline{G})$ and $d_G(u) = \Delta(G)$, where G is a c-cyclic graph.

Since $\Delta(G) \leq n-2$, there exists two vertices v, w such that $v \in N_G(u)$, $w \in N_G(v)$, and $w \notin N_G(u)$. Let $G^* = G + uw - vw$. Then, G^* is connected and thus it is a c-cyclic graph with $\Delta(G^*) = \Delta(G) + 1$. Since $f(u) \leq f(v)$, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G})$ by Lemma 2.2. This completes the proof of this result. ■

Proof of Theorem 1.4: By Lemma 2.5, Theorem 1.4 holds. ■

In the rest of this section, let $0 \leq \alpha < 1$, $0 \leq c \leq n-4$ *and* $\overline{G_0}$ *be a ρ_α-maximal graph of* $\overline{\mathbb{G}}(n,n-2;c)$. Suppose that $d_{\overline{G_0}}(u_0) = 1$ and $S_0 = V(\overline{G_0}) \setminus \{u_0\}$. Let $v_0 \in V(\overline{G_0})$ such that $u_0v_0 \in E(\overline{G_0})$. By Lemma 2.3, $\overline{G_0}[S_0]$ is a connected graph obtained from K_{n-1} by deleting $c+1$ edges and $G_0[S_0]$ is a graph with $n-1$ vertices and $c+1$ edges, as $d_{G_0}(u_0) = n-2 = \Delta(G_0)$.

Lemma 2.6: *If u_0 is not the unique vertex of G_0 with degree $n-2$, then Theorem 1.6 holds.*

Proof: Suppose that $d_{G_0}(u_0) = n-2 = d_{G_0}(w_0)$. Then, $|E(G_0)| \geq 2(n-2)-1$, with equality implying that $u_0w_0 \in E(G_0)$. Since $0 \leq c \leq n-4$, we have $|E(G_0)| = n+c-1 \leq 2(n-2)-1$, and thus $c = n-4$ and $|E(G_0)| = 2n-5$. In this case, we may suppose that $w_0x \notin E(G_0)$ and $u_0w_0 \in E(G_0)$, which follows that $v_0 \neq w_0$. If $x = v_0$, then both u_0 and w_0 are adjacent to all vertices of $V(G_0) \setminus \{u_0, w_0, v_0\}$ and $u_0w_0 \in E(G_0)$. Combining this with G_0 being connected, we have $|E(G_0)| \geq 2n-4$, a contradiction. Thus $x \neq v_0$. Now, we can conclude that $\{u_0, v_0, w_0, x\}$ are four different vertices of G_0.

Since $d_{G_0}(u_0) = n-2 = d_{G_0}(w_0)$, it follows that $v_0w_0 \in E(\overline{G_0})$, $u_0x \in E(G_0)$, $u_0w_0 \in E(G_0)$, and $y \in N_{G_0}(u_0) \cap N_{G_0}(w_0)$ holds for each vertex $y \in V(\overline{G_0}) \setminus \{u_0, v_0, w_0, x\}$. Combining this with $|E(G_0)| = 2n-5$, we can conclude that $\{v_0, x\}$ are two pendent vertices of G_0 and $d_{G_0}(y) = 2$ holds for each vertex $y \in V(\overline{G_0}) \setminus \{u_0, v_0, w_0, x\}$. Now, $G_0[S_0] = K_{1,c+1} \cup K_1$ and v_0 is a pendent vertex of $K_{1,c+1}$. This implies that Theorem 1.6 holds. ■

By Lemma 2.6, we may suppose that

$$u_0 \text{ is the unique vertex of } G_0 \text{ with degree } n-2 \tag{1}$$

in the rest of this section. By Lemma 2.3 and $0 \le c \le n-4$, $\overline{G_0}$ is connected and let $\mathbf{g} = (g(v_1), g(v_2), \ldots, g(v_n))^T$ be the Perron vector of $\overline{G_0}$ in the following.

Lemma 2.7: *If $0 \le c \le n-4$, then $G_0[S_0]$ contains exactly one component with at least two vertices.*

Proof: By contradiction, we assume that H_1 and H_2 are two components of $G_0[S_0]$ with at least two vertices. Let u_iw_i be an edge of H_i for $i \in \{1,2\}$ such that $v_0 \notin \{u_1, u_2\}$. Since $d_{G_0}(u_0) = n-2$, u_0 is adjacent to each vertex of $V(G_0) \setminus \{u_0, v_0\}$ in G_0, and hence u_0 is adjacent to the vertices $\{u_1, u_2\}$.

Recall that $\mathbf{g}$ is the Perron vector of $\overline{G_0}$. By the symmetry of u_1 and u_2, suppose that $g(u_2) \ge g(u_1)$. Let $G^* = G_0 - u_2w_2 + u_1w_2$. From Lemma 2.2, it follows that $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$. Combining $G^* = G_0 - u_2w_2 + u_1w_2$ with $\{u_1, u_2\} \subseteq N_{G_0}(u_0)$, we can conclude that G^* is also connected, and thus it is a c-cyclic graph. By (1) and since $d_{G^*}(u_0) = d_G(u_0) = n-2$, we have $\overline{G^*} \in \overline{\mathbb{G}}(n, n-2; c)$, contrary with the choice of $\overline{G_0}$. ■

From Lemma 2.7, $G_0[S_0]$ contains exactly one component with at least two vertices. In the rest of section, let H_0 *denote this unique component of* $G_0[S_0]$.

Lemma 2.8: *If $d_{H_0}(v_0) \ge 2$, then x is adjacent to every vertex of H_0 for each vertex $x \in N_{H_0}(v_0)$.*

Proof: Since $d_{G_0}(v_0) \le n-3 < n-2 = d_{G_0}(u_0)$ by (1), $d_{\overline{G_0}}(v_0) \ge 2 > 1 = d_{\overline{G_0}}(u_0)$. We first show that

$$g(v_0) = \max\{g(x) : x \in V(H_0)\}, \tag{2}$$

where $\mathbf{g}$ is the Perron vector of $\overline{G_0}$.

We assume (2) does not hold. Then, there is another vertex of H_0, say w_0, such that $g(w_0) > g(v_0)$. Since H_0 is connected and H_0 is the component of $G_0[S_0]$, u_0 is not in a path P, which is connected v_0 and w_0 in H_0. Since $u_0w_0 \in E(G_0)$ and $u_0v_0 \notin E(G_0)$, we denote by $G^* = G_0 + u_0v_0 - u_0w_0$. Then, G^* is connected. By (1), G^* is a c-cyclic graph with $\Delta(G^*) = n-2$. Since $g(w_0) > g(v_0)$ and Lemma 2.2, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$, a contradiction. This completes the proof of (2).

To complete the proof, it suffices to show that x is adjacent to every vertex of H_0 for each vertex $x \in N_{H_0}(v_0)$ in the case $d_{H_0}(v_0) \ge 2$. By contradiction, assume that $x_0y \notin E(H_0)$ for some vertex $x_0 \in N_{H_0}(v_0)$ and $y \in V(H_0)$. Let $G^* = G_0 + x_0y - v_0x_0$. Since v_0 contains at least two neighbour vertices adjacent to u_0 and u_0 is adjacent to all vertices of $V(G_0) \setminus$

$\{u_0, v_0\}$ in G_0, G^* is connected. Moreover, by (1), we can conclude that G^* is a c-cyclic graph with $\Delta(G^*) = n-2$. Since $g(v_0) \geq g(y)$ by (2), we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$ by Lemma 2.2, a contradiction. This completes the proof of this result. ■

Proof of Theorem 1.6: By Lemmas 2.6–2.8, to complete the proof of Theorem 1.6, it suffices to show that H_0 is a split graph. Recall that $\mathbf{g} = (g(v_1), g(v_2), \ldots, g(v_n))^T$ is the Perron vector of $\overline{G_0}$.

Assume H_0 has $2K_2$ as an induced subgraph. Let u_1u_2 and w_1w_2 be the two independent edges of $2K_2$. We may suppose that $v_0 \notin \{u_1, w_1\}$ and then we suppose that $g(u_1) \geq g(w_1)$ by the symmetry of u_1 and w_1. Let $G^* = G_0 + u_2w_1 - u_1u_2$. Since $v_0 \notin \{u_1, w_1\}$ and (1), G^* is a c-cyclic graph with $\Delta(G^*) = n-2$. By Lemma 2.2, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$, a contradiction.

Assume H_0 has C_4 as an induced subgraph, where $C_4 := u_1w_1u_2w_2u_1$. By Lemma 2.8, $v_0 \notin \{u_1, u_2, w_1, w_2\}$. By the symmetry of u_1 and w_1 in $\overline{G_0}$, we suppose that $g(u_1) \geq g(w_1)$. Let $G^* = G_0 + w_1w_2 - u_1w_2$. Then, G^* is a c-cyclic graph with $\Delta(G^*) = n-2$ by (1). From Lemma 2.2, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$, a contradiction.

Assume H_0 has P_4 as an induced subgraph, where $P_4 := u_1w_1u_2w_2$. By Lemma 2.8, $v_0 \notin \{w_1, u_2\}$. We first suppose that $v_0 \notin \{u_1, w_2\}$. By the symmetry of u_1 and w_2 in $\overline{G_0}$, we may suppose that $g(u_1) \geq g(w_2)$. Let $G^* = G_0 + w_1w_2 - u_1w_1$. Then, G^* is a c-cyclic graph with $\Delta(G^*) = n-2$ by (1) and $v_0 \notin \{u_1, w_2\}$. Since $g(u_1) \geq g(w_2)$, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$ by Lemma 2.2, a contradiction. We second suppose that $v_0 \in \{u_1, w_2\}$ and we may suppose that $v_0 = u_1$. If $g(u_2) \geq g(w_1)$, then let $G^* = G_0 + w_1w_2 - u_2w_2$. If $g(u_2) < g(w_1)$, then let $G^* = G_0 + u_1u_2 - u_1w_1$. In all cases, G^* is a c-cyclic graph with $\Delta(G^*) = n-2$ by (1). By Lemma 2.2, we have $\rho_\alpha(\overline{G^*}) > \rho_\alpha(\overline{G_0})$, a contradiction. ■

3. The proof of Theorem 1.5

Throughout this section, we always suppose that $\overline{G}$ is a graph of $\overline{\mathbb{G}}(n, n-1; c)$ with $d_G(w_0) = n-1$ and let $\overline{F_0} = \overline{G} - w_0$. Then, $\rho_\alpha(\overline{F_0}) = \rho_\alpha(\overline{G} - w_0) = \rho_\alpha(\overline{G})$.

Lemma 3.1: *Let $\overline{G}$ be a graph of $\overline{\mathbb{G}}(n, n-1; c)$. If $0 \leq c \leq n-3$ and $0 \leq \alpha < 1$, then $\overline{F_0}$ is connected.*

Proof: By contradiction, we assume that $\overline{F_0}$ is disconnected, then $F_0 = F_1 \vee F_2$ with $|V(F_1)| \geq |V(F_2)| \geq 1$. This implies that F_0 contains at least $|V(F_1)| \cdot |V(F_2)| \geq n-2$ edges, that is, $n + c - 1 = |E(G)| = n - 1 + |E(F_0)| \geq 2n - 3$, contrary with $0 \leq c \leq n-3$. ■

By Lemma 3.1, if $0 \leq c \leq n-3$ and $0 \leq \alpha < 1$, then $\overline{F_0}$ is connected. In the rest of this section, *let* $0 \leq c \leq n-3$, $0 \leq \alpha < 1$, $\mathbf{h} = (h(v_1), h(v_2), \ldots, h(v_{n-1}))^T$ *be the Perron vector of* $\overline{F_0}$ *and let* $W_0 = V(F_0)$.

Lemma 3.2: *Let $\overline{G}$ be a ρ_α-maximal graph of $\overline{\mathbb{G}}(n, n-1; c)$. Let u and v be two vertices of F_0 and let $\mathbf{h}$ be the Perron vector of $\overline{F_0}$. If $d_{\overline{F_0}}(u) < d_{\overline{F_0}}(v)$, then $h(u) < h(v)$.*

Proof: By contradiction, assume that $d_{\overline{F_0}}(u) < d_{\overline{F_0}}(v)$ and $h(u) \geq h(v)$. Since $\overline{G} \in \overline{\mathbb{G}}(n, n-1; c)$ and Lemma 3.1, G is a c-cyclic graph and $\overline{F_0}$ is connected.

Since $d_{\overline{F_0}}(u) < d_{\overline{F_0}}(v)$, we have $d_{F_0}(v) < d_{F_0}(u)$. Thus there exists vertex set $\{w_1, w_2, \ldots, w_s\} \subseteq N_{F_0}(u) \setminus N_{F_0}(v)$, where $s = d_{F_0}(u) - d_{F_0}(v)$. Let $F^* = F_0 + vw_1 + vw_2 + \cdots + vw_s - uw_1 - uw_2 - \cdots - uw_s$. Then, $K_1 \vee F^*$ is also a c-cyclic graph with n vertices and maximum degree $n-1$. By Lemma 2.2, $\rho_\alpha(\overline{F^*}) > \rho_\alpha(\overline{F_0})$, contrary with the choice of $\overline{G}$. ■

Lemma 3.3: *The graph F_0 contains exactly one component with at least two vertices.*

Proof: By contradiction, we assume that F_1 and F_2 are two components of F_0 with at least two vertices. Let u_iw_i be an edge of F_i for $i \in \{1, 2\}$.

By the symmetry of u_1 and u_2, suppose that $h(u_2) \geq h(u_1)$. Let $F^* = F_0 - u_2w_2 + u_1w_2$. From Lemma 2.2, it follows that $\rho_\alpha(\overline{F^*}) > \rho_\alpha(\overline{F_0})$. Since $K_1 \vee F^*$ is also a c-cyclic graph with n vertices and maximum degree $n-1$, we can get a contradiction to the choice of $\overline{G}$. ■

By Lemma 3.3, we define Z_0 *as the unique component of* F_0 *with at least two vertices* in the rest of this section.

Lemma 3.4: *There exists a vertex y of Z_0 such that $d_{Z_0}(y) = |Z_0| - 1$.*

Proof: Let y be the vertex of maximum degree of Z_0 such that $h(y) \leq h(z)$ for all $d_{Z_0}(y) = d_{Z_0}(z)$. By contradiction, assume that $y_0y \notin E(Z_0)$ for some vertex $y_0 \in Z_0$. Since Z_0 is connected, let P be a shortest path connected with y_0 and y such that $zy_0 \in E(P)$. Since $y_0y \notin E(Z_0)$, $y \neq z$. Let $F^* = F_0 + y_0y - y_0z$. Then, $K_1 \vee F^*$ is a c-cyclic graph with n vertices and maximum degree $n-1$. Since $h(z) \geq h(y)$ by Lemma 3.2 and the choice of y, we have $\rho_\alpha(\overline{F^*}) > \rho_\alpha(\overline{F_0})$ by Lemma 2.2, a contradiction. ■

Proof of Theorem 1.5: By Lemmas 3.3 and 3.4, it suffices to show that Z_0 is a split graph.

If Z_0 has $2K_2$ as an induced subgraph, then let u_1u_2 and w_1w_2 be the two independent edges of $2K_2$. If Z_0 has C_4 as an induced subgraph, then suppose that $C_4 := u_1u_2w_2w_1u_1$. If Z_0 has P_4 as an induced subgraph, then suppose that $P_4 := u_1u_2w_2w_1$. In all cases, we may suppose that $h(u_1) \geq h(w_1)$ by the symmetry of u_1 and w_1. Let $F^* = F_0 + u_2w_1 - u_1u_2$. By Lemma 2.2, we have $\rho_\alpha(\overline{F^*}) > \rho_\alpha(\overline{F_0})$, a contradiction. ■

4. The proof of Corollary 1.2

This section will be dedicated to the proof of Corollary 1.2.

Proof of Corollary 1.2: It is easily checked that $\{S_1, S_2, \ldots, S_5\}$ are all tricyclic graphs with n vertices and maximum degree $n-1$. From Theorems 1.3 and 1.5, we already know that the ρ_α-maximal graph of $\overline{\mathbb{G}}(n; 3)$ is either $\overline{S_1}$ or $\overline{S_2}$. To complete the proof of Corollary 1.2, it suffices to compare $\rho_\alpha(\overline{S_1})$ and $\rho_\alpha(\overline{S_2})$.

For $i \in \{1, 2\}$, denote by $\overline{G_i} = \overline{S_i} - v_1$. Then, $\rho_\alpha(\overline{S_i}) = \rho_\alpha(\overline{G_i})$ for $i \in \{1, 2\}$. By an elementary computation, $\rho_\alpha(\overline{G_1})$ is equal to the maximum root of $\Phi_1(x) = x^3 - (2(n-3)\alpha + n - 4)x^2 + ((n-5)(n-1)\alpha^2 + 2(n-3)^2\alpha + 8 - 2n)x - (n-5)((n+1)(n-4)$

$\alpha^2 - 2(n-6)\alpha - 2)$, and $\rho_\alpha(\overline{G_2})$ is equal to the maximum root of $\Phi_2(x) = x^2 - (n(\alpha + 1) - \alpha - 5)x + (n-4)(n\alpha + \alpha - 3)$. Thus

$$\Phi_1(x) = (x - (n-5)\alpha - 1)\,\Phi_2(x) - (x + 2 - n)(2\alpha - 1). \tag{3}$$

From Lemma 2.1, it easily follows that

$$n - 5 < \min\left\{\rho_\alpha(\overline{G_1}), \rho_\alpha(\overline{G_2})\right\} \le \max\left\{\rho_\alpha(\overline{G_1}), \rho_\alpha(\overline{G_2})\right\} < n - 2. \tag{4}$$

If $\alpha = 0.5$, since $n - 5 \ge \frac{n-5}{2} + 1$ for $n \ge 7$, $\rho_{0.5}(\overline{G_1}) = \rho_{0.5}(\overline{G_2})$ by (3) and (4).

If $0 \le \alpha < 0.5$, since $\Phi_1(\rho_\alpha(\overline{G_2})) = (n - 2 - \rho_\alpha(\overline{G_2}))(2\alpha - 1) < 0$ by (3), $\rho_\alpha(\overline{G_1}) > \rho_\alpha(\overline{G_2})$.

If $0.5 < \alpha < 1$, we first show that $\rho_\alpha(\overline{G_1}) > (n-2)\alpha$. With an elementary computation, it follows that $\Phi_1((n-2)\alpha) = (1-\alpha)\varphi_1(n)$, where $\varphi_1(n) = (3\alpha^2 - 8\alpha + 2)n - 6\alpha^2 + 34\alpha - 10$. Since $\varphi_1'(n) = 3\alpha^2 - 8\alpha + 2 < 0$, we have $\varphi_1(n) < \varphi_1(7) = 15\alpha^2 - 22\alpha + 4 < 0$. This implies that $\rho_\alpha(\overline{G_1}) > (n-2)\alpha > (n-5)\alpha + 1$. From (3) and (4), we have $(\rho_\alpha(\overline{G_1}) - (n-5)\alpha - 1)\Phi_2(\rho_\alpha(\overline{G_1})) = (\rho_\alpha(\overline{G_1}) + 2 - n)(2\alpha - 1) < 0$. Combining this with $\rho_\alpha(\overline{G_1}) - (n-5)\alpha - 1 > 0$, we have $\Phi_2(\rho_\alpha(\overline{G_1})) < 0$ and thus $\rho_\alpha(\overline{G_1}) < \rho_\alpha(\overline{G_2})$. Hence Corollary 1.2 holds. ■

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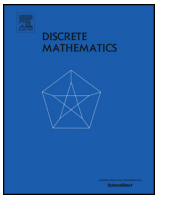
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The k-apex trees with minimum augmented Zagreb index



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ABSTRACT

For a connected graph G on at least three vertices, the augmented Zagreb index (AZI) of G is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3,$$

being a topological index well-correlated with the formation heat of alkanes. A k-apex tree G is a connected graph admitting a k-subset $X \subset V(G)$ such that $G - X$ is a tree, while $G - S$ is not a tree for any $S \subset V(G)$ of cardinality less than k. By investigating some structural properties of k-apex trees, we identify the graphs minimizing the AZI among all k-apex trees on n vertices for $k \geq 4$ and $n \geq 3(k+1)$. The latter solves an open problem posed in Cheng et al. (2021) [5].

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1. Introduction

Throughout this paper, we restrict ourselves to simple and connected graphs. For a graph $G = (V(G), E(G))$ and $v \in V(G)$, we denote by $N_G(v)$ the set of all neighbors of v, and by $|N_G(v)| = d_G(v)$ the degree of v in G. A vertex v with $d_G(v) = r$ is said to be an r-vertex. As usual, let $\Delta(G) = \max\{d_G(v) : v \in V(G)\}$ be the maximum degree of G. A 1-vertex is also called a **pendent vertex** (or leaf), a r-vertex with $r \geq 2$ is called a **non-pendent vertex**, and an r-vertex with $r \geq 3$ is referred to as a **branching vertex**. An (s,t)-edge $(\left(s^{\geq}, t^{\geq}\right)$-edge) is an edge whose end vertices have, respectively, degrees s and t (resp., at least s and t). We omit the symbol "G" from notations (as, for example, in $d_G(v)$ or $N_G(v)$) if the graph under consideration is clear from the context.

In Chemical Graph Theory, the chemical and physical properties of a molecule are studied by means of the combinatorial structure of the associated (molecular) graph. In particular, various topological indices based on the structure of a graph, are well-correlated with different chemical and physical characteristics of the corresponding molecule. Among them, the atom-bond connectivity (ABC) index, introduced in [8] in a slightly different way, is one of such topological indices. The ABC index of a graph G is defined [7] as

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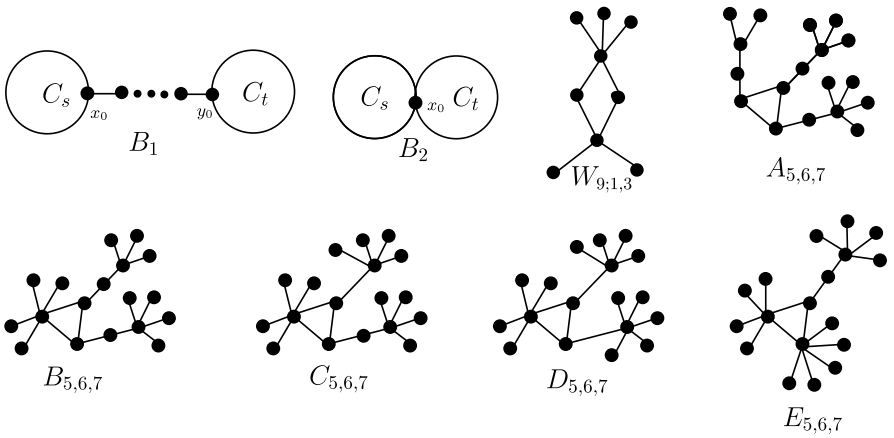


Fig. 1.1. The graphs B_1, B_2, $W_{9;1,3}$, $A_{5,6,7}$, $B_{5,6,7}$, $C_{5,6,7}$, $D_{5,6,7}$ and $E_{5,6,7}$.

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}.$$

The ABC index has been associated with the alkanes' heat of formation, and a quantum-chemical explanation for this correlation is provided in [7]. From the latter invariant Furtula et al. [9] have derived the generalized ABC index:

$$ABC_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d(u) + d(v) - 2}{d(u)d(v)}\right)^\alpha,$$

where α is a real number and G does not admit any component isomorphic to the 2-vertex path graph whenever $\alpha < 0$. The $ABC_{-3}(G)$ is called the augmented Zagreb index (AZI) of G. In particular,

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3.$$

The authors of [9] observed that the AZI outperforms the ABC index in predicting the heat of formation of heptans and octanes. For further chemical applications of the AZI, ABC index, and several other topological indices, we refer the reader to [10–12,17].

We introduce here some additional notation used in this paper. As usual, P_n, C_n, and K_n denote the path, the cycle, and the complete graph on n vertices, respectively. Let $K_{s,n-s}$ be the complete bipartite graph on n vertices with s vertices in a partition set and $n - s$ vertices in the other one. Particularly, $K_{1,n-1}$ is the star on n vertices. If G is a connected graph on n vertices and $n + c - 1$ edges, then G is said to be a c-cyclic graph. As customary, for $c = 0, 1, 2, 3$, G is a tree, unicyclic graph, bicyclic graph, tricyclic graph, respectively. Let $W_{n;c,s}$ be the c-cyclic graph obtained from $K_{2,c+1}$ by attaching $s - 1$ and $n - s - c - 2$ pendent vertices to the two $(c + 1)$-vertices, respectively, where $1 \le s \le \frac{1}{2}(n - c - 2)$ and $c \ge 1$. For instance, $W_{9;1,3}$ is shown, together with some later described graphs, in Fig. 1.1. Recently, extremal results about the AZI have been received the attention of several scholars. For example, Furtula et al. [9] showed that the star $K_{1,n-1}$ is the unique graph minimizing the AZI among all trees on $n \ge 3$ vertices. Afterwards, Huang et al. [13] and Zhan et al. [22] independently proved that the graphs obtained from $K_{1,n-1}$ by adding either one edge, or two non-adjacent edges are the graphs minimizing the AZI in the classes of unicyclic and bicyclic graphs on $n \ge 5$ vertices, respectively. Ali [1] showed that $W_{3;n,1}$ uniquely minimizes the AZI among all tricyclic graphs of order $n \ge 6$. Lin et al. [15] (see also [18]) characterize the unique tree that maximizes the AZI in the class of all trees with n vertices for $n \ge 19$, and they also pose the problem of characterizing the extremal graphs with respect to the AZI among all connected graphs on n vertices and m edges, with $m \ge n$. The latter problem was attacked by Liu et al. in [16], where it is shown that $W_{n;c,1}$ uniquely minimizes the AZI in the class of all c-cyclic graphs on n vertices for $n \ge 2c + 1$ and $c \ge 3$. The extremal tree with the maximum and minimum AZI among all trees with n vertices and k pendent vertices were recently identified in [3]. For further results on the AZI, the interested reader is referred to the survey paper [2].

Let G be a connected graph with at least one cycle. The **base graph** of G, denoted by $\mathcal{R}(G)$, is the subgraph of G obtained by recursively deleting the pendent vertices, until there is no pendent vertex left. Evidently, $\mathcal{R}(G)$ is uniquely determined and it keeps the same cyclomatic number of G. Conversely, given a graph G with at least a cycle, G is obtained from $\mathcal{R}(G)$ by attaching some hanging trees to the vertices of $\mathcal{R}(G)$. In the forthcoming discussion, by T_v we denote a rooted tree whose root is v (the root is a vertex of T_v).

Let Z_q be the unique tree with $q-2$ pendent vertices, one 2-vertex and one $(q-2)$-vertex, where $q \geq 5$, and take $Z_4 = P_4$. Hereafter, we refer to the unique pendent vertex adjacent to the 2-vertex of Z_q as the **special pendent vertex** of Z_q for $q \geq 5$. For P_4, the two pendent vertices are both special pendent vertices.

A quasi-tree is a graph G having a vertex $v \in V(G)$ such that $G - v$ is a tree [19]. Xu et al. [20] generalized the concept of quasi-tree to k-apex trees.

Definition 1.1. *[20,21]* For $k \geq 1$, a **k-apex tree** is a connected graph G admitting a k-subset $V_k \subset V(G)$, such that $G - V_k$ is a tree, but $G - X$ is not a tree whenever $X \subset V(G)$ and $|X| < k$. The set V_k is called a **k-quasi vertex set** of G.

Denote by $\mathbb{T}_n^k$ the class of k-apex trees on n vertices. In [5], two of the present paper authors and their cooperator determined the unique graphs with the minimum AZI among all graphs of $\mathbb{T}_n^k$ for $1 \leq k \leq 3$, and it was observed that providing a complete result for the general case $k \geq 4$ could be a difficult task. In this paper, we give a complete solution to the latter problem, namely, the identification of the k-apex trees of order n, with $k \geq 4$ and $n \geq 3(k+1)$, minimizing the AZI. The main result is obtained by a careful case analysis which stepwise discards c-cyclic k-apex trees for $c \geq 2$, and by identifying the AZI minimizers in the class of unicyclic k-apex trees. Hence, let $\mathscr{U}_n^k$ be the class of those unicyclic graphs on n vertices that are k-apex trees.

We now define some graphs in $\mathscr{U}_n^k$, useful to describe the obtained extremal graphs:

(i) Let A_{s_1,s_2,s_3} be the unicyclic graph with the unique cycle $C_3 := u_1u_2u_3u_1$ such that $T_{u_i} = Z_{s_i}$ and u_i is the special pendent vertex of Z_{s_i}, where $s_i \geq 4$ and $1 \leq i \leq 3$;

(ii) Let B_{s_1,s_2,s_3} be the unicyclic graph having the unique cycle $C_3 := u_1u_2u_3u_1$ such that $T_{u_1} = K_{1,s_1-1}$ with u_1 being the center vertex of K_{1,s_1-1}, and $T_{u_i} = Z_{s_i}$ with u_i being the special pendent vertex of Z_{s_i} for $i \in \{2,3\}$, where $s_1 \geq 2$ and $\min\{s_2, s_3\} \geq 4$;

(iii) Let C_{s_1,s_2,s_3} be the unicyclic graph having the unique cycle $C_3 := u_1u_2u_3u_1$ such that $T_{u_1} = K_{1,s_1-1}$ with u_1 being the center vertex of K_{1,s_1-1}, $T_{u_2} = K_{1,s_2-1}$ with u_2 being a pendent vertex of K_{1,s_2-1}, and $T_{u_3} = Z_{s_3}$ with u_3 being the special pendent vertex of Z_{s_3}, where $s_1 \geq 2$, $s_2 \geq 3$ and $s_3 \geq 4$.

For the sake of the reader, as an example of the above definitions, we depict the graphs $A_{5,6,7}$, $B_{5,6,7}$ and $C_{5,6,7}$ in Fig. 1.1. Now, we are ready to state the main result of this paper:

Theorem 1.1. *Let G_0 be a graph with minimum AZI in $\mathbb{T}_n^k$. If $k \geq 4$ and $n \geq 3k+3$, then*

$$G_0 = \begin{cases} A_{k,\left\lfloor \frac{n-k}{2} \right\rfloor, \left\lceil \frac{n-k}{2} \right\rceil} & \text{if } k \geq 7, \\ B_{6,\lceil \frac{n}{2} \rceil - 3, \lfloor \frac{n}{2} \rfloor - 3} & \text{if } k = 6, \\ C_{k,k,n-2k} & \text{if } 4 \leq k \leq 5. \end{cases}$$

Here is the remainder of this paper. In Section 2, we provide some bounds for the AZI and some related structural results useful for our investigations. In Section 3, we prove our main result restricted to the class $\mathscr{U}_n^k$ of unicyclic graphs. In Section 4, we discard the c-cyclic graphs ($c \geq 4$) in $\mathbb{T}_n^k$ as AZI minimizers. Similarly, we discard bicyclic and tricyclic graphs as AZI minimizers in Sections 5 and 6, respectively.

2. Preliminaries

Let us consider the AZI as a real function on two real variables:

$$\Psi(x, y) = \left(\frac{xy}{x+y-2} \right)^3.$$

Lemma 2.1. *Let x and y be two real numbers, where $\min\{x, y\} \geq 1$.*

(i) [14] *$\Psi(1, y)$ is decreasing for $y \geq 2$.*

(ii) [14] *$\Psi(2, y) = 8$ for any real number y.*

(iii) [14] *If $y \geq 3$ is fixed, then $\Psi(x, y) > 8$ is increasing for $x \geq 3$.*

(iv) [5] *If $y \geq 4$, then $(y-3)\Psi(1, y-1) > (y-4)\Psi(1, y-2)$.*

(v) [3] *If $x + y \geq 4$ and $x \geq 2$, then $\Psi(x, y) - \Psi(x-1, y)$ strictly decreases with $x \geq y - 1$.*

From Lemma 2.1(i)–(iii), the next result straightly follows.

Corollary 2.1. *Let G be a connected graph with e edges, p pendent vertices, and maximum degree Δ. If G contains exactly s edges such that each one of them has at least one end vertex of degree 2, then*

$$AZI(G) \geq p \left(\frac{\Delta}{\Delta - 1} \right)^3 + 8s + (e - p - s) \left(\frac{9}{4} \right)^3.$$

For a subset V_1 of $V(G)$, we denote by $G - V_1$ the graph obtained from G by removing the vertices in V_1 and all the incident edges; if H is an induced subgraph of G with $V(H) \cap V_1 = \emptyset$, then $H + V_1$ denotes the subgraph of G induced by vertex set $V(H) \cup V_1$. In particular, $G - \{v\}$ is shortened to $G - v$.

Lemma 2.2. *Let S be a k-quasi vertex set of a k-apex tree G. If $X \subset S$ such that $G - X$ is connected, then $G - X$ is a $(k - |X|)$-apex tree.*

Proof. We will prove that $G - X$ is a $(k - |X|)$-apex tree with a $(k - |X|)$-quasi vertex set $S \setminus X$. By our hypothesis, $G - X - S \setminus X = G - S$ is a tree. Contrarily, assume that there exists a subset Y of $V(G - X)$ with $|Y| \leq k - |X| - 1$ (this inequality is equivalent to $|X \cup Y| \leq k - 1$ because $X \cap Y = \emptyset$) such that $G - X - Y$ is a tree. Since $X \cup Y$ is a subset of $V(G)$ and $G - (X \cup Y) = G - X - Y$ is a tree with $|X \cup Y| \leq k - 1$, this contradicts the fact that G is a k-apex tree. □

Lemma 2.3. *Let u_0v_0 be an edge of a cycle C pertaining to a k-apex tree G such that u_0 is a 2-vertex of G. If $k \geq 2$, then $G - u_0$ is a $(k-1)$-apex tree and $G - u_0v_0$ is either a $(k-1)$-apex tree or a k-apex tree.*

Proof. Suppose that $P = v_1v_2 \cdots v_{s+1}$ $(s \geq 2)$, is a path joining v_1 and v_{s+1} (which need not be distinct) such that v_1 and v_{s+1} have degree greater than 2, while all other vertices $v_2, ..., v_s$ are of degree 2. We may further suppose that $u_0 = v_i$ and $v_0 = v_{i+1}$, where $2 \leq i \leq s$. In what follows, let C be a smallest cycle of G such that $V(P) \subseteq V(C)$, then $V(C)$ induces a cycle of G.

Clearly, $G - u_0v_0$ is connected. Let H_1 be the component of $G - \{v_1, v_{s+1}\}$ such that H_1 contains vertices $v_2, v_3, \ldots, v_s$. Since H_1 is a tree, it holds that

$$|V(G) \setminus V(H_1)| \geq k, \tag{2.1}$$

as G is a k-apex tree. We prove this lemma by the two below claims.

Claim 1. *There exists some k-quasi vertex set S of G such that $u_0 \in S$.*

Proof. Let S be a k-quasi vertex set of G. We may suppose that $u_0 \notin S$ and so $u_0 \in G - S$.

If $v_1, v_{s+1} \in S$, then $G - S$ contains no vertex of $V(G) \setminus V(H_1)$, because u_0 is not connected with any vertex of $V(G) \setminus (V(H_1) \cup \{v_1, v_{s+1}\})$ in the graph $G - \{v_1, v_{s+1}\}$. This implies that $V(G) \setminus V(H_1) \subseteq S$, which together with (2.1) yields $|V(G) \setminus V(H_1)| = k = |S|$. Let $H_2 = H_1 + V(C) \setminus V(H_1) - \{u_0\}$. Then, $|V(H_2)| \geq |V(H_1)|$ with equality if and only if $v_1 = v_{s+1}$. Since $V(C)$ induces a cycle of $\mathcal{R}(G)$, H_2 is also a tree. Since G is a k-apex tree, $|V(G) \setminus V(H_2)| \geq k$. Combining this with $|V(G) \setminus V(H_2)| \leq |V(G) \setminus V(H_1)| \leq k$, we have $|V(G) \setminus V(H_2)| = k$. Thus, $S' = V(G) \setminus V(H_2)$ is also a k-quasi vertex set such that $u_0 \in S'$, and so Claim 1 holds.

Otherwise, $v_1 \notin S$ or $v_{s+1} \notin S$. By symmetry, we suppose that $v_1 \notin S$ and so $u_0, v_1 \in G - S$. It is easily to see that $S'' = S \setminus \big(V(H_1) \cup V(C)\big) \cup \{u_0\}$ is also a vertex set of $V(G)$ such that $G - S''$ is also a tree. Since $G - S$ is a tree and C is a cycle of G, S must contain at least one vertex of C and thus $|S''| \leq k$. Combining this with G being a k-apex tree, we can conclude that $k \leq |S''| \leq k$, as $G - S''$ is a tree. Therefore, S'' is a k-quasi vertex set of G with $u_0 \in S''$, and so Claim 1 also holds. □

By Lemma 2.2 and Claim 1, we can conclude that $G - u_0$ is a $(k-1)$-apex tree. Suppose that $N_G(u_0) = \{v_0, w_0\}$.

Claim 2. *$G - u_0v_0$ is either a $(k-1)$-apex tree or a k-apex tree.*

Proof. If $G - u_0v_0$ contains a vertex set X with $|X| \leq k - 2$ such that $H_2 = G - u_0v_0 - X$ is a tree, then $X_1 = X \cup \{u_0\}$ is a subset of $V(G)$ such that $G - X_1$ is a tree when $u_0, v_0 \in V(H_2)$ and X is a subset of $V(G)$ such that $G - X$ is a tree when $u_0 \notin V(H_2)$ or $v_0 \notin V(H_2)$, which is contrary with the fact that G is a k-apex tree.

By Claim 1, let Y be a $(k-1)$-quasi vertex set of $G - u_0$. Then, $G - u_0v_0 - Y - u_0 = G - Y - u_0$ is a tree. Since $|Y \cup \{u_0\}| = k$, we can conclude that we can obtain a tree from $G - u_0v_0$ by deleting at most k vertex. Furthermore, from the former arguments, any deletion of at most $k - 2$ vertices from $G - u_0v_0$ cannot be a tree. Thus, $G - u_0v_0$ is either a $(k-1)$-apex tree or a k-apex tree. This completes the proof of Claim 2. □

Lemma 2.4. *Let u_0 be a 2-vertex of the connected graph G. If u_0 is a vertex of some cycle C of G, there exists an edge u_0v_0 of C such that $AZI(G) - AZI(G - u_0v_0) \geq 8$.*

Proof. Suppose that C is a cycle of G such that $u_0v_0 \in E(C)$, $w_0u_0 \in E(C)$ and $vv_0 \in E(C)$, where $w_0 = v$ is also permitted. Since $w_0, v \in V(C)$, it holds that $\min\{d_G(w_0), d_G(v)\} \geq 2$.

Case 1. $d_G(v_0)=2$. By Lemma 2.1(i),

$$AZI(G)-AZI(G-u_0v_0)=24-\left(\frac{d_G(w_0)}{d_G(w_0)-1}\right)^3-\left(\frac{d_G(v)}{d_G(v)-1}\right)^3\geq 24-16=8. \tag{2.2}$$

Case 2. $d_G(v_0)\geq 3$.

By Lemma 2.1(i) and Lemma 2.1(iii), for $d_G(z)\geq 3$ we have

$$\begin{aligned}\Psi\big(d_G(v_0),d_G(z)\big)-\Psi\big(d_G(v_0)-1,d_G(z)\big)&>0=\Psi\big(d_G(v_0),2\big)-\Psi\big(d_G(v_0)-1,2\big)\\&>\Psi\big(d_G(v_0),1\big)-\Psi\big(d_G(v_0)-1,1\big)\end{aligned}$$

and hence

$$\begin{aligned}&AZI(G)-AZI(G-u_0v_0)\\&\geq 16-\Psi\big(d_G(w_0),1\big)+\sum_{z\in N_G(v_0)\setminus\{u_0,v\}}\Big[\Psi\big(d_G(v_0),d_G(z)\big)-\Psi\big(d_G(v_0)-1,d_G(z)\big)\Big]\\&\geq 16-\Psi\big(d_G(w_0),1\big)+\big(d_G(v_0)-2\big)\Big[\Psi\big(d_G(v_0),1\big)-\Psi\big(d_G(v_0)-1,1\big)\Big].\end{aligned} \tag{2.3}$$

Let

$$f(x)=\big(x-2\big)\Big[\Psi\big(x,1\big)-\Psi\big(x-1,1\big)\Big]=\big(x-2\big)\left[\left(\frac{x}{x-1}\right)^3-\left(\frac{x-1}{x-2}\right)^3\right],\ \text{where } x\geq 3.$$

Since $x\geq 3$, we have $(x-1)^4(x-2)^3f'(x)=3x^5-12x^4+9x^3+18x^2-25x+4>0$, which implies that the function f is a strictly increasing function for $x\geq 3$. By Case 1, we may suppose that $d_G(w_0)\geq 3$. Combining this with Lemma 2.1(i) and (2.3), we have

$$AZI(G)-AZI(G-u_0v_0)\geq 16-\left(\frac{3}{2}\right)^3+\left(\frac{3}{2}\right)^3-8=8.$$

This completes the proof. □

Let u_0 be a vertex in the base graph of G. If $|V(T_{u_0})|=q\geq 3$, then denote by $G^*(u_0)$ the graph obtained from G by deleting all vertices of $V(T_{u_0})\setminus\{u_0\}$ and then adding one new edge between u_0 and a pendent vertex of $K_{1,q-2}$. From the definition, it is easily checked that

If G is a k-apex tree, then $G^*(u_0)$ is also a k-apex tree for $k\geq 2$.

Proposition 2.1. [5] *Let $u_0\in V(\mathcal{R}(G))$ with $N_G(u_0)\cap V(\mathcal{R}(G))=\{v_0,w_0\}$ and $d_G(v_0)\geq d_G(w_0)\geq 3$. Suppose that $|V(T_{u_0})|=q\geq 3$ and $V(T_{u_0})\setminus\{u_0\}$ contains exactly t non-pendent vertices. If $G\neq G^*(u_0)$, then we have $AZI(G)>AZI\big(G^*(u_0)\big)$ if one of the following conditions holds:*

(i) $t=0$, $d_G(v_0)=3$ and $q\geq 7$; (ii) $t=0$, $d_G(v_0)\geq 4$ and $q\geq 5$;
(iii) $t=1$, $d_G(u_0)=3$ and $q\geq 6$; (iv) $t=1$, $d_G(u_0)\geq 4$ and $q\geq 5$; (v) $t\geq 2$.

At the end of this section, we shall list the formulas of AZI for different graphs, which will be used in the sequel sections.

$$AZI(W_{n;c,s})=(n-c-2-s)\left(\frac{n-s-1}{n-2-s}\right)^3+(s-1)\left(\frac{s+c}{s+c-1}\right)^3+16(c+1), \tag{2.4}$$

$$AZI(A_{k,k,n-2k})=\frac{5259}{64}+\frac{(n-2k-2)^3}{(n-2k-3)^2}+2\frac{(k-2)^3}{(k-3)^2}, \tag{2.5}$$

$$AZI(C_{4,4,n-8})=\frac{5289}{64}+\frac{(n-10)^3}{(n-11)^2},\ AZI(C_{5,5,n-10})=\frac{6961}{78}+\frac{(n-12)^3}{(n-13)^2}, \tag{2.6}$$

$$AZI\left(A_{k,\left\lfloor\frac{n-k}{2}\right\rfloor,\left\lceil\frac{n-k}{2}\right\rceil}\right)=\frac{5259}{64}+\frac{(k-2)^3}{(k-3)^2}+\begin{cases}\frac{(n-k-4)^3}{(n-k-6)^2} & \text{if } n-k \text{ is even},\\ \frac{(n-k-3)^3}{2(n-k-5)^2}+\frac{(n-k-5)^3}{2(n-k-7)^2} & \text{if } n-k \text{ is odd},\end{cases} \tag{2.7}$$

$$AZI\left(B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3}\right)=\frac{7088}{81}+\begin{cases}\frac{(n-10)^3}{(n-12)^2} & \text{if } n \text{ is even},\\ \frac{(n-9)^3}{2(n-11)^2}+\frac{(n-11)^3}{2(n-13)^2} & \text{if } n \text{ is odd}.\end{cases} \tag{2.8}$$

3. The case of unicyclic graphs

In this section, we consider k-apex trees in $\mathscr{U}_n^k$, and we prove Theorem 1.1 under the latter restriction. The main result of this section is

Proposition 3.1. *Let G_0 have the minimum AZI in $\mathscr{U}_n^k$. If $n \geq 3k+3$, then*

$$G_0=\begin{cases}A_{k,\lfloor\frac{n-k}{2}\rfloor,\lceil\frac{n-k}{2}\rceil} & \text{if } k\geq 7,\\ B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3} & \text{if } k=6,\\ C_{k,k,n-2k} & \text{if } 4\leq k\leq 5.\end{cases}$$

To show Proposition 3.1, we need to introduce a series of lemmas.

Lemma 3.1. [5] *Let $G\in\mathscr{U}_n^k$, where $k\geq 2$. If C_g is the unique cycle of G, then $\min\{|V(T_u)|:\ u\in V(C_g)\}=k$ and $G[V_k]$ is a root tree for each k-quasi vertex set V_k of G.*

Let $G^*_{s_1,s_2}$ be the graph obtained from a connected graph G with $w_1, w_2\in V(G)$ and two stars K_{1,s_1-2} and K_{1,s_2-2} by adding an edge between w_i and one pendent vertex of K_{1,s_i-2} for each $i\in\{1,2\}$, where $w_1=w_2$ is also permitted.

Lemma 3.2. *If $s_1\geq s_2+2$ and $s_2\geq 4$, then $AZI(G^*_{s_1,s_2})>AZI(G^*_{s_1-1,s_2+1})$.*

Proof. By the definition of $G^*_{s_1,s_2}$, we have

$$\begin{aligned}AZI(G^*_{s_1,s_2})-AZI(G^*_{s_1-1,s_2+1})&=\frac{(s_1-2)^3}{(s_1-3)^2}+\frac{(s_2-2)^3}{(s_2-3)^2}-\frac{(s_1-3)^3}{(s_1-4)^2}-\frac{(s_2-1)^3}{(s_2-2)^2}\\&=\frac{(s_1-s_2-1)f(s_1)}{(s_1-3)^2(s_1-4)^2(s_2-2)^2(s_2-3)^2},\end{aligned}$$

where $f(s_1)=(3s_2^2-13s_2+13)s_1^3+(s_2-13)(3s_2^2-13s_2+13)s_1^2-(19s_2^3-238s_2^2+756s_2-672)s_1+29s_2^3-319s_2^2+960s_2-828$. Since $s_1\geq s_2+2$ and $s_2\geq 4$, we have $f'''(s_1)=6(3s_2^2-13s_2+13)>0$ and thus $f''(s_1)\geq f''(s_2+2)=2(4s_2-7)(3s_2^2-13s_2+13)>0$. Therefore, $f'(s_1)\geq f'(s_2+2)=(s_2-1)(s_2-2)(15s_2^2-69s_2+76)>0$, which implies that $f(s_1)\geq f(s_2+2)=2(s_2-2)^2(3s_2^3-15s_2^2+21s_2-7)>0$. □

Corollary 3.1. *If $n\geq 3k+1$ and $k\geq 5$, then*

$$AZI\left(A_{k,\lfloor\frac{n-k}{2}\rfloor,\lceil\frac{n-k}{2}\rceil}\right)<AZI\left(A_{k-1,\lfloor\frac{n-k+1}{2}\rfloor,\lceil\frac{n-k+1}{2}\rceil}\right)<AZI(A_{k-1,k-1,n+2-2k}).$$

Proof. Since $k-1\geq 4$ and $n+2-2k>k-1+2$, the second inequality follows from Lemma 3.2. Since $\left\lceil\frac{n-k+1}{2}\right\rceil\geq\frac{n-k+1}{2}\geq k-1+2$, we have

$$AZI\left(A_{k-1,\lfloor\frac{n-k+1}{2}\rfloor,\lceil\frac{n-k+1}{2}\rceil}\right)>AZI\left(A_{k,\lfloor\frac{n-k+1}{2}\rfloor,\lceil\frac{n-k-1}{2}\rceil}\right)=AZI\left(A_{k,\lfloor\frac{n-k}{2}\rfloor,\lceil\frac{n-k}{2}\rceil}\right)$$

by Lemma 3.2. □

Lemma 3.3. *Let $u\in V(\mathcal{R}(G))$ such that $T_u=Z_q$ with u being the special pendent vertex of Z_q and G^* be the graph obtained from G by replacing Z_q with $K_{1,q-1}$ such that u is a pendent vertex of $K_{1,q-1}$. If $4\leq q\leq 5$ and $d_G(u)=3$, then $AZI(G)>AZI(G^*)$, where $G\in\mathscr{U}_n^k$ implies that $G^*\in\mathscr{U}_n^k$.*

Proof. Clearly, if $G\in\mathscr{U}_n^k$, then $G^*\in\mathscr{U}_n^k$. Since $d_G(u)=d_{G^*}(u)=3$ and $4\leq q\leq 5$, it is easily checked that

$$AZI(G)-AZI(G^*)\geq 16+2\Psi(3,1)-3\Psi(4,1)-\Psi(3,4)>1.8,$$

thus the result holds. □

Lemma 3.4. *If $s_3 \geq 5$ and $s_1 \geq 3$, then $AZI(C_{s_1,s_2,s_3}) > AZI(C_{s_1-1,s_2,s_3+1})$.*

Proof. By Lemma 2.1, it follows that

$$\begin{aligned} AZI(C_{s_1,s_2,s_3}) - AZI(C_{s_1-1,s_2,s_3+1}) &= 2\Psi(3,s_1+1) - 2\Psi(3,s_1) + \big((s_1-1)\Psi(1,s_1+1) \\ &\quad -(s_1-2)\Psi(1,s_1)\big) + \big((s_3-3)\Psi(1,s_3-2) \\ &\quad -(s_3-2)\Psi(1,s_3-1)\big) \\ &> 2\Psi(s_1+1,3) - 2\Psi(s_1,3) - \Psi(1,s_3-2) \\ &\geq 2\Psi(3,4) - 2\Psi(3,3) - \Psi(1,3) > 0. \end{aligned}$$

This completes the proof. □

In the rest of this section, **we always suppose that G_0 has the minimum AZI in $\mathscr{U}_n^k$ and C_g is the unique cycle of G_0**, where $k \geq 2$.

Lemma 3.5. *Let u_1, u_2, u_3 be three vertices of C_g such that $u_2 \in N_{G_0}(u_1) \cap N_{G_0}(u_3)$ and let G^* be the unicyclic graph obtained from G_0 by replacing T_{u_2} with $K_{1,q-1}$ such that u_2 is the center vertex of $K_{1,q-1}$, where $3 \leq q = |V(T_{u_2})| \leq 6$. If $d_{G_0}(u_1) = d_{G_0}(u_3) = 3$, then $G_0 = G^*$.*

Proof. By contradiction, we assume that $G_0 \neq G^*$. Suppose that $V(T_{u_2}) \setminus \{u_2\}$ contains exactly t non-pendent vertices.

If $T_{u_2} = Z_q$ with u_2 being the special pendent vertex of Z_q, then $q = 6$ by the choice of G_0 and Lemma 3.3. Since $d_{G_0}(u_1) = d_{G_0}(u_3) = 3$, we have

$$AZI(G_0) - AZI(G^*) = 16 + 3\Psi(4,1) + 2\Psi(3,3) - 5\Psi(7,1) - 2\Psi(3,7) > 1.75,$$

contrary with the choice of G_0, as $G^* \in \mathscr{U}_n^k$.

If $T_{u_2} = K_{1,q-1}$ with u_2 being a pendent vertex of $K_{1,q-1}$, then

$$AZI(G_0) - AZI(G^*) \geq 4\Psi(5,1) + \Psi(3,5) + 2\Psi(3,3) - 5\Psi(7,1) - 2\Psi(3,7) > 2,$$

for $3 \leq q \leq 6$. This is contrary with the choice of G_0.

If $T_{u_2} \neq Z_q$ and $T_{u_2} \neq K_{1,q-1}$ with u_2 being a pendent vertex of $K_{1,q-1}$, then Proposition 2.1 and the choice of G_0 imply that $T_{u_2} = P_4$ with u_2 being a 2-vertex of P_4. In this case,

$$AZI(G_0) - AZI(G^*) = 16 + 2\Psi(4,3) + \Psi(4,1) - 2\Psi(5,3) - 3\Psi(5,1) > 8.5,$$

contrary with the choice of G_0. □

Lemma 3.6. *If $g \geq 4$, then there exists $G^* \in \mathscr{U}_n^k$ such that the unique cycle of G^* is C_{g-1} and $AZI(G_0) = AZI(G^*)$.*

Proof. Let $S = \{w_0, w_1, \ldots, w_{k-1}\}$ be a k-quasi vertex set of G_0. By Lemma 3.1 and $k \geq 2$, we may suppose that $G_0[S]$ is a root tree with root w_0 and each vertex of C_g is a branching vertex. Let y_1, y_2, y_3, y_4 be four vertices of C_g such that $y_1 \in N_{G_0}(w_0) \cap N_{G_0}(y_2)$, $y_2 \in N_{G_0}(y_1) \cap N_{G_0}(y_3)$ and $y_3 \in N_{G_0}(y_2) \cap N_{G_0}(y_4)$, where $y_4 = w_0$ implies that $g = 4$. We choose $z_i \in N_{G_0}(y_i) \setminus V(C_g)$ such that $d_{G_0}(z_i)$ is as small as possible, where $1 \leq i \leq 4$. Let $G_1 = G_0 + w_0y_2 + y_1z_2 - y_1w_0 - y_2z_2$. Since $g \geq 4$, then G_1 is also a k-apex tree with girth $g-1$ by Lemma 3.1.

Case 1. $d_{G_0}(y_2) \leq d_{G_0}(y_1)$.

If $d_{G_0}(z_2) \leq 2$, then Lemma 2.1 implies that

$$\begin{aligned} AZI(G_0) - AZI(G_1) &= \Psi\big(d_{G_0}(w_0), d_{G_0}(y_1)\big) + \Psi\big(d_{G_0}(z_2), d_{G_0}(y_2)\big) - \Psi\big(d_{G_0}(w_0), d_{G_0}(y_2)\big) \\ &\quad -\Psi\big(d_{G_0}(z_2), d_{G_0}(y_1)\big) \\ &\geq \Psi\big(d_{G_0}(w_0), d_{G_0}(y_1)\big) - \Psi\big(d_{G_0}(w_0), d_{G_0}(y_2)\big) \geq 0, \end{aligned}$$

as y_1, y_2, w_0 are three branching vertices of G_0. By the choice of G_0, we have

$$d_{G_0}(y_1) = d_{G_0}(y_2) \text{ and } AZI(G_0) = AZI(G_1). \tag{3.1}$$

If $d_{G_0}(z_2) \geq 3$, then by the choice of z_2, we can conclude that $d_{G_0}(w) \geq 3$ for each vertex $w \in N_{G_0}(y_2) \setminus V(C_g)$. Next, we suppose that $d_{G_0}(y_2) < d_{G_0}(y_1)$, as $AZI(G_0) = AZI(G_1)$ for $d_{G_0}(y_2) = d_{G_0}(y_1)$. By the choice of G_0, Proposition 2.1 and the choice of z_2, we can conclude that

$$N_{G_0}(y_2) \setminus V(C_g) = \{z_2\} \text{ and } d_{G_0}(y_2) = 3 < 4 \le q \le 5, \text{ where } T_{y_2} = K_{1,q-1}. \tag{3.2}$$

Let $d_{G_0}(w_0) = x$ and $d_{G_0}(y_1) = y$. Since $3 = d_{G_0}(y_2) < d_{G_0}(y_1)$, we have $y \ge 4$ and $x \ge 3$.

Subcase 1.1. $3 \le x \le 4$. Since $d_{G_0}(y_1) = y \ge 4$ and $AZI(G_0)$ is minimum, Proposition 2.1 implies that either $T_{y_1} = K_{1,r-1}$ with $3 \le r \le 6$ and y_1 being the center vertex of T_{y_1} or $T_{y_1} = P_4$ with y_1 being a 2-vertex of P_4. Let $G_2 = G_0 + w_0y_2 + y_1z - y_1w_0 - y_1y_2$, where z is a pendent vertex of T_{y_2}. Then, G_2 is also a k-apex tree with girth $g-1$ by Lemma 3.1.

We only prove the case of $x = 3$, as the case $x = 4$ can be shown similarly.

We first suppose that $T_{y_1} = K_{1,r-1}$ with $3 \le r \le 6$. By (3.2) and $4 \le q \le 5$, we have

$$\begin{aligned}
AZI(G_0) - AZI(G_2) &= 2\Psi(r+1,3) + (r-1)\Psi(r+1,1) + (q-2)\Psi(q-1,1) \\
&\quad -(r-1)\Psi(r,1) - 16 - (q-3)\Psi(q-1,1) - \Psi(3,3) \\
&\ge 2\Psi(r+1,3) + (r-1)\Psi(r+1,1) - (r-1)\Psi(r,1) + \Psi(4,1) \\
&\quad -16 - \Psi(3,3) \\
&= 2\left(\frac{3(r+1)}{r+2}\right)^3 + (r-1)\left(\frac{r+1}{r}\right)^3 - (r-1)\left(\frac{r}{r-1}\right)^3 + \left(\frac{4}{3}\right)^3 \\
&\quad -\left(\frac{9}{4}\right)^3 - 16 \\
&> 2\left(\frac{3(r+1)}{r+2}\right)^3 + (r-1)\left(\frac{r+1}{r}\right)^3 - (r-1)\left(\frac{r}{r-1}\right)^3 - \frac{51}{2} \\
&= \frac{g(r)}{2(r-1)^2 r^3 (r+2)^3} > 0,
\end{aligned}$$

where $f(r) = 57r^8 - 102r^7 - 303r^6 + 228r^5 + 300r^4 - 230r^3 + 36r^2 - 24r - 16$. This is contrary with the choice of G_0.

We second suppose that $T_{y_1} = P_4$ with y_1 being a 2-vertex of P_4. Then, $d_{G_0}(y_1) = 4$ and

$$\begin{aligned}
AZI(G_0) - AZI(G_2) &= 2\Psi(3,4) + \Psi(4,1) + \Psi(q-1,1) - \Psi(3,3) - 16 - \Psi(3,1) \\
&\ge 2\Psi(3,4) + 2\Psi(4,1) - \Psi(3,3) - 16 - \Psi(3,1) > 1.5 \text{ by Lemma 2.1},
\end{aligned}$$

contrary with the choice of G_0.

Subcase 1.2. $x \ge 5$. By (3.2), we have $4 \le q \le 5$. Since $y \ge 4$, we have

$$\Psi(3,3) - \Psi(y,3) - \Psi(3,4) + \Psi(y,4) > \Psi(y,4) - \Psi(y,3) - 2.5 = \frac{f(y)}{2(y+2)^3(y+1)^3} > 0,$$

where $f(y) = 69y^6 + 15y^5 - 429y^4 - 619y^3 - 330y^2 - 180y - 40$ and thus

$$\begin{aligned}
AZI(G_0) - AZI(G_1) &= \Psi(x,y) + \Psi(3,q-1) - \Psi(x,3) - \Psi(y,q-1) \\
&\ge \Psi(x,y) + \Psi(3,4) - \Psi(x,3) - \Psi(y,4).
\end{aligned} \tag{3.3}$$

It is not difficult to see that $\Psi(x,y) - \Psi(x,3)$ is strictly increasing with $x \ge 5$ and so

$$AZI(G_0) - AZI(G_1) \ge \Psi(5,y) + \Psi(3,4) - \Psi(5,3) - \Psi(y,4) = \frac{(y-3)g(y)}{1000(y+2)^3(y+3)^3}$$

by (3.3), where $g(y) = 59199y^5 + 324582y^4 + 578253y^3 + 457454y^2 + 367404y + 129672 > 0$. This is contrary with the choice of G_0.

Case 2. $d_{G_0}(y_2) > d_{G_0}(y_1)$. Let $G_3 = G_0 + y_1y_3 + y_2z_1 - y_2y_3 - y_1z_1$, where z_1 has minimum degree among all vertices of $N_{G_0}(y_1) \setminus V(C_g)$. Since $g \ge 4$, G_3 is also a k-apex tree with girth $g-1$ by Lemma 3.1, as $w_0 \notin \{y_1, y_2, y_3\}$.

If $d_{G_0}(z_1) \le 2$, then by a similar discussion as we made while comparing the $AZI(G_0)$ and $AZI(G_1)$, we have $AZI(G_0) > AZI(G_3)$, as $d_{G_0}(y_2) > d_{G_0}(y_1)$.

Otherwise, $d_{G_0}(w) \ge 3$ holds for any vertex $w \in N_{G_0}(y_1) \setminus V(C_g)$, then we also have $d_{G_0}(y_1) = 3$ similarly with (3.2). With the similar reason as in Case 1, we can get another k-apex tree $G_4 \in \mathscr{U}_n^k$ such that $AZI(G_0) > AZI(G_4)$, a contradiction. □

Lemma 3.7. *If $k \ge 3$, then the unique cycle of G_0 is a triangle.*

Proof. By contradiction, we assume that $g \geq 4$. If $g \geq 5$, then by applying Lemma 3.6 step by step, we can obtain a unicyclic graph $G^* \in \mathscr{U}_n^k$ such that the unique cycle of G^* is a C_4 and $AZI(G^*) = AZI(G_0)$. Thus, we may suppose that G_0 itself is a unicyclic graph with unique cycle C_4 and $V(T_{w_0})$ is a k-quasi vertex set of G_0 such that $V(C_4) = \{w_0, y_1, y_2, y_3\}$ with $N_{G_0}(y_1) \cap N_{G_0}(y_3) = \{w_0, y_2\}$. By Lemma 3.1, each vertex of C_4 is a branching vertex.

By the proof of Lemma 3.6 and the symmetry of y_1 and y_3, we have $d_{G_0}(y_1) = d_{G_0}(y_2) = d_{G_0}(y_3) = s$. Let $G_1 = G_0 + y_1y_3 + y_2z - y_1y_2 - y_2y_3$, where z is a pendent vertex of T_{y_1} such that the distance between z and y_1 is as small as possible. By Lemma 3.1, $G_1 \in \mathscr{U}_n^k$.

Case 1. $s \geq 5$. By the choice of G_0 and Proposition 2.1, we can conclude that $s = 5$ and $T_{y_i} = K_{1,3}$ with y_i being the center vertex of $K_{1,3}$ for $1 \leq i \leq 3$. This implies that

$$AZI(G_0) - AZI(G_1) = \Psi(5,5) + 4\Psi(5,1) - 16 - 3\Psi(4,1) > 15,$$

a contradiction.

Case 2. $s = 4$. By the choice of G_0 and Proposition 2.1, we can conclude that either $T_{y_i} = K_{1,2}$ with y_i being the center vertex of $K_{1,2}$ or $T_{y_i} = P_4$ with y_i being a 2-vertex of P_4, where $i \in \{1,2,3\}$. Since $T_{y_2} \in \{K_{1,2}, P_4\}$ and $zy_1 \in E(G_0)$, we have

$$AZI(G_0) - AZI(G_1) \geq \Psi(4,4) + 3\Psi(4,1) - 16 - 2\Psi(3,1) > 3 \text{ by Lemma 2.1},$$

a contradiction.

Case 3. $s = 3$. In this case, $d_{G_0}(y_1) = d_{G_0}(y_2) = d_{G_0}(y_3) = 3$ and thus $|V(T_{y_2})| \geq 7$ by Lemma 3.5 and the choice of G_0. By Proposition 2.1, we have $T_{y_2} = Z_q$ and y_2 is the special pendent vertex of Z_q, where $q \geq 7$. Suppose that w is the unique branching vertex of $V(Z_q) \setminus \{y_2\}$ and $z_1 \in N_{G_0}(y_1) \setminus V(C_4)$. Let $G_2 = G_0 + w_0y_2 + y_1w - w_0y_1 - y_2y_1$. By Lemma 3.1, G_2 is also a k-apex trees with a triangle as its unique cycle.

Since $|V(T_{y_1})| \geq k \geq 3$, we have $d_{G_0}(z_1) \geq 2$ and thus

$$\begin{aligned} AZI(G_0) - AZI(G_2) &= \Psi(3,3) + \Psi\big(d_{G_0}(z_1), 3\big) + (q-3)\Psi(q-2,1) - 16 - (q-3)\Psi(q-1,1) \\ &\geq \Psi(3,3) - 8 > 0, \end{aligned}$$

by Lemma 2.1, a contradiction. □

We need to introduce the following two classes of graphs before proceeding further:
(*i*) Let D_{s_1,s_2,s_3} be the unicyclic graph with unique cycle $C_3 = u_1u_2u_3$ such that $T_{u_1} = K_{1,s_1-1}$ with u_1 being the center vertex of K_{1,s_1-1} and $T_{u_i} = K_{1,s_i-1}$ with u_i being a pendent vertex of K_{1,s_i-1} for $i \in \{2,3\}$, where $s_1 \geq 2$ and $\min\{s_2, s_3\} \geq 3$.
(*ii*) Let E_{s_1,s_2,s_3} be the unicyclic graph with unique cycle $C_3 = u_1u_2u_3$ such that $T_{u_i} = K_{1,s_i-1}$ with u_i being the center vertex of K_{1,s_i-1} for $i \in \{1,2\}$ and $T_{u_3} = Z_{s_3}$ with u_3 being the special pendent vertex of Z_{s_3}, where $\min\{s_1, s_2\} \geq 2$ and $s_3 \geq 4$.

For instance, the graphs $D_{5,6,7}$ and $E_{5,6,7}$ are shown in Fig. 1.1.

Proof of Proposition 3.1. By Lemmas 3.1 and 3.7, $C_3 := u_1u_2u_3$ is the unique cycle of G_0 with

$$d_{G_0}(u_1) = \max\{d_{G_0}(u_i) : 1 \leq i \leq 3\} \text{ and } \min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = k.$$

Case 1. $k \geq 7$. By Proposition 2.1, we have $G_0 = A_{k,s_1,s_2}$, where $s_1 \geq s_2 \geq k \geq 7$. By Lemma 3.2, we have $G_0 = A_{k,\lfloor \frac{n-k}{2} \rfloor, \lceil \frac{n-k}{2} \rceil}$, as desired.

Case 2. $k = 6$. Since $\min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = k = 6$, by Proposition 2.1 and Lemma 3.5, we have $d_{G_0}(u_1) \geq 4$ and $d_{G_0}(u_2) = d_{G_0}(u_3) = 3$. Since $\min\{|V(T_{u_2})|, |V(T_{u_3})|\} \geq 6$, by Proposition 2.1 and Lemma 3.2, we have $G = B_{6,\lceil \frac{n}{2} \rceil - 3, \lfloor \frac{n}{2} \rfloor - 3}$.

Case 3. $k = 5$. If $d_{G_0}(u_1) = 3$, then $d_{G_0}(u_2) = d_{G_0}(u_3) = 3$. Since $\min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = 5$ and Lemma 3.5, there exists some u_i such that $T_{u_i} = K_{1,4}$ and u_i is the center vertex of $K_{1,4}$, a contradiction. Thus, $d_{G_0}(u_1) \geq 4$.

By $\min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = k = 5$, Lemma 3.3 and Proposition 2.1, we can conclude that $d_{G_0}(u_2) = d_{G_0}(u_3) = 3$ and either $T_{u_i} = K_{1,4}$ with u_i being the pendent vertex of $K_{1,4}$ or $T_{u_i} = Z_{q_i}$ with u_i being the special pendent vertex of Z_{q_i}, where $q_i \geq 6$ and $i \in \{2,3\}$. Once again, $\min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = 5$ and Proposition 2.1 imply that $T_{u_1} = K_{1,d_{G_0}(u_1)-2}$ with u_1 as the center vertex of $K_{1,d_{G_0}(u_1)-2}$ and $6 \leq d_{G_0}(u_1) \leq 7$. Next suppose that $|V(T_{u_2})| \geq |V(T_{u_3})| \geq 5$.

If $|V(T_{u_3})| = 5$, then $T_{u_3} = K_{1,4}$ with u_3 being a pendent vertex of $K_{1,4}$. Since $n \geq 18$, $G_0 = C_{d_{G_0}(u_1)-1,5,n-d_{G_0}(u_1)-4}$ by Proposition 2.1, where $n - d_{G_0}(u_1) - 4 \geq 7$ and $6 \leq d_{G_0}(u_1) \leq 7$.

If $|V(T_{u_3})| \geq 6$, then $G_0 = B_{5,s_1,s_2}$ by Proposition 2.1, as $\min\{|V(T_{u_i})| : 1 \leq i \leq 3\} = k = 5$. By Lemma 3.2, we have $G_0 = B_{5,\lceil \frac{n-5}{2} \rceil, \lfloor \frac{n-5}{2} \rfloor}$.

Since $n \geq 18$, we have $AZI(C_{5,5,n-10}) < AZI(C_{6,5,n-11})$ by Lemma 3.4. From the above arguments, we can conclude that $G_0 \in \{C_{5,5,n-10}, B_{5,\lceil \frac{n-5}{2} \rceil, \lfloor \frac{n-5}{2} \rfloor}\}$.

By an elementary computation, we have

$$\begin{aligned} AZI\left(B_{5,\lceil\frac{n-5}{2}\rceil,\lfloor\frac{n-5}{2}\rfloor}\right) - AZI(C_{5,5,n-10}) &> 16 + \frac{(n-9)^3}{(n-11)^2} - 3\left(\frac{4}{3}\right)^3 - \left(\frac{12}{5}\right)^3 - \frac{(n-12)^3}{(n-13)^2} \\ &> \frac{(n-9)^3}{(n-11)^2} - \frac{(n-12)^3}{(n-13)^2} - 5 \\ &= \frac{9n^3 - 332n^2 + 4053n - 16358}{(n-11)^2(n-13)^2} > 0, \end{aligned}$$

and thus $G_0 = C_{5,5,n-10}$.

Case 4. $k = 4$. By the choice of G_0, Lemma 3.5 and $\min\{|V(T_{u_i})| : 1 \le i \le 3\} = k = 4$, we have $d_{G_0}(u_1) \ge 4$. Suppose that $d_{G_0}(u_2) \ge d_{G_0}(u_3)$.

If $d_{G_0}(u_2) \ge 4$, then Proposition 2.1 confirms that either $T_{u_i} = K_{1,3}$ with u_i being the center vertex of $K_{1,3}$ or $T_{u_i} = P_4$ with u_i being a 2-vertex of P_4 for $i \in \{1, 2\}$. Combining this with $n \ge 15$, we have $|V(T_{u_3})| \ge 7$. By Proposition 2.1, $T_{u_3} = Z_q$ with u_3 being the special pendent vertex of Z_q for $q \ge 7$. We claim that $T_{u_i} = K_{1,3}$ with u_i being the center vertex of $K_{1,3}$ for $i \in \{1, 2\}$. Otherwise, assume that $T_{u_1} = P_4$ with u_1 being a 2-vertex of P_4. Let G_1 be the graph obtained from G_0 by replacing T_{u_1} by $K_{1,3}$ such that u_1 is the center vertex of $K_{1,3}$. Suppose that $d_{G_0}(u_2) = s$. Then, $4 \le s \le 5$ and thus

$$\begin{aligned} AZI(G_0) - AZI(G_1) &= \Psi(4,3) + \Psi(s,4) + \Psi(4,1) + 16 - \Psi(5,3) - \Psi(5,s) - 3\Psi(5,1) \\ &\ge \Psi(4,3) + \Psi(5,4) + \Psi(4,1) + 16 - \Psi(5,3) - \Psi(5,5) - 3\Psi(5,1) > 3. \end{aligned}$$

This is impossible and thus $G_0 = E_{4,4,n-8}$.

If $d_{G_0}(u_2) = 3$, then $d_{G_0}(u_3) = 3$. Since $d_{G_0}(u_1) \ge 4$, Proposition 2.1 and Lemma 3.5 imply that $T_{u_1} = K_{1,d(u_1)-2}$ with u_1 being the center vertex of $K_{1,d(u_1)-2}$ for $5 \le d_{G_0}(u_1) \le 7$.

When $6 \le d_{G_0}(u_1) \le 7$, then we suppose that $T_{u_2} = K_{1,3}$ with u_2 being a pendent vertex of $K_{1,3}$ by Lemma 3.3. By Lemmas 3.3–3.4, Proposition 2.1 and $n \ge 15$, we have $G_0 \in \{D_{6,4,5}, C_{5,4,n-9}\}$.

When $d_{G_0}(u_1) = 5$, then Lemmas 3.2–3.3 and Proposition 2.1 imply that $G_0 \in \{C_{4,4,n-8}, C_{4,5,n-9}\}$ for $n \ge 15$ or $G_0 = B_{4,\lceil\frac{n-4}{2}\rceil,\lfloor\frac{n-4}{2}\rfloor}$ for $n \ge 16$.

If $n \ge 15$, then

$$\begin{aligned} &AZI\left(B_{4,\lceil\frac{n-4}{2}\rceil,\lfloor\frac{n-4}{2}\rfloor}\right) - AZI(C_{4,4,n-8}) \ge 16 + \frac{(n-8)^3}{(n-10)^2} - \left(\frac{9}{4}\right)^3 - 2\left(\frac{3}{2}\right)^3 - \frac{(n-10)^3}{(n-11)^2} \\ &= \frac{119n^4 - 4422n^3 + 60483n^2 - 359316n + 777372}{64(n-11)^2(n-10)^2} > 0, \\ &AZI(C_{4,5,n-9}) - AZI(C_{4,4,n-8}) = \left(\frac{12}{5}\right)^3 + 3\left(\frac{4}{3}\right)^3 + \frac{(n-11)^3}{(n-12)^2} - \left(\frac{9}{4}\right)^3 - 2\left(\frac{3}{2}\right)^3 - \frac{(n-10)^3}{(n-11)^2} \\ &> 2.75 + \frac{(n-11)^3}{(n-12)^2} - \frac{(n-10)^3}{(n-11)^2} \\ &= \frac{7n^4 - 322n^3 + 5563n^2 - 42772n + 123460}{4(n-11)^2(n-12)^2} > 0, \text{ and} \\ &AZI(E_{4,4,n-8}) - AZI(C_{4,4,n-8}) = \left(\frac{25}{8}\right)^3 + 3\left(\frac{5}{4}\right)^3 - 2\left(\frac{3}{2}\right)^3 - 2\left(\frac{9}{4}\right)^3 > 6.5. \end{aligned}$$

Combining this with $AZI(D_{6,4,5}) > AZI(C_{4,4,7})$, we have $G_0 = C_{4,4,n-8}$. □

4. G_0 is not a c-cyclic graph with $c \ge 4$

In this section we discard, as AZI minimizers in $\mathbb{T}_n^k$, the k-apex trees whose cyclomatic number exceeds 3.

Proposition 4.1. *Let G_0 be a graph in $\mathbb{T}_n^k$ minimizing the AZI. Then G_0 is not a c-cyclic graph with $c \ge 4$.*

Lemma 4.1. *If $n \ge 15$, then*

$$AZI\left(A_{5,5,n-10}\right) > AZI\left(B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3}\right) > AZI(C_{5,5,n-10}) > AZI(C_{4,4,n-8}).$$

Proof. Since $\frac{6123}{64}-\frac{7088}{81}>8.15$, $\frac{7088}{81}-\frac{6961}{78}>-1.75$ and $\frac{6961}{78}-\frac{5289}{64}>6.5$, by (2.5), (2.6) and (2.8), we have

$$AZI(A_{5,5,n-10})-AZI\left(B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3}\right)>\frac{f_1(n)}{20(n-11)^2(n-13)^2}>0,$$

$$AZI\left(B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3}\right)-AZI(C_{5,5,n-10})>\frac{f_2(n)}{4(n-12)^2(n-13)^2}>0,$$

$$\text{and } AZI(C_{5,5,n-10})-AZI(C_{4,4,n-8})>\frac{f_3(n)}{2(n-11)^2(n-13)^2}>0,$$

where $f_1(n)=83n^4-4164n^3+77946n^2-645332n+1993947$, $f_2(n)=9n^4-414n^3+7081n^2-53320n+148976$ and $f_3(n)=9n^4-432n^3+7770n^2-62056n+185661$. □

Lemma 4.2. *Let G_0 be a graph in $\mathbb{T}_n^k$ minimizing the AZI with $k\geq 4$. If $n\geq 15$, then*

$$AZI(G_0)<2\left(\frac{12}{5}\right)^3+64+(n-9)\left(\frac{n-1}{n-2}\right)^3. \tag{4.1}$$

Furthermore, if $AZI(G_0)=AZI(C_{4,4,n-8})$, then

$$AZI(G_0)<3\left(\frac{9}{4}\right)^3+48+(n-8)\left(\frac{n-1}{n-2}\right)^3. \tag{4.2}$$

Proof. Assume that (4.2) does not hold. Then,

$$\begin{aligned}AZI(G_0)-AZI(C_{4,4,n-8})\geq&3\left(\frac{9}{4}\right)^3+48+(n-8)\left(\frac{n-1}{n-2}\right)^3-\frac{5289}{64}-\frac{(n-10)^3}{(n-11)^2}\\=&\frac{3f_1(n)}{32(n-11)^2(n-2)^3}>0 \text{ for } n\geq 15,\end{aligned} \tag{4.3}$$

where $f_1(n)=27n^5-948n^4+11667n^3-59170n^2+111316n-70168$. This implies that (4.2) holds. Next, assume that (4.1) does not hold, that is,

$$AZI(G_0)\geq 2\left(\frac{12}{5}\right)^3+64+(n-9)\left(\frac{n-1}{n-2}\right)^3. \tag{4.4}$$

Since $2\left(\frac{12}{5}\right)^3+64-\frac{6259}{64}>-6.15$ and $2\left(\frac{12}{5}\right)^3+64-\frac{7088}{81}>4$, we have

$$AZI(G_0)-AZI(A_{7,7,n-14})>\frac{f_2(n)}{20(n-2)^3(n-17)^2}>0 \text{ for } n\geq 21, \text{ and}$$

$$AZI(G_0)-AZI\left(B_{6,\lceil\frac{n}{2}\rceil-3,\lfloor\frac{n}{2}\rfloor-3}\right)>\frac{f_3(n)}{(n-2)^3(n-11)^2(n-13)^2}>0 \text{ for } n\geq 18,$$

where $f_2(n)=37n^5-1900n^4+33325n^3-226450n^2+477940n-318964$ and $f_3(n)=4n^7-246n^6+6060n^5-76199n^4+514188n^3-1786204n^2+2805268n-1607335$. By (4.4), we also have $AZI(G_0)>AZI(C_{5,5,n-10})$ for $15\leq n\leq 17$. This is contrary with the choice of G_0, Corollary 3.1 and Lemma 4.1. □

Lemma 4.3. [16] *Let G be a c-cyclic graph with n vertices. If $n\geq 2c+1$ and $c\geq 3$, then $AZI(G)\geq AZI(W_{n;c,1})$, where the equality holds if and only if $G=W_{n;c,1}$.*

Lemma 4.4. [4] *Let G be a connected graph with two non-adjacent vertices u and v. If $\alpha\leq 1/2$ and $\alpha\neq 0$, then $ABC_\alpha(G+uv)>ABC_\alpha(G)$.*

Lemma 4.5. *Let $n\geq 15$, then $AZI(W_{n;5,1})>AZI(A_{5,5,n-10})$.*

Proof. By (2.4) and (2.5),

$$\begin{aligned}AZI(W_{n;5,1})-AZI(A_{5,5,n-10})&=(n-8)\left(\frac{n-2}{n-3}\right)^3+96-\frac{6123}{64}-\frac{(n-12)^3}{(n-13)^2}\\&>(n-8)\left(\frac{n-2}{n-3}\right)^3-\frac{(n-12)^3}{(n-13)^2}\end{aligned}$$

$$= \frac{5f(n)}{(n-3)^3(n-13)^2} > 0,$$

where $f(n) = n^5 - 38n^4 + 517n^3 - 3056n^2 + 7816n - 7168$. □

In the following, let G_0 be the extremal graph with the minimum AZI among all k-apex trees with $n \geq 3k+3$ vertices, where $k \geq 4$.

If $\delta \geq 2$, then $c \geq 3$, otherwise, G_0 contains at most two 2-vertices in different cycles of G_0 such that the deletion of them will be resulted in a tree, contrary with $k \geq 4$. Since $n \geq 15$, by Lemma 4.4, Corollary 2.1 and (2.5),

$$\begin{aligned} AZI(G_0) - AZI(A_{5,5,n-10}) &\geq 8(n+2) - \frac{6123}{64} - \frac{(n-12)^3}{(n-13)^2} \\ &> 8n - 80 - \frac{(n-12)^3}{(n-13)^2} = \frac{7n^3 - 252n^2 + 3000n - 11792}{(n-3)^2} > 0, \end{aligned}$$

a contradiction. Combining the above fact with Proposition 3.1, we may assume that

$$c \geq 2 \text{ and } \delta = 1.$$

As in [5], a **special cycle** is a cycle with each vertex being a branching vertex. Recall that G_0 is a c-cyclic graph with exactly p pendent vertices. The following result implies that $p \geq n - 11 + c$.

Lemma 4.6. *If $2 \leq c \leq 4$, then $p \geq n - 11 + c$. Moreover, if either $k \geq 5$ or $2 \leq c \leq 3$, then G_0 contains a special cycle.*

Proof. Assume that $p \leq n - 12 + c$.

Case 1. $k = 4$. By Corollary 2.1 and (2.6), we have

$$\begin{aligned} AZI(G_0) - AZI(C_{4,4,n-8}) &\geq 8(n+c-1-p) + p\left(\frac{n-1}{n-2}\right)^3 - \frac{5289}{64} - \frac{(n-10)^3}{(n-11)^2} \\ &\geq 88 + (n-12+c)\left(\frac{n-1}{n-2}\right)^3 - \frac{5289}{64} - \frac{(n-10)^3}{(n-11)^2} \\ &\geq 88 + (n-10)\left(\frac{n-1}{n-2}\right)^3 - \frac{5289}{64} - \frac{(n-10)^3}{(n-11)^2} \qquad (4.5) \\ &> 5 + (n-10)\left(\frac{n-1}{n-2}\right)^3 - \frac{(n-10)^3}{(n-11)^2} \\ &= \frac{f_1(n)}{(n-2)^3(n-11)^2} > 0 \text{ for } n \geq 15, \end{aligned}$$

where $f_1(n) = 6n^5 - 192n^4 + 2163n^3 - 10145n^2 + 18569n - 11630$.

Case 2. $k \geq 5$. We first show that G_0 contains at least one special cycle. Otherwise, assume that G_0 contains no special cycle and thus each cycle of G_0 contains a 2-vertex. Let $G_1 = G_0 - u$, where u is a 2-vertex of some cycle of G_0. Then, G_1 is a $(c-1)$-cyclic graph with $n-1$ vertices. By our hypothesis, every cycle of G_1 is not a special cycle and thus defined $G_2 = G_1 - v$, where v is a 2-vertex of some cycle of G_2. Now, G_2 is a $(c-2)$-cyclic graph with $n-2$ vertices and G_2 contains no special cycle. With the similar reason, since $2 \leq c \leq 4$, we can obtain a tree by deleting at most c vertices from G_0, which implies that G_0 is not a k-apex tree with $k \geq 5$. Thus, G_0 contains at least one special cycle, which implies that G contains at least three $(3^{\geq}, 3^{\geq})$ edges. Combining this with Corollary 2.1, $p \leq n - 12 + c$ and (2.5), we have

$$\begin{aligned} AZI(G_0) - AZI(A_{5,5,n-10}) &\geq 3\left(\frac{9}{4}\right)^3 + 64 + (n-10)\left(\frac{n-1}{n-2}\right)^3 - \frac{6123}{64} - \frac{(n-12)^3}{(n-13)^2} \\ &= \frac{f_2(n)}{2(n-2)^3(n-13)^2} > 0 \text{ for } n \geq 15, \end{aligned}$$

where $f_2(n) = 11n^5 - 400n^4 + 5033n^3 - 25564n^2 + 48566n - 31028$. □

Hereafter, let G_0^* be the graph obtained from G_0 by deleting all the pendent vertices of G_0. Clearly, if G_0 is a c-cyclic graph with p pendent vertices and n vertices, then G_0^* is a c-cyclic graph with $n - p$ vertices.

Proof of Proposition 4.1. Let G_0 be a c-cyclic graph. In view of Lemmas 4.3, 4.4 and 4.5, for $n \geq 15$ and $c \geq 5$, we have the following chain of inequalities

$$AZI(G) \geq AZI(W_{n;c,1}) \geq AZI(W_{n;5,1}) > AZI(A_{5,5,n-10}).$$

Therefore, if $G_0 \in \mathbb{T}_n^k$ minimizes the AZI and $n \geq 15$, then $c \leq 4$.

Next, we shall prove that it is impossible that G_0 is a 4-cyclic graph. By Lemma 4.6, we have $n-7 \leq p \leq n-5$.

Case 1. $p = n-7$. If G_0 contains three $(3^{\geq}, 3^{\geq})$ edges, then

$$AZI(G_0) \geq 3\left(\frac{9}{4}\right)^3 + 56 + (n-7)\left(\frac{n-1}{n-2}\right)^3.$$

Since $3\left(\frac{9}{4}\right)^3 + 58 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). Thus, we suppose that G_0 contains at most two $(3^{\geq}, 3^{\geq})$ edges and thus $k = 4$ by Lemma 4.6.

If G_0 contains one $(3^{\geq}, 3^{\geq})$ edge, then the result follows from (4.3), as $\left(\frac{9}{4}\right)^3 + 72 > 3\left(\frac{9}{4}\right)^3 + 48$. Thus, G_0 contains no $(3^{\geq}, 3^{\geq})$ edge. Combining this with $p = n-7$ and $c = 4$, we can conclude that G_0 must be obtained from $K_{2,5}$ by attaching r and $n-7-r$ pendent vertices to the two 5-vertices of $K_{2,5}$, respectively. Combining this with $k = 4$, we have $r \geq 3$ and thus $\Delta \leq n-5$. By Corollary 2.1 and (2.6), we have

$$\begin{aligned} AZI(G_0) - AZI(C_{4,4,n-8}) &\geq 80 + (n-7)\left(\frac{n-5}{n-6}\right)^3 - \frac{5289}{64} - \frac{(n-10)^3}{(n-11)^2} \\ &> (n-7)\left(\frac{n-5}{n-6}\right)^3 - \frac{(n-10)^3}{(n-11)^2} - 3 \\ &= \frac{f(n)}{(n-11)^2(n-6)^3} > 0 \text{ for } n \geq 15, \end{aligned}$$

where $f(n) = n^5 - 43n^4 + 709n^3 - 5615n^2 + 21440n - 31717$.

Case 2. $p = n-6$. Since $p = n-6$, G_0^* is also a 4-cyclic graphs with at most six vertices. From the table of connected graphs with at most six vertices (see [6]), we can see that G_0^* contains six $(3^{\geq}, 3^{\geq})$ edges, or four $(4^{\geq}, 3^{\geq})$ edges, or three $(4^{\geq}, 4^{\geq})$ edges, or one $(4^{\geq}, 3^{\geq})$ edge and two $(5^{\geq}, 3^{\geq})$ edges, or one $(5^{\geq}, 5^{\geq})$ edge. By Corollary 2.1,

$$AZI(G_0) \geq 6\left(\frac{9}{4}\right)^3 + 24 + (n-6)\left(\frac{n-1}{n-2}\right)^3.$$

Since $6\left(\frac{9}{4}\right)^3 + 24 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4).

Case 3. $p = n-5$. Since $p = n-5$, G_0^* is also a 4-cyclic graphs with at most five vertices. From the table of connected graphs with five vertices (see [6]), we can see that G_0^* contains one $(3^{\geq}, 3^{\geq})$ edge and four $(4^{\geq}, 3^{\geq})$ edges. By Corollary 2.1,

$$AZI(G_0) \geq \left(\frac{9}{4}\right)^3 + 4\left(\frac{12}{5}\right)^3 + 24 + (n-5)\left(\frac{n-1}{n-2}\right)^3.$$

Since $\left(\frac{9}{4}\right)^3 + 4\left(\frac{12}{5}\right)^3 + 24 + 4 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). □

5. G_0 is not a bicyclic graph

For $q \geq 2$, let $Q_{s_1,s_2,\ldots,s_q}$ be a $(q-1)$-cyclic graph obtained from q non-trivial paths $P_{s_1}, P_{s_2}, \ldots, P_{s_q}$ by firstly identifying the vertices $u_1, u_2, \ldots, u_q$ and then identifying the vertices $v_1, v_2, \ldots, v_q$, where u_i, v_i are the two end vertices of P_{s_i} for $i = 1, 2, \ldots, q$, and $s_i = 2$ for at most one $i \in \{1, 2, \ldots, q\}$. In some papers, Q_{s_1,s_2,s_3} is also referred as a Θ-graph. From the definition, $Q_{s_1,s_2,\ldots,s_q}$ contains exactly two q-vertices and each of the other vertices is a 2-vertex. Since G_0 is a k-apex tree with $k \geq 4$, if $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$, then the two 3-vertices of Q_{s_1,s_2,s_3} are two vertices with degree at least four in G_0. Here is the main result of this section.

Proposition 5.1. *Let G_0 be a graph in $\mathbb{T}_n^k$ minimizing the AZI. Then G_0 is not bicyclic.*

We assume that G_0 is a bicyclic graph in the rest of this section. By Lemma 4.6, we can confirm that $p \geq n-9$ and G_0 contains a special cycle C_s. Since G_0 is a bicyclic graph, G_0 contains another cycle C_t.

Lemma 5.1. *If G_0 is a bicyclic graph, then $p \geq n-8$.*

Proof. By Lemma 4.6, assume that $p = n - 9$. If G_0 contains two $(4^{\geq}, 3^{\geq})$ edges or four $(3^{\geq}, 3^{\geq})$ edges, then Corollary 2.1 implies that (4.4) holds, contrary with Lemma 4.2. Thus, G_0 contains at most three $(3^{\geq}, 3^{\geq})$ edges and G_0 contains at most one $(4^{\geq}, 3^{\geq})$ edge. This implies that the special cycle of G_0 is a triangle, each vertex of which is a 3-vertex, and thus $\mathcal{R}(G_0) = B_1$, where $x_0y_0 \notin E(G_0)$ (see Fig. 1.1).

Since G_0 contains at most three $(3^{\geq}, 3^{\geq})$ edges, the two neighbor of y_0 in C_t are two 2-vertices of G_0. Combining this with $p = n - 9$ and G_0 being a k-apex tree with $k \geq 4$, we can conclude that C_t is also a triangle and the two 3-vertices of C_s are adjacent with one 2-vertex of G_0, which is adjacent to a pendent vertex, respectively. This implies that $k = 4$ and G_0 has three $(3^{\geq}, 3^{\geq})$ edges and night edges with a 2-vertex as their end vertex. Since $8 \times 8 + 3\left(\frac{9}{4}\right)^3 > 88$, we have $AZI(G_0) > AZI(C_{4,4,n-8})$ by (4.5). □

Lemma 5.2. *Let G_0 be a bicyclic graph. If one of the followings holds, then $p \geq n - 6$:*
(1) *G_0 contains eight $(3^{\geq}, 3^{\geq})$ edges,*
(2) *G_0 contains one $(4^{\geq}, 4^{\geq})$ edge, two $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$,*
(3) *G_0 contains four $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edges.*

Proof. Since $8\left(\frac{9}{4}\right)^3 + 2 > 4\left(\frac{12}{5}\right)^3 + \left(\frac{9}{4}\right)^3 + 24 + 2 > 2\left(\frac{12}{5}\right)^3 + \left(\frac{16}{6}\right)^3 + \left(\frac{9}{4}\right)^3 + 32 + 2 > 2\left(\frac{12}{5}\right)^3 + 64$, result follows from (4.4). □

Similarly with Lemma 5.2, we can show the following two lemmas:

Lemma 5.3. *Let G_0 be a bicyclic graph. If one of the followings holds, then $p \geq n - 5$:*
(1) *G_0 contains one $(4^{\geq}, 4^{\geq})$ edge, two $(4^{\geq}, 3^{\geq})$ edges and three $(3^{\geq}, 3^{\geq})$ edges,*
(2) *G_0 contains one $(4^{\geq}, 4^{\geq})$ edge and four $(4^{\geq}, 3^{\geq})$ edges,*
(3) *G_0 contains three $(4^{\geq}, 4^{\geq})$ edges,*
(4) *G_0 contains four $(5^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge,*
(5) *G_0 contains four $(4^{\geq}, 3^{\geq})$ edges and three $(3^{\geq}, 3^{\geq})$ edges.*

Lemma 5.4. *Let G_0 be a bicyclic graph. If one of the followings holds, then $p = n - 4$:*
(1) *G_0 contains one $(5^{\geq}, 4^{\geq})$ edges, four $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge,*
(2) *G_0 contains two $(5^{\geq}, 4^{\geq})$ edges, one $(4^{\geq}, 3^{\geq})$ edge and one $(3^{\geq}, 3^{\geq})$ edge,*
(3) *G_0 contains one $(6^{\geq}, 4^{\geq})$ edge, one $(6^{\geq}, 3^{\geq})$ edge and two $(4^{\geq}, 3^{\geq})$ edges.*

Lemma 5.5. [5] *If $G \in \mathbb{T}_n^3$ and $n \geq 14$, then $AZI(G) \geq \frac{8432}{125} + (n-8)\left(\frac{n-4}{n-5}\right)^3$.*

Lemma 5.6. *If $k \geq 5$, then no cycle of G_0 contains 2-vertex.*

Proof. By contradiction, assume that u_0v_0 is an edge of some cycle of G_0 such that u_0 is a 2-vertex of G_0. By Lemma 2.3, we have $G_0 - u_0v_0 \in \mathscr{U}_n^r$ with $k - 1 \leq r \leq k$. Combining this with Lemma 2.4 and the choice of G_0, we may suppose that

$$G_0 - u_0v_0 \in \mathscr{U}_n^{k-1} \text{ and } AZI(G_0) \geq AZI(G_0 - u_0v_0) + 8. \tag{5.1}$$

Case 1. $k \geq 8$. By (5.1), Corollary 3.1 and Proposition 3.1, we have

$$AZI(G_0) > AZI\left(A_{k-1,\left\lfloor\frac{n-k+1}{2}\right\rfloor,\left\lceil\frac{n-k+1}{2}\right\rceil}\right) > AZI\left(A_{k,\left\lfloor\frac{n-k}{2}\right\rfloor,\left\lceil\frac{n-k}{2}\right\rceil}\right),$$

and thus the result already holds.
Case 2. $6 \leq k \leq 7$. By (5.1), Lemma 4.1 and Proposition 3.1, we have

$$AZI(G_0) - AZI\left(A_{5,5,n-10}\right) \geq AZI\left(C_{5,5,n-10}\right) + 8 - AZI\left(A_{5,5,n-10}\right) > 1.5,$$

and thus the result already holds.
Case 3. $k = 5$. By (5.1), $G_0 - u_0v_0 \in \mathscr{U}_n^4$. Combining this with Proposition 3.1, we have

$$\begin{aligned} AZI(G_0) - AZI(C_{5,5,n-10}) &\geq AZI\left(C_{4,4,n-8}\right) + 8 - AZI(C_{5,5,n-10}) \\ &> \frac{(n-10)^3}{(n-11)^2} - \frac{(n-12)^3}{(n-13)^2} \end{aligned}$$

$$= \frac{2(n^4 - 48n^3 + 859n^2 - 6794n + 20044)}{(n-11)^2(n-13)^2} > 0 \text{ for } n \geq 15.$$

This completes the proof of this result. □

Lemma 5.7. *Any cycle of G_0 contains no 2-vertex of G_0.*

Proof. By contradiction, assume that u_0v_0 is an edge of some cycle of G_0 such that u_0 is a 2-vertex of G_0. By Lemma 5.6, we have $k = 4$ and thus $G_0 - u_0v_0 \in \mathscr{U}_n^r$ with $3 \leq r \leq 4$ by Lemma 2.3. Combining this with Lemma 2.4 and the choice of G_0, we may suppose that $G_0 - u_0v_0 \in \mathscr{U}_n^3$.

Since C_s is a special cycle of G_0, G_0 contains three $(3^{\geq}, 3^{\geq})$ edges. If $p \leq n-8$, then Corollary 2.1 implies that (4.3) holds, contrary Lemma 4.2. Thus, $n-4 \leq p \leq n-7$.

If $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$, then let x_0, y_0 be the two 3-vertices of Q_{s_1,s_2,s_3}. Since G_0 is a 4-apex tree, we can conclude that $|V(T_w)| \geq 3$ for each vertex $w \in \{x_0, y_0\}$, where either $d_{G_0}(w) \geq 5$ or w is adjacent with one non-pendent vertex. For convenience, we suppose that $s = s_1 + s_2 - 2$.

If $\mathcal{R}(G_0) \in \{B_1, B_2\}$, then let x_0 and y_0 be the unique cut vertex of C_s and C_t, respectively, where $x_0 = y_0$ when $\mathcal{R}(G_0) = B_2$ (see Fig. 1.1). Since C_t contains a 2-vertex and G_0 is a 4-apex tree, $|V(T_w)| \geq 3$ for each vertex $V(C_s) \setminus \{x_0\}$. This implies that either $d_{G_0}(w) \geq 4$ or w is adjacent with one non-pendent vertex.

Case 1. $p = n-7$. If G_0 contains three $(4^{\geq}, 3^{\geq})$ edges, then the result follows from (4.3), as $3\left(\frac{12}{5}\right)^3 + 40 + 1 > 3\left(\frac{9}{4}\right)^3 + 48$. Thus, we may suppose that G_0 contains at most two $(4^{\geq}, 3^{\geq})$ edges. This implies that $\mathcal{R}(G_0) \neq Q_{s_1,s_2,s_3}$.

Subcase 1.1. $\mathcal{R}(G_0) = B_2$. If $s \geq 4$, then G_0 contains two $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges and thus the result follows from (4.3), as $2\left(\frac{12}{5}\right)^3 + 2\left(\frac{9}{4}\right)^3 + 32 > 3\left(\frac{9}{4}\right)^3 + 48$. Thus, we have $s = 3$ and the two neighbors of C_t of x_0 are two 2-vertices of G_0.

If $t = 3$, then C_t contains a $(2,2)$-edge, say u_1u_2, and thus

$$AZI(G_0) \geq AZI(G_0 - u_1u_2) + 24 - 2\left(\frac{4}{3}\right)^3 > AZI(G_0 - u_1u_2) + 19 \tag{5.2}$$

by (2.2), as $d_{G_0}(x_0) \geq 4$. Since $19 + \frac{8432}{125} > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3) and Lemma 5.5. Combining this with G_0 being a 4-apex tree, we have $t \geq 4$. Since $p = n-7$, C_t contains a 2-vertex of G_0 and G_0 is a 4-apex tree, we can conclude that at least one vertex of $V(C_s) \setminus \{x_0\}$ has degree at least four and thus G_0 contains three $(4^{\geq}, 3^{\geq})$ edges, a contradiction.

Subcase 1.2. $\mathcal{R}(G_0) = B_1$. If $\max\{s,t\} = 4$, then each vertex of $V(C_s) \setminus \{x_0\}$ is a vertex with degree at least four, as C_t contains a 2-vertex of G_0 and G_0 is a 4-apex tree. This implies that G_0 contains three $(4^{\geq}, 3^{\geq})$ edges, a contradiction. Otherwise, $s = t = 3$.

Since G_0 is a 4-apex tree and G_0 contains at most two $(4^{\geq}, 3^{\geq})$ edges, we can conclude that $V(C_s) \setminus \{x_0\}$ has one vertex of degree at least four and exactly one 3-vertex, which is adjacent to one non-pendent vertex. Combining this with $p = n-7$, we have $x_0y_0 \in E(G_0)$. Thus, G_0 contains two $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges. Now, the result follows from (4.3).

Case 2. $p = n-6$.

Subcase 2.1. $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$.

We first suppose that $x_0y_0 \notin E(G_0)$. Since G_0 is a 4-apex tree and $p = n-6$, we have $\max\{d_{G_0}(x_0), d_{G_0}(y_0)\} \geq 6$ and $\min\{d_{G_0}(x_0), d_{G_0}(y_0)\} \geq 4$, and thus G_0 contains two $(6^{\geq}, 3^{\geq})$ edges and two $(4^{\geq}, 3^{\geq})$ edges. Since $2\left(\frac{18}{7}\right)^3 + 2\left(\frac{12}{5}\right)^3 + 24 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3).

We second suppose that $x_0y_0 \in E(G_0)$. If $\max\{d_{G_0}(x_0), d_{G_0}(y_0)\} \geq 5$, then G_0 contains one $(5^{\geq}, 4^{\geq})$ edge and two $(4^{\geq}, 3^{\geq})$ edges and thus the result follows from (4.3), as $2\left(\frac{12}{5}\right)^3 + \left(\frac{20}{7}\right)^3 + 32 > 3\left(\frac{9}{4}\right)^3 + 48$. Thus, x_0 and y_0 are two 4-vertices of G_0, each is adjacent with one branching vertex, respectively, as $p = n-6$ and G_0 is a 4-apex tree. Now,

$$G_0 \text{ contains one } (4^{\geq}, 4^{\geq}) \text{ edge, two } (4^{\geq}, 3^{\geq}) \text{ edges and one } (3^{\geq}, 3^{\geq}) \text{ edge.} \tag{5.3}$$

Since $2\left(\frac{12}{5}\right)^3 + \left(\frac{16}{6}\right)^3 + \left(\frac{9}{4}\right)^3 + 24 + 2 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3).

Subcase 2.2. $\mathcal{R}(G_0) = B_1$. Since G_0 is a 4-apex tree and C_t contains a 2-vertex of G_0, each vertex of $V(C_s) \setminus \{x_0\}$ has degree at least four. Thus, G_0 contains one $(4^{\geq}, 4^{\geq})$ edge, two $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge, and so the result follows from (5.3).

Subcase 2.3. $\mathcal{R}(G_0) = B_2$. If $\max\{s,t\} = 4$, then each vertex of C_s has degree at least four, as G_0 is a 4-apex tree and C_t contains a 2-vertex of G_0. This implies that G_0 contains three $(4^{\geq}, 4^{\geq})$ edges and thus the result follows from Lemma 5.3(3).

Otherwise, $s = t = 3$. Since G_0 is a 4-apex tree and C_t contains a 2-vertex of G_0, C_s contains at least two vertices with degree at least four. By (5.3), we may suppose that the two vertices of $V(C_t) \setminus \{x_0\}$ are both 2-vertices of G_0. From (5.2), the result also holds.

Case 3. $p = n - 5$. If $\mathcal{R}(G_0) = B_2$, then $s = t = 3$ and each of the three vertices of C_s has degree at least four, as G_0 is a 4-apex tree. By Lemma 5.3(3), the result also holds.

If $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$, then $\max\{d_{G_0}(x_0), d_{G_0}(y_0)\} \geq 6$, as $p = n - 5$ and G_0 is a 4-apex tree. Thus, G_0 contains one $(6^{\geq}, 4^{\geq})$ edges, one $(4^{\geq}, 3^{\geq})$ edge and one $(6^{\geq}, 3^{\geq})$ edge. Since $\left(\frac{12}{5}\right)^3 + \left(\frac{18}{7}\right)^3 + \left(\frac{24}{8}\right)^3 + 27 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3).

Case 4. $p = n - 4$. Then, $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$. Since G_0 is a 4-apex tree and $p = n - 4$, $\min\{d_{G_0}(x_0), d_{G_0}(y_0)\} \geq 6$, and thus G_0 contains one $(6^{\geq}, 6^{\geq})$ edges and two $(6^{\geq}, 3^{\geq})$ edges. Since $2\left(\frac{18}{7}\right)^3 + \left(\frac{36}{10}\right)^3 + 16 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3). □

Lemma 5.8. *$\mathcal{R}(G_0)$ contains no cut vertex.*

Proof. We assume that $\mathcal{R}(G_0)$ contains a cut vertex. By Lemma 5.7, both C_s and C_t are special cycles and each of them contains a cut vertex of G_0. By Lemma 5.1, $p \geq n - 8$. Suppose that $V(C_s) \setminus \{x_0\} = \{w_1, w_2, \ldots, w_{s-1}\}$ and $V(C_t) \setminus \{y_0\} = \{z_1, z_2, \ldots, z_{t-1}\}$, where x_0 and y_0 are the cut vertex of C_s and C_t, respectively and $x_0 = y_0$ when $\mathcal{R}(G_0) = B_2$. For convenience, we suppose that

$$d_{G_0}(w_1) \geq d_{G_0}(w_2) \cdots \geq d_{G_0}(w_{s-1}) \text{ and } d_{G_0}(z_1) \geq d_{G_0}(z_2) \cdots \geq d_{G_0}(z_{t-1}).$$

Case 1. $\mathcal{R}(G) = B_1$. Since G_0 contains six $(3^{\geq}, 3^{\geq})$ edges and $6\left(\frac{9}{4}\right)^3 + 24 > 2\left(\frac{12}{5}\right)^3 + 64$, we have $n - 7 \leq p \leq n - 6$ by (4.4).

Subcase 1.1. $p = n - 7$. By Lemma 5.2(1), we have $s = t = 3$. Since $6\left(\frac{9}{4}\right)^3 + 16 > 3\left(\frac{9}{4}\right)^3 + 48$, we have $k \geq 5$ by (4.3). By Lemma 5.2(2), we can conclude that $d_{G_0}(w_2) = d_{G_0}(z_2) = 3$. Suppose that $d_{G_0}(w_1) \geq d_{G_0}(z_1)$. By Lemma 5.2(3), we have $d_{G_0}(z_1) = 3$ and thus exactly one vertex of $\{w_2, z_1, z_2\}$ is adjacent with one non-pendent vertex, as $k \geq 5$ and $p = n - 7$. Combining this with $k \geq 5$ and $p = n - 7$, we have $d_{G_0}(w_1) \geq 4$ and thus G_0 contains two $(4^{\geq}, 3^{\geq})$ edges and five $(3^{\geq}, 3^{\geq})$ edges. Since $5\left(\frac{9}{4}\right)^3 + 2\left(\frac{12}{5}\right)^3 + 8 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4).

Subcase 1.2. $p = n - 6$. Then, $x_0y_0 \in E(G_0)$ and $s = t = 3$. Since $n \geq 15$ and $5\left(\frac{9}{4}\right)^3 + 2\left(\frac{12}{5}\right)^3 > 3\left(\frac{9}{4}\right)^3 + 48$, we have $k \geq 5$ by (4.3). Combining with $k \geq 5$ and G_0 being a k-apex tree, we may suppose that $d_{G_0}(w_1) \geq d_{G_0}(w_2) \geq 4$. This implies that G_0 contains one $(4^{\geq}, 4^{\geq})$ edge, two $(4^{\geq}, 3^{\geq})$ edges and four $(3^{\geq}, 3^{\geq})$ edges, contrary with Lemma 5.3(1).

Case 2. $\mathcal{R}(G_0) = B_2$. Then, G_0 contains four $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges. By Lemma 5.2(3), we have $n - 6 \leq p \leq n - 5$.

Subcase 2.1. $p = n - 6$. By Lemma 5.3 (2) and (5), we have $s = t = 3$ and $d_{G_0}(w) = 3$ holds for each vertex $w \in V(\mathcal{R}(G_0)) \setminus \{x_0\}$. Furthermore, Lemma 5.3(4) implies that $d_{G_0}(x_0) = 4$. Since $n \geq 15$, we may suppose that w_1 is adjacent with some branching vertex of T_{w_1}, contrary with Lemma 5.3(5).

Subcase 2.2. $p = n - 5$. Then, $s = t = 3$. If $d_{G_0}(x_0) \geq 5$, then $k \geq 5$ by (4.3), as $2\left(\frac{9}{4}\right)^3 + 4\left(\frac{15}{6}\right)^3 > 3\left(\frac{9}{4}\right)^3 + 48$. Since G_0 is a k-apex tree with $k \geq 5$ and $p = n - 5$, we may suppose that $d_{G_0}(w_1) \geq 4$, contrary with Lemma 5.4(1). Otherwise, $d_{G_0}(x_0) = 4$.

Since $n \geq 15$, we have $d_{G_0}(w_1) \geq 5$. By Lemma 5.4(2), we have $d_{G_0}(w_2) = 3$ and thus $d_{G_0}(w_1) = 5$ by Lemma 5.4(3). Since $n \geq 15$, we have $d_{G_0}(z_1) \geq 5$, which is contrary with Lemma 5.4(2). □

Proof of Proposition 5.1. By contradiction, assume that G_0 is a bicyclic graph. By Lemmas 5.7 and 5.8, we have $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3}$ and each vertex of every cycle of $\mathcal{R}(G_0)$ is a branching vertex. Since G is a k-apex tree with $k \geq 4$, we may suppose that $d_{\mathcal{R}(G)}(x_0) = d_{\mathcal{R}(G_0)}(y_0) = 3$ and $d_{G_0}(x_0) \geq d_{G_0}(y_0) \geq 4$. With the same reason, we have $\min\{|V(T_{x_0})|, |V(T_{y_0})|\} \geq k \geq 4$, and thus for $w \in \{x_0, y_0\}$, either $d_{G_0}(w) \geq 5$ or $d_{G_0}(w) = 4$, where $d_{G_0}(w) = 4$ implies that the unique neighbor vertex of w in T_w is a non-pendent vertex.

Let $s = s_1 + s_2 - 2$ and $V(C_s) = V(P_{s_1}) \cup V(P_{s_2})$. If $p = n - 4$, then $d_{G_0}(x_0) \geq d_{G_0}(y_0) \geq 6$ and thus the result follows from (4.4), as $2\left(\frac{18}{7}\right)^3 + \left(\frac{36}{10}\right)^3 + 16 > 2\left(\frac{12}{5}\right)^3 + 64$. Thus, $p \leq n - 5$.

Case 1. $u_0v_0 \in E(G)$. In this case, G_0 contains one $(4^{\geq}, 4^{\geq})$ edge and four $(4^{\geq}, 3^{\geq})$ edges. By Lemma 5.3(2), we have $p = n - 5$.

Since $\min\{|V(T_{x_0})|, |V(T_{y_0})|\} \geq k \geq 4$, $d_{G_0}(x_0) \geq 6$ and thus G_0 contains one $(6^{\geq}, 4^{\geq})$ edge, two $(6^{\geq}, 3^{\geq})$ edges and two $(4^{\geq}, 3^{\geq})$ edges, contrary with Lemma 5.4(3).

Case 2. $u_0v_0 \notin E(G)$**.** In this case, G_0 contains six $(4^{\geq}, 3^{\geq})$ edges. If $p \leq n-6$, then the result follows from Lemma 2.1 and (4.4), as $6\left(\frac{12}{5}\right)^3 + 8 + 3 > 2\left(\frac{12}{5}\right)^3 + 64$. Thus, $p = n-5$.

Since $\min\{|V(T_{x_0})|, |V(T_{y_0})|\} \geq k \geq 4$, we have $d_G(u_0) \geq d_G(v_0) \geq 6$ and so G_0 contains six $(6^{\geq}, 3^{\geq})$ edges. Since $6\left(\frac{18}{7}\right)^3 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). □

6. G_0 is not a tricyclic graph

In what follows, we shall show that G_0 is not a tricyclic. Throughout this section, we assume that G_0 is a tricyclic graph. By Lemma 4.6, we have

$n-8 \leq p \leq n-4$ and G_0 contains a special cycle C_s.

Proposition 6.1. *Let G_0 be a graph in $\mathbb{T}_n^k$ minimizing the AZI. Then G_0 is not tricyclic.*

Lemma 6.1. $\mathcal{R}(G_0) \neq K_4$ *and* $p \leq n-5$.

Proof. Since G_0 is a tricyclic graph, it suffices to show that $\mathcal{R}(G_0) \neq K_4$. Assume that $\mathcal{R}(G_0) = K_4$. Since G_0 is a k-apex tree with $k \geq 4$, K_4 contains at least three vertices with degree at least four in G_0. Thus, G_0 contains three $(4^{\geq}, 3^{\geq})$-edges and three $(4^{\geq}, 4^{\geq})$-edges. By Corollary 2.3, we have

$$AZI(G_0) \geq 3\left(\frac{12}{5}\right)^3 + 3\left(\frac{16}{6}\right)^3 + (n-4)\left(\frac{n-1}{n-2}\right)^3.$$

Since $3\left(\frac{12}{5}\right)^3 + 3\left(\frac{16}{6}\right)^3 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). □

Lemma 6.2. *If $k = 4$, then $p = n-5$ when one of the followings holds:*
(1) *G_0 contains two $(5^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge;*
(2) *G_0 contains two $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges;*
(3) *G_0 contains five $(3^{\geq}, 3^{\geq})$ edges or three $(4^{\geq}, 3^{\geq})$ edges or two $(6^{\geq}, 3^{\geq})$ edges.*

Proof. By Lemma 6.1, we assume that $p \leq n-6$. Since $2\left(\frac{15}{6}\right)^3 + \left(\frac{9}{4}\right)^3 + 40 + 2 > 2\left(\frac{18}{7}\right)^3 + 48 + 2 > 3\left(\frac{12}{5}\right)^3 + 40 + 2 > 5\left(\frac{9}{4}\right)^3 + 24 + 2 > 2\left(\frac{12}{5}\right)^3 + 2\left(\frac{9}{4}\right)^3 + 32 > 3\left(\frac{9}{4}\right)^3 + 48$, contrary with (4.3). □

Recall that G_0^* is the graph obtained from G_0 by deleting all the pendent vertices of G_0.

Lemma 6.3. *Let G_0 be a tricyclic graph with $u_0 \in \mathcal{R}(G_0)$.*
(1) *Let u_0 be a vertex of G_0^*. If $G_0^* - u_0$ is a tree, then $d_{G_0}(u_0) \geq d_{G_0^*}(u_0) + k - 1 \geq d_{G_0^*}(u_0) + 3$;*
(2) *Let u_0v_0 be a $(3^{\geq}, 3^{\geq})$ edge of G_0^* such that $u_0x_0 \in E(G_0^*)$ and $v_0y_0 \in E(G_0^*)$, where x_0 and y_0 are both branching vertices of G_0^* and $x_0 = y_0$ is also permitted. If $p = n-6$ and $G_0^* - \{u_0, v_0\}$ is a tree, then $\min\{d_{G_0^*}(x_0), d_{G_0^*}(y_0)\} = 3$ and $x_0y_0 \notin E(G_0^*)$.*

Proof. Since G_0 is a k-apex tree, if $G_0 - V(T_w)$ is a tree for some $w \in \mathcal{R}(G_0)$, then $|V(T_w)| \geq k \geq 4$. Thus, (1) hold clearly. Next we show (2) holds. Assume that $\min\{d_{G_0^*}(x_0), d_{G_0^*}(y_0)\} \geq 4$. If $d_{G_0}(v_0) \geq d_{G_0}(u_0) \geq 4$, then G_0 contains three $(4^{\geq}, 4^{\geq})$ edges. Since $3\left(\frac{16}{6}\right)^3 + 43 > 2\left(\frac{12}{5}\right)^3 + 64$, we can get a contradiction with (4.4). Thus, we may suppose that $d_{G_0}(u_0) = 3$ and thus $d_{G_0}(v_0) \geq 5$, as G_0 is a k-apex tree with $k \geq 4$. By Lemma 6.2(1), we have $k \geq 5$ and thus $d_{G_0}(u_0) = 3$ and $d_{G_0}(v_0) \geq 6$. This implies that G_0 contains one $(6^{\geq}, 4^{\geq})$ edge and one $(6^{\geq}, 3^{\geq})$ edge. Since $\left(\frac{18}{7}\right)^3 + \left(\frac{24}{8}\right)^3 + 48 > 2\left(\frac{12}{5}\right)^3 + 64$, contrary with (4.4). Now, we can conclude that $\min\{d_{G_0^*}(x_0), d_{G_0^*}(y_0)\} = 3$.

If $x_0y_0 \in E(G_0^*)$, then either $\min\{d_{G_0}(u_0), d_{G_0}(v_0)\} \geq 4$ or $\min\{d_{G_0}(u_0), d_{G_0}(v_0)\} = 3$. When $\min\{d_{G_0}(u_0), d_{G_0}(v_0)\} \geq 4$, then G_0 contains one $(4^{\geq}, 4^{\geq})$ edge, two $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge. Since $2\left(\frac{12}{5}\right)^3 + \left(\frac{9}{4}\right)^3 + \left(\frac{16}{6}\right)^3 + 35 > 2\left(\frac{12}{5}\right)^3 + 64$, we can get a contradiction with (4.4). When $\min\{d_{G_0}(u_0), d_{G_0}(v_0)\} = 3$, then $\max\{d_{G_0}(u_0), d_{G_0}(v_0)\} \geq 5$, as G_0 is a k-apex tree with $k \geq 4$. By Lemma 6.2(1), we have $k \geq 5$ and thus $\min\{d_{G_0}(u_0), d_{G_0}(v_0)\} = 3$ and

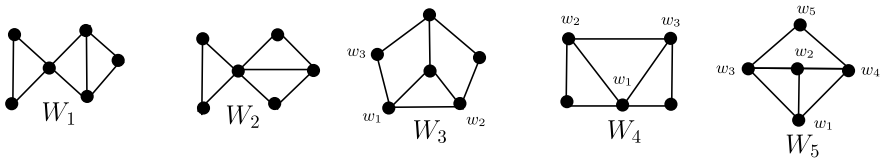


Fig. 6.1. The tricyclic graphs W_1, W_2, ..., W_5.

$\max\{d_{G_0}(u_0), d_{G_0}(v_0)\} \geq 6$. This implies that G_0 contains two $(6^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges. Since $2\left(\frac{18}{7}\right)^3 + 2\left(\frac{9}{4}\right)^3 + 35 > 2\left(\frac{12}{5}\right)^3 + 64$ and (4.4), we have $x_0y_0 \notin E(G_0^*)$. □

In what follows, let W_1, W_2, ..., W_5 be the tricyclic graphs as shown in Fig. 6.1.

Lemma 6.4. *Any cycle of G_0 contains no 2-vertex of G_0 and $n-7 \leq p \leq n-5$.*

Proof. If any cycle of G_0 contains no 2-vertex of G_0, then G_0 contains four $(3^{\geq}, 3^{\geq})$ edges. Since $4\left(\frac{9}{4}\right)^3 + 48 > 2\left(\frac{12}{5}\right)^3 + 64$, we have $p \geq n-7$ by (4.4). Combining this with Lemma 6.1, we have $n-7 \leq p \leq n-5$. Thus, to complete the proof of this result, it suffices to show that any cycle of G_0 contains no 2-vertex of G_0.

By contradiction, assume that u_0v_0 is an edge of some cycle of G_0 such that u_0 is a 2-vertex of G_0. Similar with Lemma 5.6, we have $k=4$ by Proposition 5.1. Combining $k=4$ with Lemmas 2.3 and 2.4, we may suppose that $G_0 - u_0v_0 \in \mathscr{U}_n^3$ by the choice of G_0.

Since C_s is a special cycle of G_0, G_0 contains three $(3^{\geq}, 3^{\geq})$ edges. If $p = n-7$, then Corollary 2.1 implies that

$$AZI(G_0) \geq 3\left(\frac{9}{4}\right)^3 + 48 + (n-7)\left(\frac{n-1}{n-2}\right)^3,$$

and thus the result follows from (4.3). In what follows, we assume that

$$n-6 \leq p \leq n-5.$$

Case 1. $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3,s_4}$**.** Let x_0, y_0 be the two 4-vertices of Q_{s_1,s_2,s_3,s_4} such that $d_{G_0}(x_0) \geq d_{G_0}(y_0)$. Since $n-6 \leq p \leq n-5$, we have $d_{G_0}(x_0) \geq 7$. Thus, G_0 contains two $(7^{\geq}, 3^{\geq})$ edges and one $(4^{\geq}, 3^{\geq})$ edge. Since $\left(\frac{12}{5}\right)^3 + 2\left(\frac{21}{8}\right)^3 + 32 + 2 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3).

Case 2. $\mathcal{R}(G_0)$ **contains a cut vertex.** Since $\mathcal{R}(G_0)$ is a tricyclic graph and $n-6 \leq p \leq n-5$, we have $|V(\mathcal{R}(G_0))| = 6$. In this case, $\mathcal{R}(G_0) \in \{W_1, W_2\}$ and $p = n-6$.

If $\mathcal{R}(G_0) = W_1$, then the two 3-vertices of W_1 are also two 3-vertices of G_0 by Lemma 6.2(3). Combining this with G_0 being a 4-apex tree, we can see that at least one of three 2-vertices of W_1 is a branching vertex of G_0. Thus, G_0 contains two $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges, contrary with Lemma 6.2(2).

If $\mathcal{R}(G_0) = W_2$, then G_0 contains two $(5^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge, as C_s is a special cycle of G_0. This is contrary with Lemma 6.2(1).

Case 3. $\mathcal{R}(G_0)$ **contains no cut vertex.** By Case 1 and Lemma 6.1, we have

$$\mathcal{R}(G_0) \notin \{K_4,\ Q_{s_1,s_2,s_3,s_4}\}.$$

Subcase 3.1. $p = n-6$**.** Let u_0 be a vertex of G_0^* with $d_{G_0^*}(u_0) \geq 4$. If $G_0^* - u_0$ is a tree, then $d_{G_0}(u_0) \geq 7$ by Lemma 6.3(1). By Lemma 6.2(3), u_0 has at most one branching vertex as its neighbor in G_0, and thus it has at least three 2-vertices of G_0 as its neighbors in G_0^*. This implies that we can obtain a tree from G_0 be deleting three neighbors of u_0 in G_0^*, a contradiction.

Thus, for any vertex u of G_0^*, either $d_{G_0^*}(u) \leq 3$ or $G_0^* - u$ is not a tree. Combining this with Lemma 6.3(2), we can conclude that $G_0^* = W_3$ by the table of connected graphs with six vertices (see [6]). By Lemma 6.2(2), we have $d_{G_0}(w_1) = d_{G_0}(w_2) = 3$ and thus $G_0 - \{w_1, w_2\}$ is a tree, a contradiction.

Subcase 3.2. $p = n-5$**.** Since $\mathcal{R}(G_0) \notin \{K_4,\ Q_{s_1,s_2,s_3,s_4}\}$, we have $G_0^* \in \{W_4, W_5\}$ by the table of connected graph with five vertices (see [6]).

If $G_0^* = W_4$, then $d_{G_0}(w_1) \geq 7$ by Lemma 6.3(1). Since G_0 is a 4-apex tree, we may suppose that $d_{G_0}(w_2) \geq 4$. In this case, G_0 contains one $(7^{\geq}, 4^{\geq})$ edge and one $(7^{\geq}, 3^{\geq})$ edge. Since $\left(\frac{28}{9}\right)^3 + \left(\frac{21}{8}\right)^3 + 40 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3).

If $G_0^* = W_5$, then either $d_{G_0}(w_1) \geq d_{G_0}(w_2) \geq 4$ or $d_{G_0}(w_1) \geq 5 > d_{G_0}(w_2) = 3$, as G_0 is a 4-apex tree. In both cases, G_0 contains three $(4^{\geq}, 3^{\geq})$ edges and two $(3^{\geq}, 3^{\geq})$ edges. Since $3\left(\frac{12}{5}\right)^3 + 2\left(\frac{9}{4}\right)^3 + 16 + 3 > 3\left(\frac{9}{4}\right)^3 + 48$, the result follows from (4.3). □

Lemma 6.5. *$\mathcal{R}(G_0)$ contains no cut vertex and $\mathcal{R}(G_0) \neq Q_{s_1,s_2,s_3,s_4}$.*

Proof. By Lemma 6.4, any cycle of G_0 contains no 2-vertex of G_0. By contradiction, we assume that either $\mathcal{R}(G_0)$ contains a cut vertex or $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3,s_4}$.

Case 1. $\mathcal{R}(G_0)$ contains a cut vertex. Since $\mathcal{R}(G_0)$ contains a cut vertex and $\mathcal{R}(G_0)$ is a tricyclic graph, we have $|V(\mathcal{R}(G_0))| \geq 6$ and thus $n-7 \leq p \leq n-6$ by Lemma 6.4.

Since $\mathcal{R}(G_0)$ contains a cut vertex and $\mathcal{R}(G_0)$ is a tricyclic graph, $\mathcal{R}(G_0)$ contains a cycle C_q such that each vertex of $V(C_q) \setminus \{x_0\}$ is a 2-vertex of $\mathcal{R}(G_0)$, where x_0 is a cut vertex of $\mathcal{R}(G_0)$. This implies that $\mathcal{R}(G_0) - \big(V(C_q) \setminus \{x_0\}\big)$ is a bicyclic graph containing at least four vertices and thus G_0 contains eight $(3^{\geq}, 3^{\geq})$ edges. Since $8\left(\frac{9}{4}\right)^3 + 2 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4).

Case 2. $\mathcal{R}(G_0) = Q_{s_1,s_2,s_3,s_4}$. Suppose that $d_{\mathcal{R}(G_0)}(x_0) = d_{\mathcal{R}(G_0)}(y_0) = 4$. By Lemma 6.4, $n-7 \leq p \leq n-5$. Since G_0 is a k-apex tree with $k \geq 4$, we have $\min\big\{|V(T_{x_0})|, |V(T_{y_0})|\big\} \geq k \geq 4$, and thus $d_{G_0}(x_0) \geq d_G(y_0) \geq 5$. Since no cycle of G_0 contains a 2-vertex of G_0, G_0 contains seven $(5^{\geq}, 3^{\geq})$ edges. Now, the result follows from (4.4), as $7\left(\frac{15}{6}\right)^3 > 2\left(\frac{12}{5}\right)^3 + 64$. □

Proof of Proposition 6.1. By contradiction, assume that G_0 is a tricyclic graph. From Lemmas 6.1, 6.4 and 6.5, it follows that

$$n-7 \leq p \leq n-5, \mathcal{R}(G_0) \notin \big\{Q_{s_1,s_2,s_3,s_4},\ K_4\big\} \text{ and } \mathcal{R}(G_0) \text{ contains no cut vertex.} \tag{6.1}$$

If $6 \leq |V(\mathcal{R}(G_0))| \leq 7$, then $\mathcal{R}(G_0)$ contains at least eight $(3^{\geq}, 3^{\geq})$ edges, as $\mathcal{R}(G_0)$ contains no cut vertex and each vertex of $\mathcal{R}(G_0)$ is a branching vertex by Lemmas 6.4 and 6.5. Since $8\left(\frac{9}{4}\right)^3 + 2 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). Next, suppose that $|V(\mathcal{R}(G_0))| = 5$, as $\mathcal{R}(G_0) \neq K_4$. Combining $|V(\mathcal{R}(G_0))| = 5$ and $\mathcal{R}(G_0) \neq Q_{s_1,s_2,s_3,s_4}$, we have $\mathcal{R}(G_0) \in \{W_4, W_5\}$ by the table of connected graphs with five vertices (see [6]). In this case, G_0 contains at least seven $(3^{\geq}, 3^{\geq})$ edges. Since $7\left(\frac{9}{4}\right)^3 + 16 > 2\left(\frac{12}{5}\right)^3 + 64$ and (4.4), we have $n-6 \leq p \leq n-5$.

If $\mathcal{R}(G_0) = W_4$, then $\mathcal{R}(G_0)$ contains four $(4^{\geq}, 3^{\geq})$ edges and three $(3^{\geq}, 3^{\geq})$ edges, as W_4 contains no 2-vertex of G_0. Since $4\left(\frac{12}{5}\right)^3 + 3\left(\frac{9}{4}\right)^3 + 3 > 2\left(\frac{12}{5}\right)^3 + 64$ and $p \geq n-6$, the result follows from (4.4).

Otherwise, $\mathcal{R}(G_0) = W_5$. Since G_0 is k-apex tree with $k \geq 4$, we have $\max\{d_{G_0}(w_1), d_{G_0}(w_2)\} \geq 4$, which implies that G_0 contains three $(4^{\geq}, 3^{\geq})$ edges and four $(3^{\geq}, 3^{\geq})$ edges. Since $3\left(\frac{12}{5}\right)^3 + 4\left(\frac{9}{4}\right)^3 + 8 > 2\left(\frac{12}{5}\right)^3 + 64$ and (4.4), we have $p = n-5$.

If either $d_{G_0}(w_3) = 3$ or $d_{G_0}(w_4) = 3$, then $d_{G_0}(w_1) \geq d_{G_0}(w_2) \geq 5$, as G_0 is a k-apex tree with $k \geq 4$. Thus, G_0 contains five $(5^{\geq}, 3^{\geq})$ edges. Otherwise, $d_{G_0}(w_3) \geq d_{G_0}(w_4) \geq 4$, which implies that G_0 contains six $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge.

Since $6\left(\frac{12}{5}\right)^3 + \left(\frac{9}{4}\right)^3 > 5\left(\frac{15}{6}\right)^3 + 16 > 2\left(\frac{12}{5}\right)^3 + 64$, the result follows from (4.4). □

Declaration of competing interest

There is no competing interest.

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On connected partition with degree constraints ☆

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ABSTRACT

Let s and t be nonnegative integers, and let $f(s,t)$ be the smallest positive integer such that every $f(s,t)$-connected graph G admits a vertex partition (S,T) such that $G[S]$ is s-connected and $G[T]$ is t-connected. An (s,t)-*feasible* partition of graph G is a partition (S,T) of $V(G)$ such that the minimum degree of $G[S]$ and $G[T]$ is at least s and t, respectively, and an (s,t)-feasible partition is said to be *connected* if both $G[S]$ and $G[T]$ are connected. Let $g(s,t)$ be the smallest positive integer such that every graph G with minimum degree at least $g(s,t)$ admits an (s,t)-*feasible* partition. Thomassen conjectured that $f(s,t)=s+t+1$ and $g(s,t)=s+t+1$. The later conjecture was confirmed by Stiebitz, while the former one is still open. In this paper, we improve Hajnal's upper bound $f(s,t)\le 4s+4t-13$ by showing that $f(s,t)\le\left\lceil\frac{19(s-1)}{6}\right\rceil+\left\lceil\frac{19(t-1)}{6}\right\rceil+1$ if $\min\{s,t\}\ge 3$. We also show that any connected graph with an (s,t)-feasible partition also admits a connected (s,t)-feasible partition. This implies that we can extend all the results of [4,5,7–9,11,16] to connected (s,t)-feasible partitions. Finally, we show that if $\min\{s,t\}\ge 2$, then $g(s,t)\le s+t-1$ for $\{K_3,K_{2,3},H_1,H_2,H_3\}$-free graphs, and $g(s,t)\le s+t$ for $\mathbb{K}^+_{2,3}$-free graphs, where $\mathbb{K}^+_{2,3}$ denote the set of graphs obtained from $K_{2,3}$ by adding exactly one edge joining its two vertices, and H_1, H_2 and H_3 are three specific graphs defined in the paper.

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1. Introduction

All graphs considered in this paper are finite and simple. Let G be a graph, let X be a subset of $V(G)$. We use $G[X]$ to denote the subgraph of G induced by X. For a vertex $x\in X$, we use $N_X(x)$ to denote the set of neighbors of x in X, and let $d_X(x)=|N_X(x)|$ (when $X=V(G)$, we simplify $N_X(x)$ and $d_X(x)$ as $N(x)$ and $d(x)$, respectively). Let A and B be two nonempty disjoint subsets of $V(G)$. If $A\cup B=V(G)$, then we call (A,B) a partition of $V(G)$. As usual, let C_q and K_q be the cycle and complete graph with q vertices, respectively, and let $K_{p,q}$ be the complete bipartite graph with p and q vertices in each part.

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Denote by $\mathbb{N}$ the set of nonnegative integers. Let (A, B) be a partition of $V(G)$, and let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. We say that (A, B) is an (a, b)-*feasible partition* if $d_A(x) \geq a(x)$ for each $x \in A$ and $d_B(y) \geq b(y)$ for each $y \in B$. An (a, b)-feasible partition (A, B) is said to be *connected* if both $G[A]$ and $G[B]$ are connected.

For a given graph W, we call a graph G as W-*free* if G does not contain W as its subgraph (note here that W is not necessarily an induced subgraph). Let $\mathbb{W}$ be a set of graphs. A graph is said to be $\mathbb{W}$-*free* if it is W-free for each $W \in \mathbb{W}$.

For positive integers s and t, let $g(s, t)$ be the minimum integer such that every graph G with $\delta(G) \geq g(s, t)$ admits a partition (S, T) with $\delta(G[S]) \geq s$ and $\delta(G[T]) \geq t$. In 1983, Thomassen [17] conjectured that $g(s, t) = s + t + 1$, and 13 years later this conjecture was confirmed by Stiebitz [16]. Actually, Stiebitz [16] had shown a result stronger than the Thomassen's conjecture. That is

Theorem 1.1. [16] *Let G be a graph and $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. If $d(x) \geq a(x) + b(x) + 1$ for each vertex x of G, then G has an (a, b)-feasible partition.*

Later, a series of Stiebitz-type results have been obtained [4,5,7–9,11] (interested readers are referred to recent papers [1, 12–15] for corresponding conclusions concerning with multigraphs that may have multiple edges). For instance, answering a problem of Stiebitz, Kaneko [8] showed that $g(s, t) \leq s + t$ on triangle-free graphs. Then, Diwan [4] proved that $g(s, t) \leq s + t - 1$ on the graphs with girth at least five whenever $\min\{s, t\} \geq 2$, and Gerber and Kobler [5] generalized Diwan's result to the function type. Another interesting conclusion is that Bazgan, Tuza and Vanderpooten [2] presented polynomial time algorithms to find (a, b)-feasible partitions satisfying Stiebitz's, Kaneko's, and Diwan's results, respectively.

The story does not stop. In 2017, the current authors discovered that $g(s, t) \leq s + t$ on $(K_4 - e)$-free graphs with at least four vertices, and $g(s, t) \leq s + t - 1$ on triangle-free graphs in which no two quadrilaterals share edges [11].

Theorem 1.2. [11] *Let G be a $(K_4 - e)$-free graph on at least four vertices, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions. If $d(x) \geq a(x) + b(x)$ for each vertex x, then G admits an (a, b)-feasible partition.*

Theorem 1.3. [11] *Let G be a triangle-free graph in which no two quadrilaterals share edges, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ be two functions. If $d(x) \geq a(x) + b(x) - 1$ for each vertex x, then G admits an (a, b)-feasible partition.*

Later, Hou et al. [7] improved Theorem 1.2 by proving that $g(s, t) \leq s + t$ on the set of graphs with at least five vertices and without any graph obtained by connecting a single vertex to exactly two vertices of $K_4 - e$ as subgraphs.

Theorem 1.4. [7] *Let G be a graph with at least five vertices, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions. If G has no subgraph obtained by connecting a single vertex to exactly two vertices of $K_4 - e$, and $d(x) \geq a(x) + b(x)$ for each vertex x, then G admits an (a, b)-feasible partition.*

In the same paper [7], Hou et al. also proved that, when $\min\{s, t\} \geq 2$, $g(s, t) \leq s + t$ on $K_{2,3}$-free graphs, and $g(s, t) \leq s + t - 1$ on $\{C_3, K_{2,3}, C_8\}$-free graphs.

Theorem 1.5. [7] *Let G be a $K_{2,3}$-free graph, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions. If $d(x) \geq a(x) + b(x)$ for each vertex x of G, then G admits an (a, b)-feasible partition.*

Theorem 1.6. [7] *Let G be a $\{K_3, K_{2,3}, C_8\}$-free graph, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ be two functions. If $d(x) \geq a(x) + b(x) - 1$ for each vertex x, then G admits an (a, b)-feasible partition.*

Ma and Yang [9] improved Diwan's result by showing that $g(s, t) \leq s + t - 1$ on quadrilateral-free graphs. The function type of this result is as follows.

Theorem 1.7. [9] *Let G be a simple graph without C_4, and let $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ be two functions with $d_G(x) \geq a(x) + b(x) - 1$ for each vertex x of G. Then, G admits an (a, b)-feasible partition.*

Disproving a conjecture of [11], Zu [19] discovered a $\{K_3, K_{2,3}\}$-free graph and two functions $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ such that $d(x) \geq a(x) + b(x) - 1$ for each vertex x, but G admits no (a, b)-feasible partition.

We would like to recall another related problem having closely relationship with $g(s, t)$. Let $f(s, t)$ be the smallest positive integer such that the vertex set of each graph of connectivity at least $f(s, t)$ has a partition into two sets which induce subgraphs of connectivity at least s and t, respectively. In 1983, Thomassen [17] and Szegedy (see [6,16]), independently, proved the existence of $f(s, t)$ for each pair of positive integers s and t. As $f(s, t) \geq s + t + 1$ illustrated by the complete graph K_{s+t+1}, Thomassen [18] further conjectured that $f(s, t) = s + t + 1$ for all positive integers s and t. Up to our best knowledge, the best known bound for $f(s, t)$ is

$$f(s,t) \le 4s + 4t - 13 \text{ if } s \ge 3 \text{ and } t \ge 2, \tag{1.1}$$

which is due to Hajnal [6]. Moreover, Stiebitz [16] also confirmed that

$$f(s,t) \le h(s) + h(t) + 1, \tag{1.2}$$

where $h(k)$ denotes the smallest integer such that every graph of minimum degree at least $h(k)$ contains a k-connected subgraph. However, Thomassen's conjecture is still open. In this paper, we first slightly improve (1.1) to

Theorem 1.8. *Let G be a $\left(\left\lceil \frac{19(s-1)}{6} \right\rceil + \left\lceil \frac{19(t-1)}{6} \right\rceil + 1\right)$-connected graph. If $\min\{s,t\} \ge 3$, then G admits a partition (S,T) such that $G[S]$ is s-connected and $G[T]$ is t-connected.*

For $k \ge 2$, let $\varphi(k)$ be the smallest positive real number such that every graph with $n \ge 2\varphi(k)(k-1)+1$ vertices containing no k-connected subgraphs has at most $\varphi(k)(k-1)(n-k+1)$ edges. Let $G_1 \vee G_2$ be the *join graph* of two vertex disjoint graphs G_1 and G_2, that is, $G_1 \vee G_2$ is the graph having vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv\colon u \in V(G_1), v \in V(G_2)\}$. When t is a non-negative integer, then tH denotes the union graph of t copy of the graph H. For $n = kq + r$ with $0 \le r \le k-1$ and $q \ge 1$, it is easily checked that the graph $G_0 = (q-1)K_k \cup \left(2K_r \vee K_{k-r}\right)$ containing no k-connected subgraphs. Since G_0 has n vertices and at least $0.5n(k-1)$ edges, we have $\varphi(k) \ge 0.5$. Similarly with (1.2), we will show that

$$f(s,t) \le \lceil 2\varphi(s)(s-1)\rceil + \lceil 2\varphi(t)(t-1)\rceil + 1 \text{ for } \min\{s,t\} \ge 2. \tag{1.3}$$

In [10], for $n = (k-1)q + r$ with $1 \le r \le k-1$ and $q \ge 2$, Mader discovered that the graph $(k-1)K_1 \vee \left((q-1)K_{k-1} \cup K_r\right)$ containing no k-connected subgraphs has exactly n vertices and at most $(1.5k-2)(n-k+1)$ edges. From this, he conjectured that $\varphi(k) \approx 1.5$ for sufficient large n [10]. Thus, it seems impossible to show Thomassen's conjecture (namely, $f(s,t) = s+t+1$) by (1.3). Perhaps we may try another approach, by asking further connectivity requirements in all the Stiebitz's type results, to approximate Thomassen's conjecture.

Next proposition gives very limited but positive supports to this direction.

Proposition 1.1. *For non-negative integers s and t, every connected graph with minimum degree at least $s+t+1$ has a connected (s,t)-feasible partition.*

Actually, we can extend all results of [4,5,7–9,11,16] by adding connectedness requirements. For doing this, we need to introduce some notations that have been used extensively. Let G be a graph, and let S be a subset of $V(G)$. Recall that for each vertex x of S, $d_S(x)$ denotes the degree of x in $G[S]$. Let y be a vertex in $V(G) \setminus S$. We use $e_G(y,S)$ to denote the number of edges joining y to S.

Let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. We say that S is *a-satisfactory* if $d_S(x) \ge a(x)$ for each vertex x of S, and say that S is *a-degenerate* if each nonempty subset S' of S has a vertex x with $d_{S'}(x) \le a(x)$. An *(a,b)-degenerate partition* is a partition (A,B) such that A is a-degenerate and B is b-degenerate. A pair (A,B) of disjoint subsets A and B of $V(G)$ is called an *(a,b)-feasible pair* if A is a-satisfactory and B is b-satisfactory (an (a,b)-feasible partition is just an (a,b)-feasible pair with union $V(G)$). An (a,b)-feasible pair (A,B) is said to be connected if $G[A]$ and $G[B]$ are both connected. The weight $\omega(A,B)$ of a partition (A,B), due to Stiebitz [16], is defined by

$$\omega(A,B) = |E(G[A])| + |E(G[B])| + \sum_{u \in A} b(u) + \sum_{v \in B} a(v).$$

Then, for each vertex x of A and each vertex $y \in B$,

$$\omega(A \setminus \{x\}, B \cup \{x\}) - \omega(A,B) = e_G(x,B) - d_A(x) + a(x) - b(x), \tag{1.4}$$

and

$$\omega(A \cup \{y\}, B \setminus \{y\}) - \omega(A,B) = e_G(y,A) - d_B(y) + b(y) - a(y). \tag{1.5}$$

All the proofs to results of [4,5,7–9,11,16] begin with the following Proposition 1.2, which was essentially proved by Stiebitz [16].

Proposition 1.2. [16] *Let $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions with $d(x) \ge a(x) + b(x) - 1$ for each vertex x. If G has an (a,b)-feasible pair, then it admits an (a,b)-feasible partition.*

To show Proposition 1.1, we only need to strengthen Proposition 1.2 slightly.

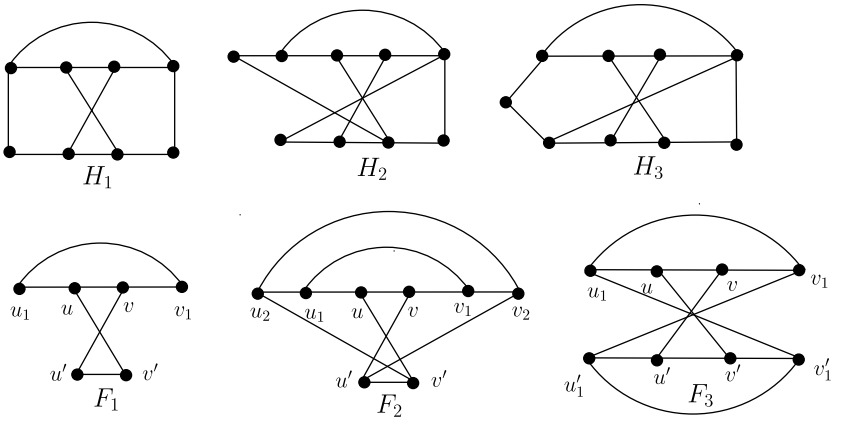


Fig. 1.1. The graphs H_1, H_2, H_3, F_1, F_2, and F_3.

Proposition 1.3. *Let $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions with $d(x) \geq a(x) + b(x) - 1$ for each vertex x, or $a, b : V(G) \longmapsto \mathbb{N}$ with $d(x) \geq a(x) + b(x)$ for each vertex x. If G is connected and has an (a, b)-feasible pair, then it admits a connected (a, b)-feasible partition.*

Following from Proposition 1.2, to show the corresponding partition result on a given graph category $\mathcal{G}$ ([4,5,7–9,11,16]), it suffices to show the existence of an (a, b)-feasible pair for each graph of $\mathcal{G}$. In view of Proposition 1.3, the existence of an (a, b)-feasible pair for each connected graph G of $\mathcal{G}$ guarantees the existence of a connected (a, b)-feasible partition of G, and thus all the proofs of [4,5,7–9,11,16] still work while adding connectedness restriction.

Hereafter, let H_1, H_2, H_3, F_1, F_2 and F_3 be the graphs as shown in Fig. 1.1, and let $\mathbb{K}^+_{2,3}$ be the set of graphs obtained from $K_{2,3}$ by adding exactly one edge joining its two vertices ($\mathbb{K}^+_{2,3}$ contains exactly two elements). Here below our results Theorems 1.9 and 1.10 generalize Theorems 1.4, 1.5 and 1.6 of [7], and Theorem 1.3 of [11], respectively.

Theorem 1.9. *Let G be a connected $\mathbb{K}^+_{2,3}$-free graph, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ two functions such that $d(x) \geq a(x) + b(x)$ for each vertex x and $\min\{a(u) + a(v), b(u) + b(v)\} \geq 3$ for each edge uv of G. Then, G admits a connected (a, b)-feasible partition.*

As mentioned in [11], by setting $a(x) = d(x) - 1$ and $b(x) = 1$ for each vertex of the graph icosahedron or $K_4 - e$, the condition $\min\{a(u) + a(v), b(u) + b(v)\} \geq 3$ is necessary in Theorem 1.9.

Theorem 1.10. *Let G be a connected $\{K_3, K_{2,3}, H_1, H_2, H_3\}$-free graph, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ two functions with $d(x) \geq a(x) + b(x) - 1$ for each vertex x. Then, G admits a connected (a, b)-feasible partition.*

Since the two graphs of $\mathbb{K}^+_{2,3}$ can be obtained from $K_4 - e$ by connecting a single vertex to exactly two vertices of $K_4 - e$, and since it has been shown that $\min\{a(u) + a(v), b(u) + b(v)\} \geq 3$ for each edge uv of any graph G as described in Theorem 1.4 (see Claim 5.1 of [7]), Theorem 1.9 improves both Theorems 1.4 and 1.5.

Since each of H_1, H_2 and H_3 contains two quadrilaterals sharing one edge, and also contains a C_8, Theorem 1.10 improves both Theorems 1.3 and 1.6. Note that each of H_1, H_2 and H_3 containing a cycle C_q for each $q \in \{5, 6, 7, 8\}$. Thus, Theorem 1.10 asserts that $g(s, t) \leq s + t - 1$ on $\{K_3, K_{2,3}, C_q\}$-free graphs for some $q \in \{5, 6, 7, 8\}$.

The paper is organized as follows. We first prove Theorem 1.8 in Section 2, and then prove Proposition 1.3 in Section 3. The proofs of Theorems 1.9 and 1.10 will be in Sections 4 and 5, respectively.

2. Proof of Theorem 1.8

This section is devoted to the proof of Theorem 1.8. We need a lemma from [3].

Lemma 2.1. [3] *If $k \geq 3$, then every graph G with $|V(G)| \geq \frac{5}{2}(k-1)$ and $|E(G)| > \frac{19}{12}(k-1)(n-k+1)$ contains a k-connected subgraph.*

For proving Theorem 1.8, we first show (1.3). Let G be a $(\lceil 2\varphi(s)(s-1)\rceil + \lceil 2\varphi(t)(t-1)\rceil + 1)$-connected graph with n vertices. Then, $\delta(G) \geq \lceil 2\varphi(s)(s-1)\rceil + \lceil 2\varphi(t)(t-1)\rceil + 1$, and so by Theorem 1.1, G admits a partition (S, T) such that $\delta(G[S]) \geq \lceil 2\varphi(s)(s-1)\rceil$ and $\delta(G[T]) \geq \lceil 2\varphi(t)(t-1)\rceil$. Then,

$$|S| \geq \delta(G[S]) + 1 \geq 2\varphi(s)(s-1) + 1, \text{ and } |E(G[S])| \geq \frac{1}{2}\delta(G[S])|S| \geq \varphi(s)(s-1)|S|.$$

Since $|E(G[S])| \geq \varphi(s)(s-1)|S| > \varphi(s)(s-1)(|S|-s+1)$, we see that $G[S]$ contains an s-connected subgraph according to the definition of $\varphi(s)$. Similarly, $G[T]$ has a t-connected subgraph.

Let A and B be two disjoin subsets of $V(G)$ such that $G[A]$ is s-connected, $G[B]$ is t-connected, and $A \cup B$ is maximum. We show that $A \cup B = V(G)$. By way of contradiction, assume that $V(G) \setminus (A \cup B) = Z \neq \emptyset$. It is certain that $G[A \cup Z]$ is not s-connected and thus has a cutset, say A', with at most $s-1$ vertices. Let G_1 be a component of $G[A \cup Z] - A'$ such that $V(G_1) \subset Z$. Since $G[A]$ is s-connected, such a G_1 must exist. Since $G[B \cup V(G_1)]$ is not t-connected, we may choose B' to be a cutset of $G[T \cup V(G_1)]$ with $|B'| \leq t-1$. Let G_2 be a component of $G[T \cup V(G_1)] - B'$ such that $V(G_2) \subseteq V(G_1)$. Since $G[T]$ is t-connected, G_2 is disjoint with any other component of $G - (A' \cup B')$. Thus, $A' \cup B'$ is a cutset of G with $|A' \cup B'| \leq s+t-2$. This contradicts the fact that $\lceil 2\varphi(s)(s-1) \rceil + \lceil 2\varphi(t)(t-1) \rceil + 1 \geq s+t-1$, as $\varphi(k) \geq 0.5$ for $k \geq 2$.

Proof of Theorem 1.8. By the proof of (1.3) and Lemma 2.1, G admits a partition (S, T) such that $|S| \geq \frac{19(s-1)}{6} + 1$, $|T| \geq \frac{19(t-1)}{6} + 1$, $|E(G[S])| > \frac{19}{12}(s-1)(|S|-s+1)$, and $|E(G[T])| > \frac{19}{12}(t-1)(|T|-t+1)$. Since $\frac{19(k-1)}{6} + 1 > \frac{5}{2}(k-1)$, we have $\varphi(k) \leq \frac{19}{12}$ by Lemma 2.1. Now, Theorem 1.8 follows from (1.3). □

3. Proof of Proposition 1.3

The proof of Proposition 1.3 is a simple slightly revision of that of Proposition 1.2 due to Stiebitz [16].

Proof of Proposition 1.3. Suppose that G has an (a, b)-feasible pair. Then, G must contain a connected (a, b)-feasible pair. Throughout this proof, we choose (A, B) as a connected (a, b)–feasible pair maximizing $|A \cup B|$, and assume that $A \cup B \neq V(G)$.

Let $C = V(G) \setminus A$, and let $D = C \setminus B$. Since $A \cup B \neq V(G)$, we have that $D \neq \emptyset$.

If C is not b-satisfactory, then there exists a vertex, say y, in D such that $d_C(y) \leq b(y) - 1$, and hence $d_{A\cup\{y\}}(y) = d(y) - d_C(y) \geq a(y)$ when $d(y) \geq a(y) + b(y) - 1$ and $d_{A\cup\{y\}}(y) \geq a(y) + 1$ when $d(y) \geq a(y) + b(y)$. In both case, $(A \cup \{y\}, B)$ is still a connected (a, b)-feasible pair of G, contradicting the choice of (A, B).

Therefore, we assume that C is b-satisfactory. By the maximality of $|A \cup B|$, $G[C]$ is not connected, of which $G[B]$ is a component. Suppose that $G[C]$ consists of $k+1$ components, say $G[B]$, $G_1, G_2, \cdots$, and G_k, where for each $i \in \{1, 2, \ldots, k\}$, G_i is connected and $V(G_i)$ is b-satisfactory. But now, $G[A \cup D]$ is connected by the connectedness of G. Since B is a component of $G[C]$, for each vertex x of D, $N_B(x) = \emptyset$ and thus $d_{G[A\cup D]}(x) = d(x) \geq a(x)$. Therefore, $(A \cup D, B)$ is a connected (a, b)-feasible partition, again contradicting the choice of (A, B). This proves Proposition 1.3. □

4. Proof of Theorem 1.9

We prove Theorem 1.9 in this section. Let $\mathcal{G}$ be the set of connected $\mathbb{K}^+_{2,3}$-free graphs, and let G be a graph in $\mathcal{G}$ throughout this section. Assume to the contrary that G has no connected (a, b)-feasible partition. By Proposition 1.3,

$$G \text{ has no } (a, b)\text{-feasible pair.} \tag{4.1}$$

Note that if there exists an $x \in V(G)$ such that $d(x) > a(x) + b(x)$, then we can reset $a(x)$ as $a'(x)$ such that $d(x) = a'(x) + b(x)$, and reset $a'(y) = a(y)$ for each vertex of G other than x. Clearly, if G admits a connected (a', b)-feasible partition, then G also admits a connected (a, b)-feasible partition. Thus, we may suppose that

$$d(x) = a(x) + b(x) \text{ for each } x \in V(G). \tag{4.2}$$

Let A be a minimum a-satisfactory subset of $V(G)$ (such an A must exist as $V(G)$ itself is $(a+1)$-satisfactory), and let $B = V(G) \setminus A$. By the minimality of A, A is a-degenerate and there exists a vertex in A, say x, such that $d_A(x) = a(x) \geq 1$. By (4.2), we have $e_G(x, B) = b(x) \geq 1$, and so $B \neq \emptyset$.

Since A is a-satisfactory, no subset of B may be b-satisfactory by (4.1). Therefore, B is $(b-1)$-degenerate, and so (A, B) is an $(a, b-1)$-degenerate partition of G.

Hereafter, we choose (A, B) to be an $(a, b-1)$-degenerate partition such that

(*i*) $\omega(A, B)$ is maximum among all $(a, b-1)$-degenerate partitions of G, and
(*ii*) subject to (*i*), $|A|$ is as small as possible.

We define $A^* = \{u \in A \mid d_A(u) \leq a(u)\}$ and $B^- = \{v \in B \mid d_B(v) \leq b(v) - 1\}$. Then $A^* \neq \emptyset \neq B^-$. Let u be a vertex of A^*, and v be a vertex of B^-. Then, $|A| \geq e_G(v, A) = d(v) - d_B(v) \geq a(v) + 1 \geq 2$ by (4.2).

If $B = \{v\}$, then $\omega(A \setminus \{u\}, B \cup \{u\}) - \omega(A, B) \geq b(u) - a(u) + a(u) - b(u) = 0$ (by (1.4)). Since $A \setminus \{u\} \neq \emptyset$, and it is still a-degenerate, by the choice of (A, B), $B \cup \{u\}$ cannot be $(b-1)$-degenerate, and thus is b-satisfactory, which implies that $b(v) \leq d_{B\cup\{u\}}(v) = 1 = d_{B\cup\{u\}}(u) \geq b(u)$ and $uv \in E(G)$. This contradicts the assumption $b(u) + b(v) \geq 3$ of Theorem 1.9. Therefore,

$$\min\{|A|, |B|\} \geq 2. \tag{4.3}$$

Let v_0 be a vertex of B^-, and let $A' = A \cup \{v_0\}$ and $B' = B \setminus \{v_0\}$. Then, $d_B(v_0) \leq b(v_0) - 1$, and by (1.5) and (4.2), $\omega(A', B') - \omega(A, B) \geq a(v_0) + 1 - (b(v_0) - 1) + b(v_0) - a(v_0) = 2$. Since B' is $(b-1)$-degenerate, A' is not a-degenerate by the choice of (A, B). So, there exists a subset A_0 of A such that $A_0 \cup \{v_0\}$ is $(a+1)$-satisfactory, which implies that A_0 is a-satisfactory. Our next claim shows that A is also a-satisfactory.

Claim 4.1. *A is a-satisfactory, and $\{u \in A \mid d_A(u) = a(u)\} \neq \emptyset$.*

Proof. We choose A'_0 to be a maximal a-satisfactory subset of A (since A_0 is a-satisfactory, $A'_0 \neq \emptyset$), and we will show that $A'_0 = A$. Otherwise, assume that $A'_0 \neq A$. Let x be a vertex in $A \setminus A'_0$ with $d_A(x) \leq a(x) - 1$. Then $e_G(x, B) \geq b(x) + 1$ by (4.2). Since $A'_0 \subseteq A \setminus \{x\}$, $B \cup \{x\}$ must be $(b-1)$-degenerate by (4.1). On the other hand, $A \setminus \{x\}$ is certainly a-degenerate, and $\omega(A \setminus \{x\}, B \cup \{x\}) - \omega(A, B) \geq b(x) + 1 - (a(x) - 1) + a(x) - b(x) = 2$ by (1.4), contradicting the maximality of $\omega(A, B)$. Therefore, $A'_0 = A$ implies that A is a-degenerate and also a-satisfactory. It is certain that $\{u \in A \mid d_A(u) = a(u)\} \neq \emptyset$. □

From Claim 4.1, we see that $d_A(u) = a(u)$ for each vertex u of A^*, i.e.,

$$A^* = \{u \in A \mid d_A(u) = a(u)\}. \tag{4.4}$$

Claim 4.2. *Let u be a vertex of A^*, and v a vertex of B^-. Then, $uv \in E(G)$, and $d_B(y) = b(y) - 1$ for each vertex y of B^-, i.e.,*

$$B^- = \{y \mid y \in B \text{ and } d_B(y) = b(y) - 1\}. \tag{4.5}$$

Proof. Since $\omega\big(A \setminus \{u\}, B \cup \{u\}\big) - \omega(A, B) \geq b(u) - a(u) + a(u) - b(u) = 0$, and $\omega\big(A \cup \{v\}, B \setminus \{v\}\big) - \omega(A, B) \geq a(v) + 1 - \big(b(v) - 1\big) + b(v) - a(v) = 2$ (by (1.4) and (1.5)), by the choice of (A, B), we can conclude that $B \cup \{u\}$ is not $(b-1)$-degenerate and $A \cup \{v\}$ is not a-degenerate. Consequently, we may choose A' to be an $(a+1)$-satisfactory subset of $A \cup \{v\}$, and choose B' to be a b-satisfactory subset of $B \cup \{u\}$.

If $uv \notin E(G)$, then $u \notin A'$ and $v \notin B'$ which imply that (A', B') is an (a, b)-feasible pair of G, a contradiction. Therefore, $uv \in E(G)$.

Since every b-satisfactory subset of $B \cup \{u\}$ must contain v (as $uv \in E(G)$ and $e_G(u, B) = b(u)$ by (4.2) and (4.4)), we have $d_B(v) = b(v) - 1$ and so (4.5) holds. □

Claim 4.3. *Let v_0 be a vertex of B^-, and let A_0 be an a-satisfactory subset of A such that $A_0 \cup \{v_0\}$ is $(a+1)$-satisfactory. Then, $A^* \subseteq N_{A_0}(v_0)$.*

Proof. Since $A_0 \cup \{v_0\}$ is $(a+1)$-satisfactory and $e_G(v_0, A) = a(v_0) + 1$ by (4.2) and (4.5), every neighbor of v_0 in A belongs to $A_0 \cup \{v_0\}$. Combining this with $A^* \subseteq N(v_0)$ by Claim 4.2, it follows that $A^* \subseteq N_{A_0}(v_0)$. □

Claim 4.4. *For each vertex $u \in A^*$, $N_{A^*}(u) \neq \emptyset$, and $|A| \geq 3$.*

Proof. Let u be a vertex of A^*, and assume that $N_{A^*}(u) = \emptyset$. By (4.3), $A \setminus \{u\}$ is not empty and is a-satisfactory since A is a-satisfactory by Claim 4.1. On the other hand, since $e_G(u, B) = d(u) - d_A(u) = b(u)$ by (4.2) and (4.4), $B \cup \{u\}$ is b-satisfactory by Claim 4.2, and so $(A \setminus \{u\}, B \cup \{u\})$ is an (a, b)-feasible partition of G. This contradiction shows that $N_{A^*}(u) \neq \emptyset$. Let x be a neighbor of u in A^*. Now, $d_A(u) + d_A(x) = a(u) + a(x) \geq 3$, and so $|A| \geq 3$. □

Now, let us choose $x_0 \in A^*$ and $v_0 \in B^-$, and let $S_1 = (A \setminus \{x_0\}) \cup \{v_0\}$ and $T_1 = (B \setminus \{v_0\}) \cup \{x_0\}$.

Claim 4.5. *(S_1, T_1) is also a maximum $(a, b-1)$-degenerate partition of G.*

Proof. Since every $(a+1)$-satisfactory subset of $A \cup \{v_0\}$ must contain v_0 and so contains all its neighbors in A by (4.2) and (4.5), and since every b-satisfactory subset of $B \cup \{x_0\}$ must contain x_0 and so contains all its neighbors in B by (4.2) and (4.4), (S_1, T_1) is also an $(a, b-1)$-degenerate partition of G as $v_0x_0 \in E(G)$ by Claim 4.2. By Claims 4.1 and 4.2, $\omega(S_1, T_1) - \omega(A, B) = b(x_0) - 1 + a(v_0) + a(x_0) + b(v_0) - (a(x_0) + b(v_0) - 1 + b(x_0) + a(v_0)) = 0$. Thus, (S_1, T_1) is also a maximum $(a, b-1)$-partition of G. □

By Claim 4.4, $G[A^*]$ has at least one edge. Since $G \in \mathcal{G}$, and since the complete bipartite graph $K_{|A^*|,|B^-|}$ is a subgraph of $G[A^* \cup B^-]$ by Claim 4.2, $|B^-| \leq 2$.

Claim 4.6. $|B^-| = 1$.

Proof. If it is not the case, we may assume that $B^- = \{v_0, w_0\}$. By Claim 4.4, A^* has a pair of adjacent vertices. Since $G \in \mathcal{G}$, and since $G[A^* \cup B^-]$ is a complete bipartite graph, we may assume that $A^* = \{x_0, y_0\}$ with $x_0y_0 \in E(G)$.

Now, Claim 4.4 implies that $A \setminus \{x_0, y_0\} \neq \emptyset$ and each vertex in $A \setminus \{x_0, y_0\}$ is adjacent to at most one of x_0 and y_0. So, $A \setminus \{x_0, y_0\}$ is a-satisfactory (note $A^* = \{x_0, y_0\}$). By Claim 4.2 and (4.4), $B \cup \{x_0, y_0\}$ is b-satisfactory, and an (a, b)-feasible partition $(A \setminus \{x_0, y_0\}, B \cup \{x_0, y_0\})$ appears, a contradiction. Therefore, $|B^-| = 1$. □

Claim 4.7. *Let $B^- = \{v_0\}$, and let $v_1 \in N_B(v_0)$ with $d_B(v_1) = b(v_1)$. Then, $A^* \subseteq N(v_1)$ and $|A^*| = 2$.*

Proof. Suppose that $A^* \nsubseteq N(v_1)$, let x_0 be a vertex of A^* with $x_0v_1 \notin E(G)$. As before, denote by $S_1 = (A \setminus \{x_0\}) \cup \{v_0\}$ and $T_1 = (B \setminus \{v_0\}) \cup \{x_0\}$. By Claim 4.5, (S_1, T_1) is a maximum $(a, b-1)$-degenerate partition of G, and $|S_1| = |A|$. Recall that Claim 4.6 holds on all $(a, b-1)$-degenerate partition satisfying both (i) and (ii). But now, since $x_0v_1 \notin E(G)$, $T_1^- = \{v_1, x_0\}$, contradicting Claim 4.6. Therefore, $A^* \subseteq N(v_1)$.

Since $G[A^*]$ contains at least one edge by Claim 4.4, and since the complete bipartite graph $K_{|A^*|,2}$ is a subgraph of $G[A^* \cup \{v_0, v_1\}]$ by Claim 4.2, $|A^*| = 2$ as otherwise a member of $\mathbb{K}^+_{2,3}$ would appear in G. □

Now, we proceed to complete the proof of Theorem 1.9. Since $|B^-| = 1$ by Claim 4.6, we suppose that $B^- = \{v_0\}$. Since B is $(b-1)$-generate, and since $|B| \geq 2$ by (4.3), we may choose a vertex, say v_1, in $N_B(v_0)$ with $d_B(v_1) = b(v_1)$. By Claims 4.4 and 4.7, we suppose that $A^* = \{x_0, y_0\}$ with $x_0y_0 \in E(G)$. Then, $G[\{x_0, y_0, v_0, v_1\}] = K_4$ by Claims 4.2 and 4.7.

Since $A \setminus \{x_0, y_0\} \neq \emptyset$ by Claim 4.4, and since every vertex of $A \setminus \{x_0, y_0\}$ is adjacent to at most one of x_0 and y_0, $A \setminus \{x_0, y_0\}$ is a-satisfactory, as $A^* = \{x_0, y_0\}$. By Claim 4.2, $B \cup \{x_0, y_0\}$ is b-satisfactory. Now, an (a, b)-feasible partition appears. This contradiction to (4.1) proves Theorem 1.9. □

5. Proof of Theorem 1.10

This section is dedicated to the proof of Theorem 1.10. Throughout this section, we suppose that G is a connected $\{K_3, K_{2,3}, H_1, H_2, H_3\}$-free graph, and let $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ be two functions with $d(x) \geq a(x) + b(x) - 1$ for each vertex x of G.

By Proposition 1.3, we suppose that (4.1) still holds, and by using the same argument as used to prove (4.2), we may suppose that, for every vertex v of G,

$$d(v) = a(v) + b(v) - 1. \tag{5.1}$$

Since G is triangle-free, we have $|N(u) \cap N(v)| = \emptyset$ for every edge uv of G. This observation will be used frequently during the proof.

Recall that, for functions $p, q : V(G) \longmapsto \mathbb{N}$, a partition (S, T) is said to be (p, q)-degenerate if S is p-degenerate and T is q-degenerate simultaneously. In what follows, an $(a-1, b-1)$-degenerate partition will be simplified as an (a, b)-*partition*.

Claim 5.1. *G admits an (a, b)-partition.*

Proof. Let S be an a-satisfactory subset of $V(G)$ of minimum size, and let $T = V(G) \setminus S$. Then, $T \neq \emptyset$ as $d(w) = a(w) + b(w) - 1 \geq a(w) + 1$ for each vertex w, and T must be $(b-1)$-degenerate as otherwise we would have an (a, b)-feasible pair. By the minimality of $|S|$, each proper subset of S is $(a-1)$-degenerate, and S must have a vertex, say x, with $d_S(x) = a(x)$. Since $e_G(x, T) = b(x) - 1$ by (5.1), $(S \setminus \{x\}, T \cup \{x\})$ is an (a, b)-partition in G. □

An (a, b)-partition (A, B) is called a *maximum* (a, b)-*partition* if $\omega(A, B)$ reaches maximum among all (a, b)-partitions. From now on, we always assume that (A, B) is a maximum (a, b)-partition.

Let $A^- = \{x \,|\, x \in A, d_A(x) \leq a(x) - 1\}$, $A^= = \{x \,|\, x \in A, d_A(x) = a(x)\}$, and let $A^+ = A \setminus (A^- \cup A^=)$. Analogously, we define B^-, $B^=$ and B^+.

Since (A, B) is an (a, b)-partition, $A^- \neq \emptyset \neq B^-$. Let $u \in A^-$ and $v \in B^-$. Then, $e_G(u, B) \geq b(u) \geq 2$ and $e_G(v, A) \geq a(v) \geq 2$ by (5.1), and thus $|A| \geq 2$ and $|B| \geq 2$. It follows from (1.4) and (1.5) that

$$\omega(A \setminus \{u\}, B \cup \{u\}) - \omega(A, B) \geq b(u) - (a(u) - 1) - b(u) + a(u) = 1, \tag{5.2}$$

and

$$\omega(A \cup \{v\}, B \setminus \{v\}) - \omega(A, B) \geq a(v) - (b(v) - 1) - a(v) + b(v) = 1. \tag{5.3}$$

So, $A \cup \{v\}$ cannot be $(a-1)$-degenerate, and $B \cup \{u\}$ cannot be $(b-1)$-degenerate. Let A' be an a-satisfactory subset of $A \cup \{v\}$, and B' a b-satisfactory subset of $B \cup \{u\}$. If $u \notin A'$ and $v \notin B'$, then (A', B') is an (a, b)-feasible pair. Therefore, for each pair of vertices $u \in A^-$ and $v \in B^-$, either every a-satisfactory subset of $A \cup \{v\}$ must include u, or every b-satisfactory subset of $B \cup \{u\}$ must include v. Actually, we can have more than that.

Claim 5.2. *Let u be a vertex of A^-, and v a vertex of B^-. Then,*

(*i*) *$A \cup \{v\}$ is not $(a-1)$-degenerate and every a-satisfactory subset of $A \cup \{v\}$ must include u, and $B \cup \{u\}$ is not $(b-1)$-degenerate and every b-satisfactory subset of $B \cup \{u\}$ must include v.*
(*ii*) *$uv \in E(G)$, and*

$$A^- = \{x \mid x \in A, d_A(x) = a(x) - 1\} \text{ and } B^- = \{y \mid y \in B, d_B(y) = b(y) - 1\}.$$

Proof. By (5.3), $A \cup \{v\}$ is not $(a-1)$-degenerate. If there exists some a-satisfactory subset of $A \cup \{v\}$ not including u, then every b-satisfactory subset of $B \cup \{u\}$ must include v (as otherwise an (a,b)-feasible pair would appear), and hence $d_G(v) \geq a(v) + b(v)$, contradicting (5.1). A similar contradiction occurs if there exists some b-satisfactory subset of $B \cup \{u\}$ not including v. Therefore, (*i*) holds. Since $u \in A^-$ and $v \in B^-$, $uv \in E(G)$, and $d_A(u) = a(u) - 1$ and $d_B(v) = b(v) - 1$ as desired in (*ii*). □

Claim 5.3. *Let u be a vertex of A^- with a neighbor $u_1 \in A^=$, and v be a vertex of B^- with a neighbor $v_1 \in B^=$. Then, $u_1v_1 \in E(G)$.*

Proof. Let $A_1 = (A \cup \{v\}) \setminus \{u\}$ and $B_1 = (B \cup \{u\}) \setminus \{v\}$. Since $\omega(A_1, B_1) - \omega(A, B) = (b(u) - 1 + a(v) - 1 + a(u) + b(v)) - (a(u) - 1 + b(v) - 1 + b(u) + a(v)) = 0$ by Claim 5.2 (*ii*) and (5.1), (A_1, B_1) is also a maximum (a,b)-partition by Claim 5.2 (*i*). Since G is triangle-free, $u_1v \notin E(G)$ and $uv_1 \notin E(G)$, which imply that $u_1 \in A_1^-$ and $v_1 \in B_1^-$. Now, $u_1v_1 \in E(G)$ by Claim 5.2 (*ii*). □

Recall that (A, B) always denotes a maximum (a,b)-partition of G. For a subset $S \subseteq V(G)$, let $N(S) = \cup_{x \in S} N(x)$. If $\min\{|A^-|, |B^-|\} = 2$, we define

$$f(A, B) = \left|N(A^-) \cap A^=\right| + \left|N(B^-) \cap B^=\right|.$$

Claim 5.4. $\min\{|A^-|, |B^-|\} = 1$.

Proof. If it is not the case, we may assume that G has a maximum (a,b)-partition (A, B) with $|A^-| = |B^-| = 2$ since G is $K_{2,3}$-free, and choose such an (A, B) with $f(A, B)$ maximum. Let $A^- = \{u, u'\}$ and $B^- = \{v, v'\}$. Then, $uvu'v'u$ is a quadrilateral by Claim 5.2 (*ii*).

If $N(A^-) \cap A^= = \emptyset$, then the $(a-1)$-degeneracy of A implies the existence of vertex $x \in A^+$ such that $x \in N(u) \cap N(u')$ and so $\{x, u, u', v, v'\}$ contains a $K_{2,3}$, a contradiction. Therefore, $N_{A^=}(A^-) \neq \emptyset$, and $N_{B^=}(B^-) \neq \emptyset$ by symmetry.

Without loss of generality, let u_1 be a vertex in $N_{A^=}(u)$, and let v_1 be a vertex in $N_{B^=}(v)$. By Claim 5.3, we have $u_1v_1 \in E(G)$, and so G contains F_1 as its subgraph (see Fig. 1.1).

Since G is $K_{2,3}$-free,

$$N_{A^=}(u) = \{u_1\} \text{ and } N_{B^=}(v) = \{v_1\} \tag{5.4}$$

by Claim 5.3. With the similar reason, it follows that

$$|N_{A^=}(u')| \leq 1 \text{ and } |N_{B^=}(v')| \leq 1.$$

We first prove the following.

$$\text{If } u_2 \in N_{A^=}(u_1), \text{ then } u_2v' \in E(G) \text{ and } N_{B^=}(v') = \emptyset. \tag{5.5}$$

If $u_2v \in E(G)$, then G would have a $K_{2,3}$ with partite sets $\{u_1, v\}$ and $\{u, u_2, v_1\}$. Therefore, $u_2v \notin E(G)$. Let $(A_1, B_1) = (A \cup \{v\}) \setminus \{u\}, B \cup \{u\}) \setminus \{v\})$. By Claim 5.2 (*ii*), (A_1, B_1) is also a maximum (a,b)-partition such that $u \in B_1^-$ with $v' \in N_{B_1^=}(u)$, and $u_1 \in A_1^-$ with $u_2 \in N_{A_1^=}(u_1)$, and so $u_2v' \in E(G)$ by Claim 5.3.

If $N_{B^=}(v') \neq \emptyset$, let v_1' be a vertex in $N_{B^=}(v')$, then $u_1v_1' \in E(G)$ by Claim 5.3, implying that $G[\{u_2, u_1, u, v', v_1'\}]$ contains a $K_{2,3}$. Therefore, $N_{B^=}(v') = \emptyset$, and so (5.5) holds.

Suppose that there are $u_2 \in N_{A^=}(u_1)$ and $u_3 \in N_{A^=}(u_2) \setminus \{u_1\}$. If $vu_3 \in E(G)$ and $x \in N_B(v') \cap N_B(v_1)$, then $G[\{v, u, u_1, v_1, x, v', u_2, u_3\}]$ contains an H_1, a contradiction. Therefore, we have that

$$\text{if } u_2 \in N_{A^=}(u_1) \text{ and } u_3 \in N_{A^=}(u_2) \setminus \{u_1\} \text{ with } vu_3 \in E(G), \text{ then } N_B(v') \cap N_B(v_1) = \emptyset. \tag{5.6}$$

We distinguish three cases depending upon the elements of $N_{A^=}(u_1) \cup N_{B^=}(v_1)$. In what follows, let $(A_1, B_1) = (A \cup \{v\}) \setminus \{u\}, B \cup \{u\}) \setminus \{v\})$.

Case 1. First, we suppose that there exist $u_2 \in N_{A^=}(u_1)$ and $v_2 \in N_{B^=}(v_1)$.

By (5.5) and by the symmetry between u_2 and v_2, we have $\{u_2v', u'v_2\} \subseteq E(G)$ and $N_{A^=}(u') = \emptyset = N_{B^=}(v')$. Then, (A_1, B_1) is also a maximum (a, b)-partition such that $u_1 \in A_1^-$ with $u_2 \in N_{A_1^=}(u_1)$, and $v_1 \in B_1^-$ with $v_2 \in N_{B_1^=}(v_1)$. By Claim 5.3, we have $u_2v_2 \in E(G)$, and so

G contains F_2 as its subgraph. (5.7)

Let u_3 be a vertex in $N_{A^=}(u_2)\backslash\{u_1\}$, and v_3 be a vertex in $N_{B^=}(v_2)\backslash\{v_1\}$. We will show that

$$vu_3 \in E(G) \text{ and } N_B(v') \cap N_B(v_1) = \emptyset, \text{and } uv_3 \in E(G) \text{ and } N_A(u') \cap N_A(u_1) = \emptyset. \tag{5.8}$$

By symmetry, we only prove the former conclusion. Suppose $vu_3 \notin E(G)$. Let $(A_2, B_2) = ((A \cup \{v\}) \setminus \{u_1\}, (B \cup \{u_1\}) \setminus \{v\})$. Since $e_G(u_1, B) = b(u_1) - 1$ by (5.1), and since every a-satisfactory subset of $A \cup \{v\}$ must contain u by Claim 5.2 (i) (so contains all its neighbors in A), (A_2, B_2) is an (a, b)-partition, and so a maximum (a, b)-partition as $\omega(A_2, B_2) - \omega(A, B) = (b(u_1) - 1 + a(v) + a(u_1) + b(v)) - (a(u_1) + b(v) - 1 + b(u_1) + a(v)) = 0$. If $\{u_2, u_3\} \cap N(v) = \emptyset$, then $u_2 \in A_2^-$ with $u_3 \in N_{A_2^=}(u_2)$, and $u_1 \in B_2^-$ with $v_1 \in N_{B_2^=}(u_1)$. By Claim 5.3, $v_1u_3 \in E(G)$ and so $G[\{v_2, v_1, u_1, u_2, u_3\}]$ contains a $K_{2,3}$, a contradiction. Therefore, $\{u_2, u_3\} \cap N(v) \neq \emptyset$, and so $vu_2 \in E(G)$ as $vu_3 \notin E(G)$. But now, $G[\{u_2, u_1, u, v, v_1\}]$ contains a $K_{2,3}$. This contradiction shows that $vu_3 \in E(G)$, and (5.8) follows directly from (5.6).

If $N_{A^=}(u_2) = \{u_1\}$ and $N_{B^=}(v_2) = \{v_1\}$, since G is triangle-free, and since F_2 is a subgraph of G by (5.7), then $N(v_2) \cap \{v, v', v_1\} = \{v_1\}$ which implies that $B\backslash\{v, v', v_1, v_2\} \neq \emptyset$ (since $d_B(v_2) = b(v_2) \geq 2$). By (5.4), $N_{B^=}(v) = \{v_1\}$. Since G is $\{K_3, K_{2,3}\}$-free, we have $N_{B^=}(v_1) = \{v_2\}$ and $N(v) \cap N(v_1) = N_B(v) \cap N_B(v') = N_B(v) \cap N_B(v_2) = N_B(v') \cap N_B(v_2) = N(v_1) \cap N(v_2) = \emptyset$. Combining this with $N_{B^=}(v') = \emptyset$ by (5.5), with $N_{B^=}(v_2) = \{v_1\}$, and with the $(b-1)$-degeneracy of B, we can conclude the existence of vertex, say y, in $N_{B^+}(v') \cap N_{B^+}(v_1)$. By symmetry, the similar argument shows that there exists a vertex, say z, in $N_{A^+}(u') \cap N_{A^+}(u_1)$. Now, one can easily check that $G[\{u_1, u, v, v_1, y, v', u', z\}]$ contains an H_1. This contradiction shows that

either there exists $u_3 \in N_{A^=}(u_2) \setminus \{u_1\}$ or there exists $v_3 \in N_{B^=}(v_2) \setminus \{v_1\}$.

If both u_3 and v_3 exist, then by applying (5.8) to u_3 and v_3 respectively, we have $\{uv_3, vu_3\} \subseteq E(G)$, which implies that $G[\{u, u_1, u_2, u_3, v, v_1, v_2, v_3\}]$ contains an H_1, a contradiction. So, we suppose, by symmetry, the existence of u_3, and suppose that $N_{B^=}(v_2) = \{v_1\}$. Since G is triangle-free, and since F_2 is a subgraph of G by (5.7), $N(v_2) \cap \{v, v', v_1\} = \{v_1\}$, and so $B\backslash\{v, v', v_1, v_2\} \neq \emptyset$ (as $d_B(v_2) = b(v_2) \geq 2$). Note that $N_{B^=}(v_2) = \{v_1\} = N_{B^=}(v)$ and $N_{B^=}(v') = \emptyset$ by (5.5). The $(b-1)$-degeneracy of B implies the existence of vertex, say z_1, in B^+ that is adjacent to at least two vertices of $\{v, v', v_1, v_2\}$. Since G is triangle-free and $K_{2,3}$-free, one can conclude that z_1 is adjacent to both v' and v_1, contrary with (5.8). This completes the proof of Case 1.

Case 2. In this case, we suppose that,

either there exists $u_2 \in N_{A^=}(u_1)$ with $N_{B^=}(v_1) = \emptyset$ or $N_{A^=}(u_1) = \emptyset$ with $v_2 \in N_{B^=}(v_1)$.

Without loss of generality, we suppose that there exists $u_2 \in N_{A^=}(u_1)$ and $N_{B^=}(v_1) = \emptyset$.
By (5.5), we have $N_{B^=}(v') = \emptyset = N_{B^=}(v_1)$ and $u_2v' \in E(G)$. We will prove that

$$N_{A^=}(u') \neq \emptyset. \tag{5.9}$$

Otherwise, assume to the contrary of (5.9) that $N_{A^=}(u') = \emptyset$ and so $f(A, B) = 2$. Recall that $(A_1, B_1) = ((A \cup \{v\}) \setminus \{u\}, (B \cup \{u\}) \setminus \{v\})$. It is straightly checked that $A_1^- = \{u_1, v\}$ with $N_{A_1^=}(u_1) = \{u_2\}$ and $N_{A_1^=}(v) = \{u'\}$, and $B_1^- = \{u, v_1\}$ with $N_{B_1^=}(u) = \{v'\}$. Thus, (A_1, B_1) is a maximum (a, b)-partition with $\min\{|A_1^-|, |B_1^-|\} = 2$ and $f(A_1, B_1) = 3 > 2 = f(A, B)$, contrary with the choice of (A, B). This contradiction confirms (5.9) and we suppose that $u_1' \in N_{A^=}(u')$.

Since G is $K_{2,3}$-free, we have $N(v_1) \cap \{v, v'\} = \{v\}$ and $N_{B^=}(v) = \{v_1\}$, and so $B \setminus \{v, v', v_1\} \neq \emptyset$ (since $d_B(v_1) = b(v_1) \geq 2$). Now, the $(b-1)$-degeneracy of $B \setminus \{v, v', v_1\}$ implies the existence of vertex, say w_1, in B^+ which has at least two neighbors in $\{v, v', v_1\}$. Since G contains neither K_3 not $K_{2,3}$, one can easily check that $w_1 \in N(v') \cap N(v_1)$. Combining this with $\{u_1'v_1, u_1v_1\} \subseteq E(G)$ by Claim 5.3, $G[\{u_2, u_1, u, v, u', v', u_1', v_1, w_1\}]$ contains an H_2, a contradiction. This completes the proof of Case 2.

Case 3. Finally, we suppose that $N_{A^=}(u_1) = \emptyset = N_{B^=}(v_1)$.

If $N_{A^=}(u') = \emptyset = N_{B^=}(v')$, since $N_{A^-}(u_1) = \{u\}$ and $d_A(u_1) = a(u_1) \geq 2$, then $A \neq \{u, u', u_1\}$ and the $(a-1)$-degeneracy of A implies the existence of vertex, say w_2, in A^+ that has at least two neighbors in $\{u, u_1, u'\}$. Since G is triangle-free and $K_{2,3}$-free, we can conclude that w_2 is adjacent to u' and u_1. Similarly, there exists a vertex, say w_3, in B^+ that is adjacent to v' and v_1. Now, $G[\{u_1, u, v, v_1, w_3, v', u', w_2\}]$ contains an H_1, a contradiction. This implies that

either $N_{A^=}(u') \neq \emptyset$ or $N_{B^=}(v') \neq \emptyset$.

Without loss of generality, suppose that there exists $u_1' \in N_{A^=}(u')$. By the symmetry between u_1 and u_1', we may further suppose that $N_{A^=}(u_1') = \emptyset$ (as otherwise the case can be deduced to Case 1 or Case 2).

If $N_{B^=}(v') \neq \emptyset$, then in view of Case 2 and the symmetry of v and v', we may suppose that there exists $v'_1 \in N_{B^=}(v')$ with $N_{B^=}(v'_1) = \emptyset$. Claim 5.3 implies that $\{u_1v_1, u_1v'_1, u'_1v'_1, u'_1v_1\} \subseteq E(G)$ and so

G contains F_3 as its subgraph.

Since G is triangle-free and $K_{2,3}$-free, $N_A(u_1) \cap \{u, u', u'_1\} = \{u\}$ and so $A \setminus \{u, u', u_1, u'_1\} \neq \emptyset$, as $d_A(u_1) = a(u_1) \geq 2$. Combining this with $N_{A^=}(u_1) = \emptyset = N_{A^=}(u'_1)$, $N_{A^=}(u) = \{u_1\}$ and $N_{A^=}(u') = \{u'_1\}$, the $(a-1)$-degeneracy of A implies the existence of a vertex, say w_4, in A^+ that has at least two neighbors in $\{u, u_1, u', u'_1\}$. Since G is triangle-free and $K_{2,3}$-free and by symmetry, we may suppose that w_4 is adjacent to u' and u_1. Similarly, there exists a vertex, say w_5, in B^+ that is adjacent to v and v'_1 by symmetry. Now, $G[\{u_1, u, v', v'_1, w_5, v, u', w_4\}]$ contains an H_1, a contradiction. Therefore,

$$N_{B^=}(v') = \emptyset = N_{A^=}(u'_1).$$

G being triangle-free and $K_{2,3}$-free, the $(b-1)$-degeneracy of B implies the existence of vertex, say w_6, in B^+ that has exactly two neighbors in $\{v, v_1, v'\}$ and $d_A(w_6) = a(w_6) + 1$. The $(a-1)$-degeneracy of A implies the existence of vertex, say w_7, in A^+ that has exactly two neighbors in $\{u, u', u_1, u'_1\}$ and $d_A(w_7) = a(w_7) + 1$. Since $G \in \mathcal{G}$, it follows that $\{v', v_1\} \subseteq N(w_6)$ and $\{u_1, u'_1\} \subseteq N(w_7)$. Thus, G contains H_3 as its subgraph, a contradiction. This completes the proof of Case 3. □

We proceed to finish the proof of Theorem 1.10.

Let (A, B) be a maximum (a, b)-partition, and suppose by symmetry that $|A^-| \geq |B^-|$. Then, $|B^-| = 1$ by Claim 5.4. Let $B^- = \{v\}$. Since $B \neq B^-$ as $|B| \geq 2$, we may choose a vertex, say v_1, in $N_{B^=}(v)$. Since G is triangle-free and $d_B(v_1) = b(v_1) \geq 2$, $B \setminus (N(v) \cup \{v\}) \neq \emptyset$. If $N_B(w) \setminus \{v\} \subseteq B^+$ for each vertex $w \in N_{B^=}(v)$, then the $(b-1)$-degeneracy of B guarantees the existence of two vertices, say $\{v_1, v_2\} \subseteq N_{B^=}(v)$, and $w \in B^+$ such that $d_B(w) = b(w) + 1$ and $N(v_1) \cap N(v_2) = \{v, w\}$, as G is $K_{2,3}$-free. Therefore, either

$$\text{there exists a vertex } v_2 \in N_{B^=}(v_1), \tag{5.10}$$

or there exist two vertices $\{v_1, v_2\}$ of $N_{B^=}(v)$ and $w \in B^+$ such that

$$d_B(w) = b(w) + 1 \text{ and } N(v_1) \cap N(v_2) = \{v, w\}. \tag{5.11}$$

If there is a vertex $u \in A^-$ and a vertex $u_1 \in N_{A^=}(u)$, since G is triangle-free, then $u_1v \notin E(G)$ and $uv_1 \notin E(G)$. Thus, (A_1, B_1) is a maximum (a, b)-partition with $\{u_1, v\} \subseteq A_1^-$ and $\{v_1, u\} \subseteq B_1^-$, which contradicts Claim 5.4. Therefore, $A \cap N(A^-) \subseteq A^+$.

Since G is $K_{2,3}$-free, each vertex of $A \setminus A^-$ has at most two neighbors in A^-. The $(a-1)$-degeneracy of A implies that A^- contains two vertices, say u and u', and a vertex z of A^+ such that $d_A(z) = a(z) + 1$ and $N(u) \cap N(u') = \{z, v\}$.

If (5.10) holds, since $N(v_1) \cap \{u, u'\} = \emptyset$ and $|N(v_2) \cap \{u, u'\}| \leq 1$ (as G is $K_{2,3}$-free and triangle-free), we may suppose that $uv_2 \notin E(G)$, and let $(A_3, B_3) = ((A \cup \{v_1\}) \setminus \{u\}, (B \cup \{u\}) \setminus \{v_1\})$, then, (A_3, B_3) is also a maximum (a, b)-partition by Claim 5.2. But now, $\{u', v_1\} \subseteq A_3^-$ and $\{v, v_2\} \subseteq B_3^-$, which contradicts Claim 5.4.

Therefore, (5.11) holds. Let $(A_4, B_4) = ((A \cup \{v_1, v_2\}) \setminus \{u, u'\}, (B \cup \{u, u'\}) \setminus \{v_1, v_2\})$. Since $\omega(A_4, B_4) - \omega(A, B) = (b(u) + b(u') + a(v_1) + a(v_2) - 2 + a(u) + a(u') + b(v_1) + b(v_2)) - (a(u) + a(u') - 2 + b(v_1) + b(v_2) + b(u) + b(u') + a(v_1) + a(v_2)) = 0$, (A_4, B_4) is also a maximum (a, b)-partition by Claim 5.2 (as $d_{B_4}(v) = b(v) - 1$, and $d_{A_4}(v_i) = a(v_i) - 1$ for every $1 \leq i \leq 2$). Since G is triangle-free and $K_{2,3}$-free, there are no edges between $\{u, u'\}$ and $\{w, v_1, v_2\}$, which implies that $\{v_1, v_2\} \subseteq A_4^-$ and $\{v, w\} \subseteq B_4^-$, which contradicts Claim 5.4 again. This contradiction proves Theorem 1.10. □

Declaration of competing interest

There is no conflict of interest.

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Note

Spectral strengthening of a theorem on transversal critical graphs

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ABSTRACT

A transversal set of a graph G is a set of vertices incident to all edges of G. The transversal number of G, denoted by $\tau(G)$, is the minimum cardinality of a transversal set of G. A simple graph G with no isolated vertex is called τ-critical if $\tau(G-e) < \tau(G)$ for every edge $e \in E(G)$. For any τ-critical graph G with $\tau(G) = t$, it has been shown that $|V(G)| \le 2t$ by Erdős and Gallai and that $|E(G)| \le \binom{t+1}{2}$ by Erdős, Hajnal and Moon. Most recently, it was extended by Gyárfás and Lehel to $|V(G)| + |E(G)| \le \binom{t+2}{2}$. In this paper, we prove stronger results via spectrum. Let G be a τ-critical graph with $\tau(G) = t$ and $|V(G)| = n$, and let λ_1 denote the largest eigenvalue of the adjacency matrix of G. We show that $n + \lambda_1 \le 2t + 1$ with equality if and only if G is tK_2, $K_{s+1} \cup (t-s)K_2$, or $C_{2s-1} \cup (t-s)K_2$, where $2 \le s \le t$; and in particular, $\lambda_1(G) \le t$ with equality if and only if G is K_{t+1}. We then apply it to show that for any nonnegative integer r, we have $n\left(r + \frac{\lambda_1}{2}\right) \le \binom{t+r+1}{2}$ and characterize all extremal graphs. This implies a pure combinatorial result that $r|V(G)| + |E(G)| \le \binom{t+r+1}{2}$, which is stronger than Erdős-Hajnal-Moon Theorem and Gyárfás-Lehel Theorem. We also have some other generalizations.

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1. Introduction

Throughout the paper, let $G = (V, E)$ be a simple graph. For terminology not defined here, we refer readers to [1]. For any $v \in V(G)$, let $d_G(v)$ or simply $d(v)$ denote the degree of v. A d-regular graph is a graph with the degree of each vertex equals to d. A *transversal set* of G is a vertex subset $X \subseteq V(G)$ such that every edge of G is incident to some vertex of X. The *transversal number* of G, denoted by $\tau(G)$, is the minimum cardinality of a transversal set of G. A transversal set and the transversal number are also called a *vertex covering* and the *covering number*, respectively (see [1]). An *independent set* is a set of non-adjacent vertices and the *independence number* of G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set in G. Clearly, T is a transversal set of G if and only if $V(G) - T$ is an independent set of G, and therefore $\tau(G) + \alpha(G) = |V(G)|$. A simple graph G with no isolated vertex is called *τ-critical* if $\tau(G-e) < \tau(G)$ for every edge $e \in E(G)$. Since $\tau(G-e) \ge \tau(G) - 1$, it follows that if G is τ-critical, then $\tau(G-e) = \tau(G) - 1$ for every edge $e \in E(G)$. Furthermore, $\tau(G) \le |V(G)| - 1$ with equality if and only if G is a complete graph. More properties of τ-critical graphs can be found in Chapter 12 of [8] by Lovász and Plummer.

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In the following, we always assume that t is a positive integer. Let K_n, C_n, tK_2 denote the complete graph on n vertices, the cycle on n vertices and t disjoint copies of K_2, respectively. For any τ-critical graph G with $\tau(G) = t$, it has been shown that $|V(G)| \leq 2t$ and conjectured that $|E(G)| \leq \binom{t+1}{2}$ by Erdős and Gallai [4]. The conjecture was settled by Erdős, Hajnal and Moon [5].

Theorem 1.1 *(Erdős, Hajnal and Moon [5]). For any τ-critical graph G with $\tau(G) = t$,*

$$|E(G)| \leq \binom{t+1}{2},$$

where the equality holds if and only if G is K_{t+1}.

The theorem was recently extended by Gyárfás and Lehel [6] with a very short proof using the sum of order and size. This combined bound immediately implies Theorem 1.1 since $|V(G)| \geq t+1$.

Theorem 1.2 *(Gyárfás and Lehel [6]). For any τ-critical graph G with $\tau(G) = t$,*

$$|V(G)| + |E(G)| \leq \binom{t+2}{2},$$

with equality if and only if G is K_{t+1}, $2K_2$, or C_5.

We will prove an extension of Theorems 1.2, as shown below. Clearly, Theorem 1.3 implies Theorems 1.1 and 1.2 when $r = 0, 1$, respectively.

Theorem 1.3. *Let r be a nonnegative integer. Suppose that G is a τ-critical graph with $\tau(G) = t \geq r$ and $|V(G)| = n$. Then*

$$r|V(G)| + |E(G)| \leq \binom{t+r+1}{2},$$

with equality if and only if G is K_{t+1} when $r = 0$; K_{t+1}, $2K_2$, or C_5 when $r = 1$; and rK_2, $(r+1)K_2$, C_{2r+1}, or C_{2r+3} when $r \geq 2$.

In fact, we discover stronger results involving the largest eigenvalue of adjacency matrix that strengthen Theorems 1.1, 1.2 and 1.3, with all extremal graphs characterized. This will be done in Section 3, and Theorem 1.3 will be proved there.

In the last section, we make some remarks that our results can be further extended to more general forms and to eigenvalues of signless Laplacian matrix. We start with some combinatorial tools on τ-critical graphs in the next section.

2. Combinatorial preliminaries

In this section, we present two useful theorems on τ-critical graphs, and prove a combinatorial lemma, which will play an important role in the proofs of our main results. Theorem 2.1 is the complement version of a theorem of Hajnal [7]. Theorem 2.2 was discovered by Surányi [9], but can also be found in [8].

Theorem 2.1 *(Hajnal [7]). Let G be a τ-critical graph with $\tau(G) = t$ and $|V(G)| = n$. Then the degree $d(v) \leq 2t + 1 - n$ for every $v \in V(G)$.*

Theorem 2.2 *(Surányi [9]; see also Theorem 12.1.13 of [8]). Let G be a τ-critical graph and S be an independent set of G. Then for any vertex $v \in S$, $d_G(v) \leq |N(S)| - |S| + 1$.*

Theorem 2.2 actually implies Theorem 2.1. To see this, notice that for any vertex v, we can find a maximum independent set S containing v (by Lemma 12.1.2 of [8]). Then $N(S)$ is a minimum transversal set of G, where $N(S)$ denotes the set of vertices that are adjacent to some vertex of S.

Lemma 2.3. *Let G be a τ-critical graph with $\tau(G) = t$ and $|V(G)| = n$. If G contains a $(2t+1-n)$-regular component, then G is tK_2, $K_{s+1} \cup (t-s)K_2$ or $C_{2s-1} \cup (t-s)K_2$, where $2 \leq s \leq t$.*

Proof. Let $d = 2t + 1 - n$ and let G' be a d-regular component of G. Let $u \in V(G')$. Since G is τ-critical, G' is also τ-critical and we suppose that $\tau(G') = s$. Notice that if X is a transversal set of G', then $V(G') - X$ is an independent set, and thus the independence number $\alpha(G') = p - s$, where $|V(G')| = p$.

Notice that $G - G'$ is τ-critical and so $|V(G - G')| \leq 2\tau(G - G')$, that is, $n - p \leq 2(t - s)$. It follows that $2s - p \leq 2t - n$. By Theorem 2.1, we have

$$2s+1-p \le 2t+1-n = d = d(u) \le 2s+1-p$$

and thus

$$2(t-s) = n-p \text{ and } d = 2s+1-p.$$

It follows that $|V(G-G')| = 2\tau(G-G') = 2(t-s)$. By Theorem 2.1, the degree of each vertex of $G-G'$ is at most $2\tau(G-G') - |V(G-G')| + 1 = 1$, and thus $G-G' = (t-s)K_2$.

To complete the proof, it suffices to show that G' is K_2, K_{s+1} or C_{2s-1} for $s \ge 2$. If $d = 1$, then G' is K_2 and so the result already holds. Thus, we may suppose that $d \ge 2$ in the following.

Let $v_1, v_2, \ldots, v_d$ be all neighbors of u, and let $e_i = uv_i$ for $i = 1, 2, \ldots, d$. Since G' is τ-critical, we have $\tau(G'-e_i) = s-1$. In other words, we can find an independent set S_i of $G'-e_i$ with $|S_i| = p-s+1$. By the τ-criticality of G', we have $u, v_i \in S_i$. (Otherwise if one of $\{u, v_i\}$ is not in S_i, then adding e_i back does not affect the independence of S_i and thus S_i is also an independent set of G', violating the fact that $\alpha(G') = p-s$.)

Now for all $j \ne i$, v_j is adjacent to u in $G'-e_i$, and thus $v_j \notin S_i$ since $u \in S_i$. Let $T_i = S_i - u$. Since T_i is an independent set of G' with $|T_i| = p-s$, it turns out that T_i is a maximum independent set of G'.

We claim that $T_i \cap T_j = \emptyset$ for all $i \ne j$. If not, then let $w \in T_i \cap T_j$. Since $T_i \cap T_j$ is an independent set, by Theorem 2.2, we have

$$2s+1-p = d = d(w) \le |N(T_i \cap T_j)| - |T_i \cap T_j| + 1,$$

whence

$$|N(T_i \cap T_j)| \ge |T_i \cap T_j| + 2s - p = |T_i \cap T_j| + p - |T_i| - |T_j| = p - |T_i \cup T_j|.$$

Observing that $N(T_i \cap T_j)$ is a subset of $V(G') \setminus (T_i \cup T_j)$, we can conclude that every vertex of G' outside of $T_i \cup T_j$ is adjacent to some vertex in $T_i \cap T_j$. This is impossible, since u is not adjacent to any vertex in $T_i \cap T_j$. Thus $T_i \cap T_j = \emptyset$ for all $i \ne j$.

Hence

$$p = |V(G')| \ge 1 + \sum_{i=1}^{d} |T_i| = 1 + d(p-s) = 1 + (2s+1-p)(p-s),$$

yielding

$$(p-s-1)(2s-1-p) \le 0.$$

Notice that we always have $p \ge s+1$. Hence $p = s+1$ or $2s-1-p \le 0$.

If $p = s+1$, then

$$d = 2s+1-p = s = p-1$$

and so G' is $K_p = K_{s+1}$.

If $2s-1-p \le 0$, then

$$2 \le d = 2s+1-p \le 2,$$

yielding that $p = 2s-1$, and so $G' = C_p = C_{2s-1}$. This completes the proof of the lemma. □

3. Spectral strengthening

In this section, we present spectral analogues that strengthen Theorems 1.1 and 1.2, and determine all extremal graphs. Theorem 3.2, Corollaries 3.3 and 3.4 are the main results, and Theorem 1.3 will be proved at the end of the section.

Let $\lambda_1 := \lambda_1(G)$ denote the largest eigenvalue of the adjacency matrix of G, which is called the *spectral radius* of G. The following lemma is well-known (see also Theorem 3.2.1 of [3]).

Lemma 3.1. *For any graph G with maximum degree Δ,*

$$\frac{2|E(G)|}{|V(G)|} \le \lambda_1 \le \Delta,$$

with the first equality if and only if G is regular, and the second equality if and only if G has a Δ-regular component.

Now we are ready to prove a spectral extremal theorem on τ-critical graphs with respect to the sum of the order and spectral radius, which strengthens Theorem 1.2.

Theorem 3.2. *For any τ-critical graph G with $\tau(G) = t$ and $|V(G)| = n$,*

$$n + \lambda_1 \leq 2t + 1,$$

with equality if and only if G is tK_2, $K_{s+1} \cup (t-s)K_2$, or $C_{2s-1} \cup (t-s)K_2$ for $2 \leq s \leq t$.

Proof. By Theorem 2.1 and Lemma 3.1, we have $\lambda_1 \leq \Delta \leq 2t + 1 - n$, and thus $n + \lambda_1 \leq 2t + 1$. It is easily checked that the equality holds when G is one of these extremal graphs as described. Conversely, if the equality holds, then $\lambda_1 = \Delta = 2t + 1 - n$, and thus Lemma 3.1 implies that G contains a $(2t + 1 - n)$-regular component. The result then follows from Lemma 2.3. □

The following corollary is a simple extremal result with respect to solely spectral radius, and it can be considered as a spectral analogue of Theorem 1.1.

Corollary 3.3. *If G is a τ-critical graph with $\tau(G) = t$, then $\lambda_1(G) \leq t$ with equality if and only if G is K_{t+1}.*

Proof. Since $|V(G)| \geq t + 1$, we have $\lambda_1(G) \leq t$ by Theorem 3.2. The equality holds if and only if $|V(G)| = t + 1$, that is, if and only if G is K_{t+1}. □

The following result looks more general, however, it can be derived from Theorem 3.2.

Corollary 3.4. *Let r be a nonnegative integer. Suppose that G is a τ-critical graph with $\tau(G) = t \geq r$ and $|V(G)| = n$. Then*

$$n\left(r + \frac{\lambda_1}{2}\right) \leq \binom{t+r+1}{2},$$

with equality if and only if one of the following holds:
(1) K_{t+1} when $r = 0$;
(2) K_{t+1}, $K_t \cup K_2$ for $t \geq 2$, or C_5, when $r = 1$;
(3) rK_2, $(r+1)K_2$, $K_{t-r+2} \cup (r-1)K_2$, $K_{t-r+1} \cup rK_2$ with $r \leq t-2$, $C_{2s-1} \cup (r+1-s)K_2$ for $2 \leq s \leq r+1$, or $C_{2s-1} \cup (r+2-s)K_2$ for $2 \leq s \leq r+2$, when $r \geq 2$.

Proof. Since $\lambda_1 \leq 2t - n + 1$ by Theorem 3.2, we have $n\left(r + \frac{\lambda_1}{2}\right) \leq \frac{n(2t+2r+1-n)}{2}$. Since $\frac{n(2t+2r+1-n)}{2}$ is maximized when $n = t + r$ or $n = t + r + 1$, we have

$$n\left(r + \frac{\lambda_1}{2}\right) \leq \frac{(t+r+1)(t+r)}{2} = \binom{t+r+1}{2}.$$

If G is one of the graphs listed in the statement, then it is easily checked that the equality holds. Next we suppose that the equality holds. Then $\lambda_1 = 2t - n + 1$ and either $n = t + r$ or $n = t + r + 1$. By Theorem 3.2, we can deduce the following:

(1) $r = 0$. Notice that $n \geq t + 1$ by the definition of transversal number, it follows that $n = t + 1$. Thus G is K_{t+1}.

(2) $r = 1$. Then $n = t + 1$ or $n = t + 2$. By verifying all extremal graphs in Theorem 3.2, it follows that G is K_{t+1} if $n = t + 1$; and G is $2K_2$ (i.e. $K_2 \cup K_2$), $K_t \cup K_2$ for $t \geq 3$, or C_5 if $n = t + 2$.

(3) $r \geq 2$. Then $n = t + r$ or $n = t + r + 1$. Again, it suffices to verify all extremal graphs in Theorem 3.2. If $n = t + r$, then G is $tK_2 = rK_2$, $K_{t-r+2} \cup (r-1)K_2$ or $C_{2s-1} \cup (t-s)K_2 = C_{2s-1} \cup (r+1-s)K_2$ for $2 \leq s \leq r+1$; and if $n = t + r + 1$, then G is $tK_2 = (r+1)K_2$, $K_{t-r+1} \cup rK_2$ provided that $r \leq t-2$, or $C_{2s-1} \cup (t-s)K_2 = C_{2s-1} \cup (r+2-s)K_2$ for $2 \leq s \leq r+2$. □

In the rest of this section, we present a proof of Theorem 1.3.

Proof of Theorem 1.3. By Lemma 3.1, we have $|E(G)| \leq n\lambda_1/2$ and so $r|V(G)| + |E(G)| \leq n\left(r + \frac{\lambda_1}{2}\right)$. By Corollary 3.4, it follows that $r|V(G)| + |E(G)| \leq \binom{t+r+1}{2}$. The equality holds if and only if the equalities hold in both Lemma 3.1 and Corollary 3.4. In other words, the extremal graphs are those graphs in Corollary 3.4 that are regular. By verifying the graphs listed in Corollary 3.4, we conclude that the equality holds if and only if G is K_{t+1} when $r = 0$; K_{t+1}, $2K_2$, or C_5 when $r = 1$; and rK_2, $(r+1)K_2$, C_{2r+1}, or C_{2r+3} when $r \geq 2$. □

4. Remarks

In this paper, we proved spectral extremal results for τ-critical graphs. The results also imply a combinatorial theorem which is stronger than former results by Erdős, Hajnal and Moon [5] and by Gyárfás and Lehel [6]. We make some remarks to show further generalizations.

Remark 1. In the proof of Corollary 3.4, notice that r is nonnegative but not necessary to be integral. In fact, $\frac{n(2t+2r+1-n)}{2}$ is maximized when $n=(2t+2r+1)/2$, and thus we have

$$n\left(r+\frac{\lambda_1}{2}\right)\leq\frac{(2t+2r+1)^2}{8}.$$

The equality is attained only if $(2t+2r+1)/2$ is an integer, i.e., $2r$ is odd. By Theorem 3.2, it is not hard to show that the extremal graphs are K_{t+1} for $r=\frac{1}{2}$ as well as $\frac{2r+1}{2}K_2$, $K_{t-r+3/2}\cup(r-\frac{1}{2})K_2$ or $C_{2s-1}\cup\frac{3+2r-2s}{2}K_2$ where $2\leq s\leq r+\frac{3}{2}$, for other values r such that $2r$ is odd.

More general forms like $n\left(r_1+r_2\frac{\lambda_1}{2}\right)$ and $r_1|V(G)|+r_2|E(G)|$ may be done similarly with more complicated arguments, but we did not put effort on it.

Remark 2. The matrix $Q(G)=D(G)+A(G)$ is the *signless Laplacian matrix* of G, where $D(G)$ is the diagonal degree matrix and $A(G)$ is the adjacency matrix of G. Let $q_1:=q_1(G)$ be the largest eigenvalue of $Q(G)$, which is called the *signless Laplacian spectral radius* of G. It is known that (see [2]) $2\lambda_1\leq q_1\leq 2\Delta$, where Δ is the maximum degree of G. Furthermore, the second equality holds if and only if G has a Δ-regular component. Thus, with the same method, we can extend Theorem 3.2, Corollaries 3.3 and 3.4 by showing that

$$n+\frac{q_1}{2}\leq 2t+1,\ \ q_1\leq 2t\ \text{ and }\ n\left(r+\frac{q_1}{4}\right)\leq\binom{t+r+1}{2},$$

with the same extremal graphs as those in Theorem 3.2, Corollaries 3.3 and 3.4.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Minimum augmented Zagreb index of c-cyclic graphs☆

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ABSTRACT

The augmented Zagreb index (*AZI*) has proved its applicability potential in various chemical researches. Its mathematical features are being investigated vigorously. Here, the unique graph that minimizes the *AZI* among all c-cyclic graphs with fixed order is characterized.

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1. Introduction

The history of degree-based molecular descriptors can be traced back to the very beginning of the applications of topological indices in chemistry. The oldest degree–based index was introduced in 1952 and nowadays is known as the Platt index [11]. The most popular among them is certainly the Randić index, which appeared in 1975 [12]. The success of the Randić index led researchers to focus their efforts on improving its capabilities. A number of degree-based topological indices has appeared as descendants of the Randić index. According to popularity, the best-known successor of the Randić index is the atom-bond connectivity index [4]. In the seminal paper, an improvement in predicting the heat of formation of alkanes using the *ABC* index compared with Randić index has been demonstrated. An investigation of its peculiar mathematical features had been initiated in [5]. A dozen of years after the introduction of the *ABC* index, its modifications appeared that outperformed its prediction of the heat of formation of alkanes. This modification was named as augmented Zagreb index [6] and defined as:

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3,$$

where $d(u)$ and $d(v)$ are the degrees of the end-vertices of an edge uv.

Moreover, the comparative survey of the prediction ability of more than a dozen of well-established degree-based topological indices (tested on the physico–chemical properties of alkanes) showed the supremacy of the augmented Zagreb index [7].

Mathematical features of the *AZI* have been extensively investigating, which resulted in dozens of scientific contributions (e.g. see [3] and references cited therein). It was shown in [6] that among trees of order n the star has minimum

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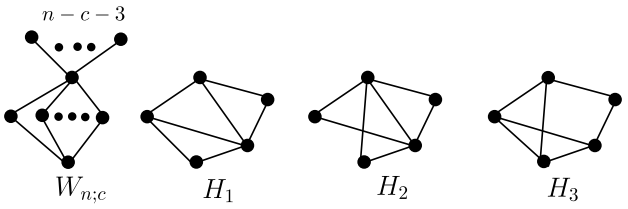


Fig. 1. The graphs $W_{n;c}$, H_1, H_2 and H_3.

AZI . The unique unicyclic or bicyclic graph, having $n \geq 5$, with minimum *AZI* can be constructed from the star by adding an edge or two nonadjacent edges, respectively [8,14]. Recently, it was proven that double-star maximizes the *AZI* among all trees of order $n \geq 19$ [10]. In this paper, the following problem was put forward:

Problem 1. Characterizing extremal graphs of *AZI* among all connected graphs with m edges and n vertices for $m \geq n$.

A connected graph G with n vertices and $n + c - 1$ edges will be referred as a c-cyclic graph. Denote by $K_{s,t}$ be the complete bipartite graph with s and t vertices in each vertex partition. $W_{n;c}$ is the c-cyclic graph with n vertices obtained from $K_{2,c+1}$ by attaching $n - c - 3$ pendent vertices to a $(c + 1)$-vertex (A k-vertex is a vertex with degree k). The $W_{n;c}$ graph is depicted in Fig. 1, as well as three tricyclic graphs with five vertices.

Motivated by Problem 1, Ali [1] showed that $W_{n;3}$ uniquely has the minimum *AZI* among all tricyclic graphs with $n \geq 6$.

In this note, it is going to be shown that

Theorem 1. *Let G be a c-cyclic graph with n vertices. If $n \geq 2c + 1$ and $c \geq 3$, then*

$$AZI(G) \geq AZI(W_{n;c}) = (n - c - 3)\left(\frac{n-2}{n-3}\right)^3 + 16(c + 1), \tag{1}$$

with equality iff G is isomorphic to the graph $W_{n;c}$.

2. Proof of Theorem 1

Let

$$\Psi(x, y) = \left(\frac{xy}{x + y - 2}\right)^3.$$

Lemma 1 ([9])**.**
(*i*) $\Psi(1, y)$ *is decreasing for* $y \geq 2$.
(*ii*) $\Psi(2, y) = 8$ *for any real number* y.
(*iii*) *If* $y \geq 3$ *is fixed, then* $\Psi(x, y)$ *is increasing and* $\Psi(x, y) > 8$ *for* $x \geq 3$.

An edge uv of G with $\min\{d(u), d(v)\} = 1$ (resp., $\min\{d(u), d(v)\} \geq 2$) is called a pendent (resp., non-pendent) edge. For $s \neq t$, a graph G is said to be (s, t)-biregular if each vertex has degree s or t, and each s-vertex is adjacent to some t-vertex and vice versa. Let $\mathcal{G}_1$ be the class of connected graphs whose pendent vertices are adjacent to the vertices of maximum degree and each of non-pendent edges contains at least one 2-vertex as its end vertex. Let $\mathcal{G}_2$ be the class of connected graphs with minimum degree at least two such that each edge contains at least one 2-vertex as its end vertex.

Lemma 2 ([13])**.** *Let G be a connected graph with n vertices, e edges, p pendent vertices and maximum degree Δ. If the minimum non-pendent vertex degree of G is δ_1, then*

$$AZI(G) \geq p\left(\frac{\Delta}{\Delta - 1}\right)^3 + (e - p)\left(\frac{\delta_1^2}{2\delta_1 - 2}\right)^3,$$

with equality iff G is isomorphic to a $(1, \Delta)$-biregular graph or G is regular or $G \in \mathcal{G}_1$ or $G \in \mathcal{G}_2$.

From Lemma 2, it follows that

Corollary 1. *Let G be a c-cyclic graph with n vertices and minimum degree at least two. If $n \geq c + 3$ and $c \geq 3$, then*

$$AZI(G) \geq (n - c - 3)\left(\frac{n-2}{n-3}\right)^3 + 16(c + 1), \tag{2}$$

with equality iff G is isomorphic to the graph $K_{2,c+1}$.

Proof. From Lemmas 1 and 2 it follows that

$$AZI(G) \geq 8|E(G)| = 8(n+c-1) \geq (n-c-3)\left(\frac{n-2}{n-3}\right)^3 + 16(c+1).$$

If $G = K_{2,c+1}$, then it is easily checked that equality holds in (2).

Next, we suppose that the equality holds in (2). Then, by Lemma 2 and $c \geq 3$, we have $\delta = 2 < \Delta$ and $n = c+3$. From Lemma 2, each edge of G contains at least one 2-vertex as its end vertex. Since the number of edges in G is $n+c-1 = 2(c+1)$, it follows that G has at least $c+1$ vertices with degree two as well. On the other hand, since $\Delta > 2$ and $n = c+3$, G should have at most $c+2$ vertices of degree two. If G has $c+2$ vertices of degree two, then $\Delta = 2|E(G)| - 2(c+2) = 2c \geq c+3 = n$, which is a contradiction. Thus, G has exactly $c+1$ vertices of degree two. Let u and v be other two vertices of G such that $d(u) = \Delta \geq d(v) > 2$. Since all neighbors of u and v are 2-vertices, we have $d(v) \leq d(u) \leq n-2 = c+1$. Combining this with $d(u) + d(v) = 2|E(G)| - 2(c+1) = 2(c+1)$, we can conclude that $d(u) = d(v) = c+1$ and thus $G = K_{2,c+1}$. □

Lemma 3. *If $3 \leq x \leq n-2$ and $n \geq 7$, then*

$$\Phi(x) = \left(\frac{x(n-1)}{x+n-3}\right)^3 - \left(\frac{(x-1)(n-1)}{x+n-4}\right)^3 > 8.$$

Proof. Since

$$\Phi(n-2) = \frac{(12n^2-54n+61)(n-1)^3}{8(2n-5)^3} > 8,$$

we may assume that $3 \leq x \leq n-3$.

By an elementary computation, it follows that

$$\Phi'(x) = \frac{3(n-3)(n-1)^3\left((n-3)^2 - x(x-1)\right)f(x)}{(n+x-4)^4(n+x-3)^4},$$

where $f(x) = 2x^3 + (4n-15)x^2 + (2n^2-16n+31)x - (n-3)^2$. Note that $f(x) \geq f(3) = 5n^2 - 6n + 3 > 0$. Thus, $\Phi'(x) > 0$ and

$$\Phi(x) \geq \Phi(3) = \frac{(n-3)(19n^2-24n+9)}{n^3} > 8,$$

for $n \geq 7$. □

Lemma 4 ([2])**.**

For a real number p, let

$$f(x,y) = \left(\frac{xy}{x+y-2}\right)^3 - \left(\frac{(x-p)y}{x+y-p-2}\right)^3,$$

where $\min\{x,y\} \geq 2$ and $x > p \geq 1$. Then, the function $f(x,y)$ is increasing on y for $y \geq 2$.

Lemma 5. *Let G be a c-cyclic graph with n vertices and $\Delta = n-1$. If $n \geq \min\{2c+1, 7\}$, then*

$$AZI(G) \geq (n-2c-1)\left(\frac{n-1}{n-2}\right)^3 + 24c\,, \tag{3}$$

where the equality holds iff G is obtained from the star $K_{1,n-1}$ by adding c independent edges.

Proof. Let G be an extremal graph with minimum *AZI* among all c-cyclic graphs with n vertices and maximum degree $n-1$. Denote by $(d_1, d_2, \ldots, d_n)$ the degree sequence of G, where $d_1 = n-1$. If $\delta \geq 2$, then $2(n+c-1) = \sum_{i=1}^{n} d_i \geq n-1+2(n-1)$. Combining this with $n \geq 2c+1$, we can conclude that $d_2 = d_3 = \cdots = d_n = 2$ and $d_1 = n-1 = 2c$. Thus, G is obtained from the star $K_{1,2c}$ by adding c independent edges.

Let us suppose that $\delta = 1$. Assume that $d(u_0) = n-1$ and v_0 is a pendent vertex of G. It suffices to show that, for each non-pendent edge uv with $u_0 \notin \{u,v\}$, $d(u) = d(v) = 2$. By contradiction, let uv be a non-pendent edge with $u_0 \notin \{u,v\}$ such that $d(v) \geq 3$ and $d(u) \geq 2$. Let $G_1 = G - uv + uv_0$. Then, G_1 is also a c-cyclic graph with n vertices. Since $d(u_0) = n-1$, every neighbor of v is a non-pendent vertex. Denote by $N(v)$ the neighbor set of vertex v in G. From Lemma 1 and Lemmas 3–4, it follows that

$$\begin{aligned} &AZI(G) - AZI(G_1) \\ &= \sum_{w \in N(v)\setminus\{u_0,u\}} \left(\left(\frac{d(w)d(v)}{d(w)+d(v)-2}\right)^3 - \left(\frac{d(w)(d(v)-1)}{d(w)+d(v)-3}\right)^3\right) \end{aligned}$$

$$
\begin{aligned}
&+\left(\frac{n-1}{n-2}\right)^3+\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3+\left(\frac{d(v)(n-1)}{d(v)+n-3}\right)^3-\left(\frac{(d(v)-1)(n-1)}{d(v)+n-4}\right)^3-16\\
&>\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3+\left(\frac{d(v)(n-1)}{d(v)+n-3}\right)^3-\left(\frac{(d(v)-1)(n-1)}{d(v)+n-4}\right)^3-16\\
&\geq\left(\frac{d(v)(n-1)}{d(v)+n-3}\right)^3-\left(\frac{(d(v)-1)(n-1)}{d(v)+n-4}\right)^3-8>0\,,
\end{aligned}
$$

which is contrary to the choice of G. □

Lemma 6. *Let G be a c-cyclic graph with n vertices and $\Delta=n-1$. If $n\geq 2c+1$ and $c\geq 3$, then $AZI(G)>AZI(W_{n;c})$.*

Proof. Let $g(n)=(n-3)(14n^5-171n^4+828n^3-1983n^2+2346n-1097)$. By Lemma 5, it follows that

$$
\begin{aligned}
&AZI(G)-AZI(W_{n;c})\\
\geq&(n-2c-1)\left(\frac{n-1}{n-2}\right)^3+24c-\left((n-c-3)\left(\frac{n-2}{n-3}\right)^3+16(c+1)\right)\\
=&\frac{(7n^6-108n^5+690n^4-2328n^3+4362n^2-4296n+1738)c-g(n)}{(n-2)^3(n-3)^3}\\
\geq&\frac{3(7n^6-108n^5+690n^4-2328n^3+4362n^2-4296n+1738)-g(n)}{(n-2)^3(n-3)^3}\\
=&\frac{7n^6-111n^5+729n^4-2517n^3+4791n^2-4753n+1923}{(n-2)^3(n-3)^3}>0.\quad\square
\end{aligned}
$$

If uv is an edge of G such that $d(u)\geq d(v)\geq 3$, then uv is called a **special edge** of G. A cycle C of G is called a **pendent cycle** if C contains exactly one vertex with degree at least three.

Lemma 7. *Let G be a c-cyclic graph with at most $c+2$ vertices and minimum degree at least two. If $c\geq 2$, then G has at least one special edge.*

Proof. We prove this result by induction on c. If $c=2$, then K_4-e is the unique bicyclic graph with four vertices, and thus the result holds. Now, we suppose that the result holds for all k-cyclic graphs with $k\leq c-1$ and G is a c-cyclic graph with n vertices, where $n\leq c+2$ and $c\geq 3$. We assume to the contrary that G has no special edge.

We claim that G has at least two vertices with degree at least three. Otherwise, $2(n+c-1)\leq n-1+2(n-1)$, and thus $2c+1\leq n\leq c+2$, which is a contradiction. Thus, we can define u and v as two vertices with degree at least three such that the distance between u and v is as large as possible. Since G contains no special edge, all neighbors of u are 2-vertices.

Case 1. u **is a cut vertex of** G**.** By the choice of u, it lies in a pendent cycle C, that is, each vertex of $V(C)\setminus\{u\}$ is a 2-vertex.

If $d(u)\geq 4$, then denote by G_1 the graph obtained from G by deleting all vertices of $V(C)\setminus\{u\}$. In this case, G_1 is a $(c-1)$-cyclic graph with $n+1-|V(C)|$ vertices and minimum degree at least two. Since $n+1-|V(C)|\leq n-2<c-1+2$, by the induction hypothesis, G_1 has at least one special edge, and thus G also contains a special edge, which is a contradiction.

Let us suppose that $d(u)=3$. Recall that each neighbor of u is a 2-vertex and $c\geq 3$. Thus, there exist vertices $\{w,u_1,u_2,\ldots,u_t\}$ with $t\geq 1$ such that $d(w)\geq 3>2=d(u_1)=d(u_2)=\cdots=d(u_t)$ and $wu_1u_2\cdots u_tu$ is the unique path of G connecting w and u. Let G_2 be the graph obtained from G by deleting all vertices of $V(C)\cup\{u_1,u_2,\ldots,u_t\}$. Then, G_2 is also a $(c-1)$-cyclic graph with $n-t-|V(C)|$ vertices and minimum degree at least two. Since $n-t-|V(C)|\leq n-4<c-1+2$, by the induction hypothesis, G_2 has at least one special edge, and thus G also has a special edge, which is a contradiction.

Case 2. u **is not a cut vertex of** G**.** In this case, there exist vertices $\{w,u_1,u_2,\ldots,u_t\}$ with $t\geq 1$ such that $d(w)\geq 3>2=d(u_1)=d(u_2)=\cdots=d(u_t)$, and $wu_1u_2\cdots u_tu$ is a path connecting w and u that is a part of some cycle of G. Let G_3 be the graph obtained from G by deleting all vertices of $\{u_1,u_2,\ldots,u_t\}$. Then, G_3 is a $(c-1)$-cyclic graph with $n-t$ vertices and minimum degree at least two. Since $n-t\leq n-1\leq c-1+2$, by the induction hypothesis, G_3 has at least one special edge, and thus G also has a special edge, which is a contradiction. □

As special edge uv of G is called **good** if uv satisfies the followings:

(*i*) Either $d(u)\geq d(v)\geq 4$ or $d(u)\geq 5>3=d(v)$;

(*ii*) If $d(u)=d(v)=3$, then $d(w)\geq 3$ for each $w\in N(u)\cup N(v)$;

(*iii*) If $d(u)=4>3=d(v)$, then there exist vertices $w\in N(u)\setminus\{v\}$ and $z\in N(v)\setminus\{u\}$ such that $\min\{d(w),d(z)\}\geq 3$ (Here, $w=z$ is also possible).

Lemma 8. *Let G be a c-cyclic graph with at most $c+2$ vertices and minimum degree at least two. If $c \geq 3$, then G has a good special edge.*

Proof. We show this result by induction on c.

If $c = 3$, then K_4 is the unique tricyclic graph with four vertices and there are three tricyclic graphs with five vertices (See H_1, H_2 and H_3 of Fig. 1), and thus we can check straightforwardly that the result holds. In what following, we suppose that the result already holds for all k-cyclic graphs with $k \leq c-1$ and G is a c-cyclic graph with n vertices, where $n \leq c+2$.

By Lemma 7, G has at least one special edge uv. If $d(u) \geq d(v) \geq 4$ or $d(u) \geq 5 > 3 = d(v)$, then uv is a good special edge and thus we only need to consider the case of $d(u) = 4 > 3 = d(v)$ or $d(u) = d(v) = 3$. We assume that G contains no good special edge. We first prove the following claim:

Claim 1. Every vertex of G lies on some cycle of G.

Proof of Claim 1. By contradiction, we assume that G has at least one vertex not lying on any cycle of G. Then, denote by G_1 the graph obtained from G by deleting all these vertices not lying on any cycle of G. Then, G_1 is a disconnected graph such that each component of G_1 is a graph with every vertex lying on some cycle of G_1. Suppose that $F_1, F_2, \ldots, F_q$ are all components of G_1 and F_i is a c_i-cyclic graph for $1 \leq i \leq q$. Then,

$$\sum_{i=1}^{q} c_i = c, \text{ and } n \geq 1 + \sum_{i=1}^{q} |V(F_i)|, \text{ where } q \geq 2.$$

For $1 \leq i \leq q$, if $c_i = 1$, then F_i is a cycle and thus $|V(F_i)| \geq c_i + 2$; if $c_i = 2$, then F_i is a bicyclic graph and thus $|V(F_i)| \geq c_i + 2$; if $c_i \geq 3$, then $|V(F_i)| \geq c_i + 3$ according to $c_i < c$ and the induction hypothesis (otherwise, F_i and thus G contains a good special edge). This implies that

$$n \geq 1 + \sum_{i=1}^{q} |V(F_i)| \geq 1 + \sum_{i=1}^{q} (c_i + 2) = c + 2q + 1 \geq c + 5,$$

which is opposite to the condition $n \leq c + 2$. Thus, Claim 1 holds.

We choose $z \in \{u, v\}$. Since G contains no good special edge, uv is not a good special edge of G, and thus there exists neighbor w_1 of z such that w_1 is a 2-vertex.

Let us assume that z lies on a pendent cycle C. If $d(z) = 3$, let G_2 be the graph obtained from G by deleting all vertices of $V(C)$. If $d(z) = 4$, let G_2 be the graph obtained from G by deleting all vertices of $V(C) \setminus \{z\}$. In both cases, by Claim 1, G_2 is a $(c-1)$-cyclic graph with at most $n + 1 - |V(C)|$ vertices and minimum degree at least two. Since $n + 1 - |V(C)| \leq n - 2 < c - 1 + 2$, by the induction hypothesis, G_2 has at least one good special edge, and thus G also has a good special edge, which is a contradiction.

Let us assume that z does not lie on any pendent cycle of G. Then, there exist vertices $\{w_1, w_2, \ldots, w_t, w\}$ with $t \geq 1$ such that $d(w) \geq 3 > 2 = d(w_1) = d(w_2) = \cdots = d(w_t)$ (here, $w = \{u, v\} \setminus \{z\}$ is possible) and $zw_1w_2 \cdots w_t w$ is a path connecting z and w. By Claim 1, we may suppose that $\{z, w_1, w_2, \ldots, w_t, w\}$ are in the same cycle of G. Let G_3 be the graph obtained from G by deleting all vertices of $\{w_1, w_2, \ldots, w_t\}$. Then, G_3 is also a $(c-1)$-cyclic graph with $n - t$ vertices and minimum degree at least two. Since $n - t \leq n - 1 \leq c - 1 + 2$, from the induction hypothesis, G_3 has at least one good special edge, and thus G also has a good special edge, which is a contradiction. □

Proof of Theorem 1. This result will be proved by induction on n. Let G be the extremal graph with minimum AZI among all c-cyclic graph with n vertices. If $G = W_{n;c}$, then it is evident that equality holds in (1). Furthermore, since the result already holds for $c = 3$ [1], we may suppose $G \neq W_{n;c}$ for $c \geq 4$ as well.

From Corollary 1 and Lemma 6, we may assume that $\Delta \leq n-2$ and $\delta = 1$. Since $\delta = 1$, we choose u_0 as a non-pendent vertex of G such that u_0 is the neighbor of some pendent vertex. Suppose that $\{u_1, u_2, \ldots, u_p\}$ are all these pendent vertices adjacent to u_0, and $\{u_{p+1}, u_{p+2}, \ldots, u_r\}$ are all these non-pendent neighbors of u_0. This implies that

$$d(u_0) = r \text{ and } 1 \leq p \leq r - 1,$$

by the choice of u_0. Denote by G_1 be the graph obtained from G by deleting all these pendent vertices $\{u_1, u_2, \ldots, u_p\}$. Then, G_1 is also a c-cyclic graph with $n - p$ vertices. By the induction hypothesis, we have

$$AZI(G_1) \geq (n - p - c - 3)\left(\frac{n - p - 2}{n - p - 3}\right)^3 + 16(c + 1), \tag{4}$$

with equality iff G is isomorphic to the graph $W_{n-p;c}$.

Claim 1. $p \geq n - c - 2$.

Proof of Claim 1. By contradiction, let us assume that $p \leq n - c - 3$. Since

$$r \leq \Delta \leq n - 2, \ p \leq n - c - 3 \text{ and } \frac{n - p - 2}{n - p - 3} > \frac{n - 2}{n - 3} > 1,$$

from the definition of $AZI(G)$ and (4), we have

$$\begin{aligned}
&AZI(G)\\
=&\sum_{i=p+1}^{r}\left(\left(\frac{rd(u_i)}{r+d(u_i)-2}\right)^3-\left(\frac{d(u_i)(r-p)}{r+d(u_i)-p-2}\right)^3\right)+p\left(\frac{r}{r-1}\right)^3+AZI(G_1)\\
\geq&p\left(\frac{r}{r-1}\right)^3+(n-p-c-3)\left(\frac{n-p-2}{n-p-3}\right)^3+16(c+1)\quad\text{(by Lemma 4)}\\
\geq&p\left(\frac{n-2}{n-3}\right)^3+(n-p-c-3)\left(\frac{n-p-2}{n-p-3}\right)^3+16(c+1)\quad\text{(by Lemma 1 (i))}\\
=&(n-c-3)\left(\frac{n-2}{n-3}\right)^3+16(c+1)+(n-p-c-3)\left(\left(\frac{n-p-2}{n-p-3}\right)^3-\left(\frac{n-2}{n-3}\right)^3\right)\\
\geq&AZI(W_{n;c}).
\end{aligned}$$

By the choice of G, we can conclude that $AZI(G)=AZI(W_{n;c})$, and thus $r=n-2=\Delta$ and $p=n-c-3$. Furthermore, by Lemma 4 and (4), $G_1=W_{c+3;c}=K_{2,c+1}$. Since $r=n-2$ and from the structure of G_1, we can conclude that $G=W_{n;c}$, which is a contradiction. This completes the proof of Claim 1.

If there exists other vertex v_0 with $u_0\neq v_0$ such that v_0 is adjacent to $s\geq 1$ pendent vertex, then similarly to Claim 1 and by the symmetry of u_0 and v_0, we have $s\geq n-c-2$. Furthermore, since $c\geq 3$, G has at least four non-pendent vertices, and thus $n\geq s+p+4\geq 2n-2c$, which is in contradiction to $n\geq 2c+1$. This implies that

all pendent vertices are adjacent to u_0 of G.

Let H_0 be the base graph of G, that is, H_0 is obtained from G by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. Since $p\geq n-c-2$ by Claim 1, H_0 is also a c-cyclic graph with at most $c+2$ vertices and minimum degree at least two, and thus it contains a good special edge v_0w_0 by Lemma 8. This implies that v_0w_0 is also a good special edge of G.

Case 1. $u_0\notin\{v_0,w_0\}$. We may suppose that v_0 and u_0 are in the same component of $G-v_0w_0$. Denote by $G_2=G-v_0w_0+u_1w_0$. Then, G_2 is also a c-cyclic graph. From the definition of AZI, we have

$$\begin{aligned}
&AZI(G)-AZI(G_2)\\
=&\sum_{w\in N(v_0)\setminus\{w_0\}}\left(\left(\frac{d(v_0)d(w)}{d(v_0)+d(w)-2}\right)^3-\left(\frac{(d(v_0)-1)d(w)}{d(v_0)+d(w)-3}\right)^3\right)\\
&+\left(\frac{d(u_0)}{d(u_0)-1}\right)^3+\left(\frac{d(v_0)d(w_0)}{d(v_0)+d(w_0)-2}\right)^3-16.
\end{aligned}\tag{5}$$

We rewrite $\{v_0,w_0\}$ as $\{x_0,y_0\}$ such that $d(x_0)=\max\{d(v_0),d(w_0)\}$ and $d(y_0)=\min\{d(v_0),d(w_0)\}$.
If either $d(x_0)\geq d(y_0)\geq 4$ or $d(x_0)\geq 5>3=d(y_0)$, then Eq. (5), Lemmas 1 and 4 imply that

$$AZI(G)-AZI(G_2)>\left(\frac{d(v_0)d(w_0)}{d(v_0)+d(w_0)-2}\right)^3-15\geq\left(\frac{5}{2}\right)^3-15>0,$$

as each neighbor of v_0 is a non-pendent vertex. This is contrary to the choice of G.

If $d(x_0)=d(y_0)=3$, then $d(w)\geq 3$ for each $w\in N(v_0)\cup N(w_0)$ since v_0w_0 is a good special edge. In this case, (5) and Lemma 1 suggest that

$$AZI(G)-AZI(G_2)>2\left(\left(\frac{9}{4}\right)^3-8\right)+1+\left(\frac{9}{4}\right)^3-16>0,$$

which is a contradiction.

If $d(x_0)=4>3=d(y_0)$, then $d(w)\geq 3$ for some $w\in N(v_0)\setminus\{w_0\}$ since v_0w_0 is a good special edge. In this case, (5), Lemmas 1 and 4 imply that

$$\begin{aligned}
&AZI(G)-AZI(G_2)\\
>&\min\left\{\left(\left(\frac{9}{4}\right)^3-8\right),\left(\left(\frac{12}{5}\right)^3-\left(\frac{9}{4}\right)^3\right)\right\}+1+\left(\frac{12}{5}\right)^3-16>0,
\end{aligned}$$

which is a contradiction.

Case 2. $u_0 \in \{v_0, w_0\}$. Let us suppose that $u_0 = w_0$ and thus, u_0v_0 is a good special edge of H_0. Denote by $G_3 = G - u_0v_0 + u_1v_0$. Then, G_3 is also a c-cyclic graph. Recall that u_0 is adjacent to exactly p pendent vertices and $\{u_{p+1}, u_{p+2}, \ldots, u_r\}$ are all these non-pendent neighbors of u_0. Then,

$$d(u_0) = r \geq p + 3 \geq n - c - 2 + 3 \geq 2c + 1 - c - 2 + 3 = c + 2 \geq 6,$$

since u_0v_0 is a good special edge of H_0.

Suppose that $v_0 = u_r$. Then, from the definition of *AZI*, we have

$$\begin{aligned} AZI(G) - AZI(G_3) = &\sum_{i=p+1}^{r-1} \left(\left(\frac{d(u_i)r}{d(u_i)+r-2} \right)^3 - \left(\frac{(r-1)d(u_i)}{d(u_i)+r-3} \right)^3 \right) \\ &+ p\left(\frac{r}{r-1} \right)^3 - (p-1)\left(\frac{r-1}{r-2} \right)^3 \\ &+ \left(\frac{rd(v_0)}{r+d(v_0)-2} \right)^3 - 16. \end{aligned} \tag{6}$$

Denote by

$$f(p) = p\left(\frac{r}{r-1} \right)^3 - (p-1)\left(\frac{r-1}{r-2} \right)^3,$$

where $n - c - 2 \leq p \leq r - 1$. Then, $f'(p) = \left(\frac{r}{r-1}\right)^3 - \left(\frac{r-1}{r-2}\right)^3 < 0$ and thus

$$\begin{aligned} f(p) \geq f(r-1) =& (r-1)\left(\frac{r}{r-1} \right)^3 - (r-2)\left(\frac{r-1}{r-2} \right)^3 \\ =& \frac{r^4 - 6r^3 + 10r^2 - 5r + 1}{(r-1)^2(r-2)^2} > 0, \ (\text{as } r \geq 6). \end{aligned} \tag{7}$$

Now, since $r \geq 6$ and $d(v_0) \geq 3$, by Lemmas 1 and 4, (6) and (7) we have

$$AZI(G) - AZI(G_3) > \left(\frac{rd(v_0)}{r+d(v_0)-2} \right)^3 - 16 \geq \left(\frac{18}{7} \right)^3 - 16 > 0,$$

contrary to the choice of G. □

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On a conjecture of Schweser and Stiebitz☆

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ABSTRACT

Let G be a graph (which may have multiple edges but no loops), let the multiplicity $\mu_G(u, v)$ between two different vertices u and v be the number of edges joining u and v, and let $\mu_G(u) = \max\{\mu_G(u, v) : v \in V(G) \setminus \{u\}\}$. In this paper, we prove that if G is triangle-free in which no two quadrangles share edges, then for any two integral functions $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0, 1\}$ with $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 3$ for each vertex v of G, there is a partition (A, B) of $V(G)$ such that $d_{G[A]}(u) \geq a(u)$ for each $u \in A$ and $d_{G[B]}(v) \geq b(v)$ for each $v \in B$. Consequently, we confirm two conjectures of Schweser and Stiebitz (2019).

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1. Introduction

All graphs considered in this paper are finite and undirected, may have multiedges but no loops. We refer the readers to [3] for undefined terms and notations.

Let G be a graph. We use $N_G(v)$ to denote the neighbor set of a vertex v in G, and use $d_G(v)$ to denote the degree of v (which is the number of edges incident with v). Let $\Delta(G)$ and $\delta(G)$, respectively, be the maximum and the minimum degree of G. The *multiplicity* $\mu_G(u, v)$ of two different vertices u and v is defined to be the number of edges joining u and v, and the weight $\mu_G(u)$ of a vertex u is defined as

$$\mu_G(u) = \max\{\mu_G(u, v) : v \in V(G) \setminus \{u\}\}.$$

A graph is said to be *simple* if every pair of different vertices has multiplicity at most one.

We use $\mathbb{N}$ to denote the set of nonnegative integers. Let $f : V(G) \longrightarrow \mathbb{N}$ be a function, X be a subset of $V(G)$, and let v be a vertex of G. We use $G[X]$ to denote the subgraph of G induced by X, write $d_X(v)$ for the degree of v in $G[X]$ if $v \in X$, and write $e_G(v, X)$ for the number of edges between v and X if $v \notin X$ (in another words, $e_G(v, X) = d_{X\cup\{v\}}(v)$). We say that (i) X is *f-meager* if for every nonempty subset Y of X, Y has a vertex u with $d_Y(u) \leq f(u) + \mu_G(u) - 1$, (ii) X is *f-nice* if $d_X(u) \geq f(u) + \mu_G(u) - 1$ for each vertex $u \in X$, (iii) X is *f-feasible* if $d_X(u) \geq f(u)$ for each vertex $u \in X$, (iv) X is *f-suitable* if $d_X(u) \leq f(u) + \mu_G(u) - 1$ for each $u \in X$, and (v) X is *f-degenerate* if for each non-empty subset Y of X, Y has a vertex u with $d_Y(u) \leq f(u)$. From these definitions, if G has no isolated vertices, then each f-nice subset is also f-feasible, and each f-degenerate subset is also f-meager.

Let a, b: $V(G) \longrightarrow \mathbb{N}$ be two functions. Let A and B be two disjoint nonempty subsets of $V(G)$. We call (A, B) an *(a, b)-feasible pair* if A is a-feasible and B is b-feasible, and call (A, B) a partition of G if $A \cup B = V(G)$. A partition (A, B) of

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G is said to be (i) (a, b)-*feasible* if A is a-feasible and B is b-feasible, (ii) (a, b)-*suitable* if A is a-suitable and B is b-suitable, and (iii) (a, b)-*meager* if A is a-meager and B is b-meager.

In 1983, Thomassen [16] conjectured that for each pair of nonnegative integers s and t, if a simple graph has minimum degree at least $s + t + 1$ then it admits a partition (S, T) such that $\delta(G[S]) \geq s$ and $\delta(G[T]) \geq t$. In 1996, Stiebitz [15] proved a stronger functional version and confirmed the conjecture.

Theorem 1.1 ([15]). *Let G be a simple graph, and let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. If $d_G(v) \geq a(v) + b(v) + 1$ for each vertex v, then G admits an (a, b)-feasible partition.*

Since then, quite a few Stiebitz' type theorems have appeared concerning partitions of special families of simple graphs under minimum degree restrictions (see [2,5–9,11,14]), and Ban [1] proved a similar conclusion on weighted simple graphs.

A cycle of length four is referred to as a *quadrangle*, and K_4^- denotes the graph obtained from K_4 by removing an edge. In [12], Schweser and Stiebitz generalized some results of partitions of simple graphs to multigraphs, and they succeeded in proving that

Theorem 1.2 ([12]). *Let G be a graph with $\delta(G) \geq 1$, and let $a, b : V(G) \longrightarrow \mathbb{N}$ be two functions with $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 1$ for every vertex v. Then, G has an (a, b)-feasible partition.*

Theorem 1.3 ([12]). *Let G be a graph without K_4^- and having $\delta(G) \geq 1$, and let $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0\}$ be two functions with $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 2$ for every vertex v. Then, G has an (a, b)-feasible partition.*

Schweser and Stiebitz [12] also put forward the following two conjectures.

Conjecture 1.1 ([12]). *Let G be a graph with neither triangles nor quadrangles, and let $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0, 1\}$ be two functions such that $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 3$ for every vertex v. Then, G has an (a, b)-feasible partition.*

Conjecture 1.2 ([12]). *Let G be a triangle-free graph of which each edge is contained in at most one quadrangle, and let $a, b : V(G) \longrightarrow \mathbb{N}\setminus\{0, 1\}$ be two functions such that $d_G(v) \geq a(v)+b(v)+2\mu_G(v)-3$ for every vertex v. Then, G has an (a, b)-feasible partition.*

It is certain that the validity of Conjecture 1.2 implies that of Conjecture 1.1. In this paper, we confirm Conjecture 1.2.

Theorem 1.4. *Let G be a triangle-free graph in which no two quadrangles share edges, and let $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0, 1\}$ be two functions. If $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 3$ for every vertex v, then G has an (a, b)-feasible partition.*

Note that the requirement of no two quadrangles sharing edges excludes two subgraphs: one is $K_{2,3}$, and the other is the bipartite graph obtained from a cycle of length 6 by adding exactly one chord. In [17], Zu presented an example showing that there exists a simple graph G with neither triangles nor $K_{2,3}$ and two functions $a, b : V(G) \longrightarrow \mathbb{N}\setminus\{0, 1\}$ such that $d_G(v) \geq a(v) + b(v) - 1$ for every vertex v, but G does not admit an (a, b)-feasible partition. This negatively answers a question of [9] (see also [14]), and also shows that Theorem 1.4 is best possible in the sense that the requirements 'triangle-free and no two quadrangles sharing edges' are necessary.

Contrary to a partition, in a weak partition also empty sets are allowed. As early as in 1966, Lovász [10] concerned with partitions with maximum degree restrictions subject to constant functions, and he proved the following result.

Theorem 1.5 ([10]). *Let $d_1, d_2, \ldots, d_p$ be non-negative integers. If $p \geq 2$, then each simple graph G with $\Delta(G) \leq d_1 + d_2 + \cdots + d_p + p - 1$ has a weak partition $(A_1, A_2, \ldots, A_p)$ such that $\Delta(G[A_i]) \leq d_i$ for each $i \in \{1, 2, \ldots, p\}$.*

Later, Borodin and Kostochka [4] conveyed this outcome to the case of variable functions, and Schweser and Stiebitz [12] generalized Theorem 1.5 to graphs with multiedges. In what follows, we present another extension of Theorem 1.5, that is,

Theorem 1.6. *Let G be a graph with $\delta(G) \geq 1$, and let $a, b : V(G) \longrightarrow \mathbb{N}$ be two functions. If $2\mu_G(v) - 1 \leq d_G(v) \leq a(v) + b(v) + 2\mu_G(v) - 1$ holds for every vertex v, then G admits an (a, b)-suitable partition.*

The proofs of Theorems 1.4 and 1.6 will be given in Section 2.

2. The proofs of Theorems 1.4 and 1.6

Let G be a graph, let $a, b : V(G) \longrightarrow \mathbb{N}$ be two functions, and let (A, B) be a partition of G. As in [12], we define the weight $\omega(A, B)$ of (A, B) as

$$\omega(A, B) = |E(G[A])| + |E(G[B])| + \sum_{v\in A} b(v) + \sum_{v\in B} a(v). \tag{2.1}$$

The following result due to Schweser and Stiebitz will play an important role in our proof of Theorem 1.4.

Lemma 2.1 ([12]). *Let G be a graph with $\delta(G) \geq 1$, and let $a, b : V(G) \longrightarrow \mathbb{N}$ be two functions with $d_G(v) \geq a(v) + b(v) + 2\mu_G(v) - 3$ for every vertex v. If G has an (a, b)-feasible pair, then it has an (a, b)-feasible partition.*

Proof of Theorem 1.4. Let $\mathcal{G}$ be the set of graphs with neither triangles nor two quadrangles sharing common edges. Suppose that Theorem 1.4 does not hold, let G be a graph in $\mathcal{G}$, and let a, b be two functions as claimed such that G does not have (a, b)-feasible partition. Then, it follows from the degree condition that $\delta(G) \geq 1$. By Lemma 2.1,

$$G \text{ has no } (a, b)\text{-feasible pair.} \tag{2.2}$$

We may suppose that for every vertex $v \in V(G)$,

$$d_G(v) = a(v) + b(v) + 2\mu_G(v) - 3. \tag{2.3}$$

Otherwise, if $d_G(v_0) > a(v_0) + b(v_0) + 2\mu_G(v_0) - 3$ for some vertex v_0, we may reset $a'(v_0)$ such that $a'(v_0) + b(v_0) + 2\mu_G(v_0) - 3 = d_G(v_0)$, and let $a'(w) = a(w)$ for any vertex w other than v_0, then the existence of an (a', b)-feasible partition would certainly guarantee that of an (a, b)-feasible partition of G. We first show that

Claim 1. *G has an $(a - 1, b - 1)$-meager partition.*

Proof. Let $V(G) = V$, and $v \in V$ be an arbitrary vertex. For any vertex $x \neq v$, $d_{G-v}(x) \geq d_G(x) - \mu_G(x) \geq a(x) + b(x) + \mu_G(x) - 3 \geq a(x) + \mu_G(x) - 1$ since $b(x) \geq 2$. Hence, $V \setminus \{v\}$ is an a-nice set. Let S be a minimal a-nice subset of V. Then, $S \subsetneq V$, and hence $T = V \setminus S$ is nonempty.

Since G has no (a, b)-feasible pair, and since S is an a-feasible subset, T must be $(b - 1)$-degenerate and hence is $(b-1)$-meager. Let u be a vertex of S. Then, $d_S(u) \geq a(u)+\mu_G(u)-1 \geq \mu_G(u)+1$, as S is a-nice. This implies that $|S| \geq 2$. The minimality of S shows that

$$S \setminus \{u\} \text{ is } (a - 1)\text{-meager.}$$

Since $d_G(u) = a(u)+b(u)+2\mu_G(u)-3$ by (2.3), $d_{T\cup\{u\}}(u) \leq b(u)+\mu_G(u)-2$ which implies that $T\cup\{u\}$ is $(b-1)$-meager. Therefore, $\big(S \setminus \{u\}, T \cup \{u\}\big)$ is an $(a - 1, b - 1)$-meager partition of G. ■

An $(a - 1, b - 1)$-meager partition (A, B) is called a *maximum (a, b)-partition* if $\omega(A, B)$ reaches maximum among all $(a - 1, b - 1)$-meager partitions of G.

From now on, we always suppose that (A, B) is a maximum (a, b)-partition. Let $A^- = \big\{x | \, x \in A,\ d_A(x) \leq a(x)+\mu_G(x)-2\big\}$, $A^= = \big\{x | \, x \in A,\ d_A(x) = a(x) + \mu_G(x) - 1\big\}$, and let $A^+ = A \setminus \big(A^- \cup A^=\big)$. Analogously, we can define B^-, $B^=$ and B^+.

Since (A, B) is a maximum (a, b)-partition, $A^- \neq \emptyset$ and $B^- \neq \emptyset$. Let u be an arbitrary vertex in A^-, and v be an arbitrary vertex in B^-. Then, $e_G(u, B) \geq b(u) + \mu_G(u) - 1 \geq \mu_G(u) + 1$ and $e_G(v, A) \geq a(v) + \mu_G(v) - 1 \geq \mu_G(v) + 1$, which implies that

$$|A| \geq 2 \quad \text{and} \quad |B| \geq 2.$$

It follows from (2.1) and (2.3) that

$$\begin{aligned} &\omega\big(A \setminus \{u\}, B \cup \{u\}\big) - \omega(A, B) \\ \geq &b(u) + \mu_G(u) - 1 - \big(a(u) - 2 + \mu_G(u)\big) + a(u) - b(u) = 1, \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} &\omega\big(A \cup \{v\}, B \setminus \{v\}\big) - \omega(A, B) \\ \geq &a(v) + \mu_G(v) - 1 - \big(b(v) - 2 + \mu_G(v)\big) + b(v) - a(v) = 1. \end{aligned} \tag{2.5}$$

Claim 2. *Let (A, B) be a maximum (a, b)-partition. Then, for each pair of vertices $u \in A^-$ and $v \in B^-$, the following statements hold:*
(i) $A' = A \cup \{v\}$ is not $(a - 1)$-meager, and so A' has an a-nice subset. Moreover, every a-nice subset of A' contains both u and v;
(ii) $B' = B \cup \{u\}$ is not $(b - 1)$-meager, and so B' has a b-nice subset. Moreover, every b-nice subset of B' contains both u and v;
(iii) $uv \in E(G)$, both A^- and B^- are independent sets of G, and both sets $A \setminus A^-$ and $B \setminus B^-$ are nonempty;
(iv) If $\min\{|A^-|, |B^-|\} \geq 2$, then $|A^-| = |B^-| = 2$.

Proof. Recall that (A, B) is an $(a - 1, b - 1)$-meager partition. Thus, v is contained in every a-nice subset of A' and u is contained in every b-nice subset of B'. By (2.4) and (2.5), A' cannot be $(a - 1)$-meager, and B' cannot be $(b - 1)$-meager. Let A^* be an arbitrary a-nice subset of A' and B^* an arbitrary b-nice subset of B'. Since $u \notin A^*$ and $v \notin B^*$ would imply

that (A^*, B^*) is an (a, b)-feasible pair, by (2.2), either every a-nice subset of A' must include u, or every b-nice subset of B' must include v.

Now, we suppose that $(A \cup \{v\}) \setminus \{u\}$ has an a-nice subset. Then, every b-nice subset of $B \cup \{u\}$ must contain v, which indicates that $d_G(v) \geq d_{B\cup\{u\}}(v) + e_G(v, A \setminus \{u\}) \geq (b(v) + \mu_G(v) - 1) + (a(v) + \mu_G(v) - 1) = a(v) + b(v) + 2\mu_G(v) - 2$, contradicting (2.3). This proves (i) and (ii) by the symmetry of u and v.

Since $uv \notin E(G)$ implies that $d_{A'}(u) = d_A(u) \leq a(u) + \mu_G(u) - 2$ and so $u \notin A^*$ (and, similarly, $v \notin B^*$), it follows directly that

$$uv \in E(G). \tag{2.6}$$

Recall that G is a graph with neither triangles nor two quadrangles sharing edges. Thus, A^- and B^- are independent sets of G, and if $\min\{|A^-|, |B^-|\} \geq 2$, then $|A^-| = |B^-| = 2$ by (2.6). Thus, (iv) holds.

To complete the proof of (iii), to the contrary, we suppose by the symmetry of $A \setminus A^-$ and $B \setminus B^-$ that $A \setminus A^- = \emptyset$. By (i), A' is not $(a-1)$-meager and every a-nice subset of A' must contain u, this implies that $\mu_G(u) \geq d_{A'}(u) \geq a(u) + \mu_G(u) - 1 \geq \mu_G(u) + 1$, as A^- is an independent set of G. This contradiction implies that (iii) holds. ■

Claim 3. *Let (A, B) be a maximum (a, b)-partition, let $u \in A^-$, and let $v \in B^-$. If $d_A(u) \leq a(u) - 1$ or $d_B(v) \leq b(v) - 1$, then the partition $(\widetilde{A}, \widetilde{B})$ with $\widetilde{A} = (A \cup \{v\}) \setminus \{u\}$ and $\widetilde{B} = (B \cup \{u\}) \setminus \{v\}$ is also a maximum (a, b)-partition. Furthermore, the following statements hold:*
(i) If $d_A(u) \leq a(u) - 1$, then $\mu_G(u) = \mu_G(u, v)$, $d_{\widetilde{B}}(u) = b(u) + \mu_G(u) - 2$, and $d_{\widetilde{A}}(v) = a(v) - 1 + \mu_G(v) - \mu_G(u, v) \leq a(v) + \mu_G(v) - 2$.
(ii) If $d_B(v) \leq b(v) - 1$, then $\mu_G(v) = \mu_G(v, u)$, $d_{\widetilde{A}}(v) = a(v) + \mu_G(v) - 2$, and $d_{\widetilde{B}}(u) = b(u) - 1 + \mu_G(u) - \mu_G(u, v) \leq b(u) + \mu_G(u) - 2$.

Proof. By Claim 2, $(\widetilde{A}, \widetilde{B})$ is an $(a-1, b-1)$-meager partition of G. By symmetry, we may suppose that $d_A(u) \leq a(u) - 1$. Since $d_G(u) = a(u) + b(u) + 2\mu_G(u) - 3$ and $d_G(v) = a(v) + b(v) + 2\mu_G(v) - 3$ by (2.3) and since $uv \in E(G)$ by Claim 2(iii), $\omega(\widetilde{A}, \widetilde{B}) - \omega(A, B) \geq (b(u) + 2\mu_G(u) - 2 - \mu_G(u, v)) + (a(v) - 1 + \mu_G(v) - \mu_G(u, v)) + a(u) + b(v) - (a(u) - 1 + b(v) + \mu_G(v) - 2 + a(v) + b(u)) = 2\mu_G(u) - 2\mu_G(u, v) \geq 0$, $(\widetilde{A}, \widetilde{B})$ is also a maximum (a, b)-partition, $\mu_G(u) = \mu_G(u, v)$, $d_{\widetilde{B}}(u) = b(u) + \mu_G(u) - 2$, and $d_{\widetilde{A}}(v) = a(v) - 1 + \mu_G(v) - \mu_G(u, v) \leq a(v) + \mu_G(v) - 2$ (as otherwise, we would have $\omega(\widetilde{A}, \widetilde{B}) > \omega(A, B)$). Now, we can conclude that Claim 3 holds. ■

Claim 4. *Let (A, B) be a maximum (a, b)-partition, u_1 be a vertex in $N_{A=}(u)$ and v_1 be a vertex in $N_{B=}(v)$, where $u \in A^-$ and $v \in B^-$. If either $d_A(u) \leq a(u) - 1$ or $d_B(v) \leq b(v) - 1$, then $u_1v_1 \in E(G)$.*

Proof. Let $(A_1, B_1) = ((A \cup \{v\}) \setminus \{u\}, (B \cup \{u\}) \setminus \{v\})$. By Claim 3, (A_1, B_1) is also a maximum (a, b)-partition. Since $u_1v \notin E(G)$ and $uv_1 \notin E(G)$ (otherwise, G would contain a triangle), $u_1 \in A_1^-$ and $v_1 \in B_1^-$, and thus $u_1v_1 \in E(G)$ by Claim 2(iii). ■

Let X and Y be two subsets of $V(G)$. We define $N_Y(X) = \cup_{x\in X} N_Y(x)$, where $N_Y(x)$ is the set of neighbors of x in Y.

Claim 5. *If (A, B) is a maximum (a, b)-partition, then $\min\{|A^-|, |B^-|\} = 1$.*

Proof. By Claim 2(iv), either $\min\{|A^-|, |B^-|\} = 1$, or $|A^-| = |B^-| = 2$.

Suppose that $|A^-| = |B^-| = 2$. Let $A^- = \{u, u'\}$ and $B^- = \{v, v'\}$. Now, $G[\{u, v, u', v'\}]$ is a quadrangle by Claim 2(iii), and thus

$$\text{every other vertex has at most one neighbor in } \{u, v, u', v'\} \tag{2.7}$$

as $G \in \mathcal{G}$. Since $A \cup B^-$ is not $(a-1)$-meager by Claim 2(i), $B \setminus B^-$ must be $(b-1)$-degenerate and non-empty by Claim 2(iii), which indicates the existence of a vertex $v_1 \in B \setminus \{v, v'\}$ such that

$$d_B(v_1) \geq b(v_1) + \mu_G(v_1) - 1 \text{ and } d_{B\setminus\{v,v'\}}(v_1) \leq b(v_1) - 1.$$

Combining this with (2.7), we have $b(v_1) + \mu_G(v_1) - 1 \leq d_B(v_1) \leq b(v_1) - 1 + \mu_G(v_1)$, confirming that v_1 is a vertex in $N_{B=}(B^-)$. The similar argument shows that $N_{A=}(A^-) \neq \emptyset$.

Since G has no (a, b)-feasible pair, we may suppose by symmetry that B is $(b-1)$-degenerate, and suppose further that $d_B(v) \leq b(v) - 1$. If $N_{B=}(v) = \emptyset$ and $d_B(v') \geq b(v')$, then $B\setminus\{v\}$ contains a b-feasible subset by (2.7) and $A \cup \{v\}$ is not $(a-1)$-meager by Claim 2(i), which indicates that G has an (a, b)-feasible pair, contradicting (2.2). Therefore, we may suppose further, by symmetry between v and v', that $N_{B=}(v) \neq \emptyset$. Let v_1 be a vertex in $N_{B=}(v)$, and let u_1 be a vertex in $N_{A=}(u)$ by symmetry. Then, $u_1v_1 \in E(G)$ following from Claim 4, and hence uv appears in two quadrangles of $G[\{u, u', u_1, v, v', v_1\}]$, contradicting $G \in \mathcal{G}$. ■

Let (A, B) be a maximum (a, b)-partition. If $B^- = \{v\}$, then let

$$D = \{w \in B \mid d_{B\setminus\{v\}}(w) \leq b(w) - 1\}.$$

Claim 6. *Let (A, B) be a maximum (a, b)-partition. If $B^- = \{v\}$, then D is a nonempty independent set of $B^=$ and $\mu_G(w, v) = \mu_G(w) \geq 1$ for all $w \in D$.*

Proof. By Claim 2(iii), $B \neq \{v\}$. Since G has no (a, b)-feasible pair, and since $A \cup \{v\}$ is not $(a-1)$-meager by Claim 2(i), $B \setminus \{v\}$ is $(b-1)$-degenerate, and so has a vertex, say w, with $d_{B\setminus\{v\}}(w) \leq b(w) - 1$. Combining this with $w \notin B^-$, we have $b(w) + \mu_G(w) - 1 \leq d_B(w) \leq d_{B\setminus\{v\}}(w) + \mu_G(w, v) \leq b(w) + \mu_G(w) - 1$. Therefore,

$$d_B(w) = b(w) + \mu_G(w) - 1 \text{ and } \mu_G(w, v) = \mu_G(w) \geq 1. \tag{2.8}$$

Since G is triangle-free, D is a nonempty independent set of $B^=$, and thus Claim 6 holds. ■

Let (A, B) be a maximum (a, b)-partition with $B^- = \{v\}$. By Claim 6, we can choose $w \in D$. Since $d_B(w) = b(w) + \mu_G(w) - 1 \geq \mu_G(w, v) + 1$ by (2.8) and G is triangle-free, we have $B \setminus \big(N(v) \cup \{v\}\big) \neq \emptyset$.

If $N_{B^=}(D) = \emptyset$, then $N_B(D) \setminus \{v\} \subseteq B^+$. Since $B \setminus \big(\{v\} \cup D\big)$ is $(b-1)$-degenerate by Claim 2(i), and since each vertex but v has at most two neighbors in D (as $G \in \mathcal{G}$), B^+ has a vertex, say v_3, which has exactly two neighbors, say v_1 and v_2, in D such that $b(v_3) + \mu_G(v_3) \leq d_B(v_3) \leq b(v_3) - 1 + \mu_G(v_2, v_3) + \mu_G(v_1, v_3)$ and $N_B(v_1) \cap N_B(v_2) = \{v, v_3\}$.

From the above arguments and Claim 6, there exists $v_1 \in D$ satisfies the following two possibilities: either
(C1) $N_{B^=}(v_1)$ has a vertex v_2; or
(C2) there exists a vertex other than v_1, say v_2, in $N_{B^=}(v)$, and a vertex, say v_3, in B^+ such that $N(v_1) \cap N(v_2) = \{v, v_3\}$, and $b(v_3) + \mu_G(v_3) \leq d_B(v_3) \leq b(v_3) - 1 + \mu_G(v_1, v_3) + \mu_G(v_2, v_3)$.

Below Claim 7 tells that under appropriate assumption to A, (C1) holds.

Claim 7. *Let (A, B) be a maximum (a, b)-partition with $B^- = \{v\}$. Let u and w be two vertices in A^-, and let z be a vertex in $N_{A^+}(u) \cap N_{A^+}(w)$. Suppose that $d_A(w) \leq a(w) - 1$ and $d_A(z) \leq a(z) - 1 + \mu_G(u, z) + \mu_G(w, z)$. If either $d_A(u) \leq a(u) - 1$ or $d_B(v) \leq b(v) - 1$, then* (C1) *holds.*

Proof. Suppose that $d_A(u) \leq a(u) - 1$ or $d_B(v) \leq b(v) - 1$, but (C1) does not hold. Then, we have (C2).

Since $G \in \mathcal{G}$, $N_A(u) \cap N_A(w) = \{z\}$, $N(u) \cap \{v_1, v_2, v_3\} = \emptyset$, and $N(v_i) \cap \{u, w, z\} = \emptyset$ for $i \in \{1, 2\}$, where $\{v_1, v_2, v_3\}$ are as defined in (C2).

Let $\big(A_2, B_2\big) = \big((A \cup \{v_1\}) \setminus \{u\}, (B \cup \{u\}) \setminus \{v_1\}\big)$. We first show that

$$\big(A_2, B_2\big) \text{ is also an } (a-1, b-1)\text{-meager partition of } G. \tag{2.9}$$

Since $d_B(v_1) = b(v_1) + \mu_G(v_1) - 1$, $e_G(v_1, A) = a(v_1) + \mu_G(v_1) - 2$ by (2.3) which implies that A_2 is $(a-1)$-meager. To prove (2.9), it suffices to show that B_2 is $(b-1)$ meager.

If $d_B(v) \leq b(v) - 1$, then every b-nice subset of $B \cup \{u\}$ must contain v and v_1 by Claim 2(ii), and so B_2 is $(b-1)$ meager. So, we suppose that $d_B(v) \geq b(v)$, which implies that $d_A(u) \leq a(u) - 1$ by our assumption.

Let $\big(A_3, B_3\big) = \big((A \cup \{v\}) \setminus \{u\}, (B \cup \{u\}) \setminus \{v\}\big)$. By Claim 3(i), $\big(A_3, B_3\big)$ is also a maximum (a, b)-partition, $\mu_G(u) = \mu_G(u, v)$, $d_{A_3}(v) = a(v) - 1 + \mu_G(v) - \mu_G(u, v) \leq a(v) + \mu_G(v) - 2$, and $d_{B_3}(u) = b(u) + \mu_G(u) - 2$. Since $N_G(u) \cap \{v_1, v_2\} = \emptyset$, $\{v_1, v_2, u\} \subseteq B_3^-$ and $v \in A_3^-$, and thus every b-nice subset of $B_3 \cup \{v\}$ must contain $\{v_1, v_2, u\}$ by Claim 2(ii).

Since $B_3 \cup \{v\} = B \cup \{u\}$, every b-nice subset of $B \cup \{u\}$ must contain both v and v_1. This confirms that B_2 is indeed $(b-1)$-meager, and thus proves (2.9).

Combining (2.9) with the fact that $\omega\big(A_2, B_2\big) - \omega(A, B) \geq \big(a(v_1) + \mu_G(v_1) - 2\big) + \big(b(u) + \mu_G(u) - 1\big) + a(u) + b(v_1) - \big(b(v_1) + \mu_G(v_1) - 1 + a(u) + \mu_G(u) - 2 + a(v_1) + b(u)\big) = 0$, we see that $\big(A_2, B_2\big)$ is also a maximum (a, b)-partition, $e_G\big(v_1, A\big) = a(v_1) + \mu_G(v_1) - 2$ and $e_G\big(u, B\big) = b(u) + \mu_G(u) - 1$, which implies that

$$\{w, v_1\} \subseteq A_2^-.$$

If $\big(N_B(v_1) \setminus \{v\}\big) \cap B_2^-$ contains a vertex, say v', then $wv' \in E(G)$ by Claim 2(iii) (as $w \in A_2^-$), and so vw would be in two quadrangles $G\big[\{v, u, w, z\}\big]$ and $G\big[\{v, w, v_1, v'\}\big]$, a contradiction. Suppose so that $\big(N_B(v_1) \setminus \{v\}\big) \cap B_2^- = \emptyset$. Note that $d_{B_2}(u) = e_G\big(u, B\big) = b(u) + \mu_G(u) - 1$ and $d_{B_2}(v_2) = d_B(v_2) = b(v_2) + \mu_G(v_2) - 1$. The only possibility is that $v \in B_2^-$. Since $d_{A_2}(z) \leq a(z) - 1 + \mu_G(w, z)$, either $z \in A_2^-$ yielding the triangle $G\big[\{w, v, z\}\big]$ by Claim 2(iii), or $z \in A_2^=$ yielding that $zv_2 \in E(G)$ by Claim 4 (as $v_2 \in B_2^= \cap N_G(v)$ and $d_{A_2}(w) = d_A(w) \leq a(w) - 1$). In the latter case, vw lies in two quadrangles of $G\big[\{v, u, z, w, v_2\}\big]$, contradicting $G \in \mathcal{G}$. This contradiction completes the proof of Claim 7. ■

In what follows, by Claims 5 and 6, we suppose that (A, B) is a maximum (a, b)-partition such that u is a vertex in A^-, $B^- = \{v\}$, and $v_1 \in D$ such that there is a vertex v_2 satisfying (C1) or vertices $v_2 \in N_{B^=}(v)$ and $v_3 \in B^+$ satisfying (C2). To finish the proof of Theorem 1.4, we distinguish two cases depending on the value of $d_B(v)$. Let

$$W = \big\{u' \mid u' \in A^- \text{ and } d_A\big(u'\big) \leq a\big(u'\big) - 1\big\}.$$

Case 1. We first suppose that $d_B(v) \leq b(v) - 1$, and will deduce a contradiction to Claim 2(ii) by showing that

$$\big(B \cup \{w\}\big) \setminus \{v\} \text{ has a } b\text{-nice subset for some } w \in A^-. \tag{2.10}$$

Suppose that (2.10) is not true. By Claim 2(ii), every b-nice subset of $B\cup\{u\}$ must contain v and hence

$$d_B(v)=b(v)-1,\ \ \mu_G(u,v)=\mu_G(v),\ \ \big(B\cup\{u\}\big)\setminus\{v\}\text{ is }(b-1)\text{-meager},\tag{2.11}$$

and

$$\big(B\cup\{u\}\big)\setminus\{v'\}\text{ is }(b-1)\text{-meager for each }v'\in N_B(v).\tag{2.12}$$

In particular, $\big(B\cup\{u\}\big)\setminus\{v_1\}$ is $(b-1)$-meager.

Case 1.1. Suppose that $N_{A=}(A^-)\neq\emptyset$. Since $u\in A^-$ was chosen arbitrarily, we may suppose that u_1 is a vertex in $N_{A=}(u)$. By Claim 2(ii), $\big(B\cup\{u\}\big)\setminus\{v\}$ is $(b-1)$-meager. By (2.3), $d_G(v)=a(v)+b(v)+2\mu_G(v)-3$. So, $e_G\big(v,A\setminus\{u\}\big)=a(v)+\mu_G(v)-2$ by (2.11), which implies that $\big(A\cup\{v\}\big)\setminus\{u\}$ is $(a-1)$-meager. Recall that $\big(A_1,B_1\big)=\big((A\cup\{v\})\setminus\{u\},(B\cup\{u\})\setminus\{v\}\big)$. By Claim 3(ii), $\big(A_1,B_1\big)$ is also a maximum (a,b)-partition with $d_{A_1}(v)=a(v)+\mu_G(v)-2$ and $d_{B_1}(u)=b(u)-1+\mu_G(u)-\mu_G(v)\le b(u)-2+\mu_G(u)$. Since $u_1v,uv_1\notin E(G)$ as $G\in\mathcal{G}$, $u_1\in A_1^-$ and $v_1\in B_1^-$. Now, $\min\big\{|A_1^-|,|B_1^-|\big\}\ge 2$ as $v\in A_1^-$ and $u\in B_1^-$, contradicting Claim 5.

Case 1.2. Now, we suppose that $N_{A=}(A^-)=\emptyset$, i.e., $N_A(A^-)\subseteq A^+$.

Since $A^-\neq A$ by Claim 2(iii), and since $B\cup\{u\}$ is not $(b-1)$-meager by Claim 2(ii), $|A^-|\ge 2$ by the $(a-1)$-degeneracy of $A\setminus\{u\}$. Note that each vertex but v has at most two neighbors in A^- by Claim 2(iii). Since $A\setminus\{u\}$ and therefore $A\setminus A^-$ are $(a-1)$-degenerate, there are two vertices $x,y\in A^-$ and a vertex $z\in A^+$ such that

$$N_A(x)\cap N_A(y)=\{z\},\ \text{ and }a(z)+\mu_G(z)\le d_A(z)\le a(z)-1+\mu_G(x,z)+\mu_G(y,z).\tag{2.13}$$

Now, we have a quadrangle $vxzyv$.

Let w be a vertex in $\{x,y\}$, and let $\big(A_4,B_4\big)=\big((A\cup\{v\})\setminus\{w\},(B\cup\{w\})\setminus\{v\}\big)$. By Claim 3(ii), $\big(A_4,B_4\big)$ is also a maximum (a,b)-partition with $e_G\big(v,A\big)=a(v)+2\mu_G(v)-2$ and $e_G\big(w,B\big)=b(w)+\mu_G(w)-1$, which imply that

$$d_A(x)=a(x)+\mu_G(x)-2\text{ and }d_A(y)=a(y)+\mu_G(y)-2.\tag{2.14}$$

We claim that

$$\text{either }d_A(x)\le a(x)-1\text{ or }d_A(y)\le a(y)-1.\tag{2.15}$$

Suppose to the contrary that (2.15) does not hold, i.e., $d_A(x)\ge a(x)$ and $d_A(y)\ge a(y)$. Recall that $d_A(u')\le a(u')-1$ for each vertex $u'\in W$. If $W=\emptyset$, then $A\setminus\{x\}$ is an a-feasible subset (as $N_{A=}(A^-)=\emptyset$). On the other hand, $B\cup\{x\}$ is not $(b-1)$-meager by Claim 2(ii), and thus there is a b-nice subset of $B\cup\{x\}$, which leads to an (a,b)-feasible pair, contradicting (2.2). Similarly, if $W=\{x'\}$, then $A\setminus\{x'\}$ is also an a-feasible subset. So, we suppose that $|W|\ge 2$. For each pair of vertices x' and y' of W, either $N_A(x')\cap N_A(y')=\emptyset$, or $N_A(x')\cap N_A(y')$ consists of a single vertex z' with $d_A(z')\ge a(z')+\mu_G(z',x')+\mu_G(z',y')$ (as otherwise (2.15) holds with $\{x',y',z'\}$ taking the role of $\{x,y,z\}$). In both situations, $A\setminus W$ contains an a-feasible subset (as $N_A(A^-)\subseteq A^+$ in this subcase), contradicting the fact that $B\cup W$ is not $(b-1)$-meager by Claim 2(ii). Therefore, (2.15) holds.

Without loss of generality, we suppose that $d_A(y)\le a(y)-1$. Then, (C1) holds by Claim 7, i.e., there exists a vertex v_2 satisfying (C1).

Next, we show $(B\cup\{x\})\setminus\{v\}$ has a b-nice subset, that is, x is a vertex satisfying (2.10), and thus finish the proof of Case 1.

If it is not the case, then we define $(A_4,B_4)=\big((A\cup\{v\})\setminus\{x\},(B\cup\{x\})\setminus\{v\}\big)$, and thus $d_A(x)=a(x)+\mu_G(x)-2$ by (2.14). Since $G\in\mathcal{G}$, $vz,xv_1,xv_2\notin E(G)$, and hence $v_1\in B_4^-$, $d_{B_4}(v_1)=b(v_1)-1$ and $v_2\in N_{B_4^=}(v_1)$ by Claim 6. Following from (2.11), $e_G\big(v,A\setminus\{x\}\big)=a(v)+\mu_G(v)-2$, and so $v\in A_4^-$. Now, $d_{A_4}(y)\le d_A(y)+\mu_G(v,y)\le a(y)-1+\mu_G(y)$. Either $y\in A_4^-$ yielding the triangle $G\big[\{v,y,v_1\}\big]$ by Claim 2(iii) and $v_1\in B_4^-$, or $y\in N_{A_4^=}(v)$ which implies $yv_2\in E(G)$ by Claim 4 and produces another quadrangle vv_1v_2yv. Then, yv is contained in two quadrangles $vxzyv$ (see (2.13)) and vv_1v_2yv, contradicting $G\in\mathcal{G}$.

Case 2. Now, we suppose that $b(v)\le d_B(v)\le b(v)+\mu_G(v)-2$. Then, B is b-feasible.

Since G has no (a,b)-feasible pair, A is $(a-1)$-degenerate, and thus $W\neq\emptyset$. Without loss of generality, we suppose that $d_A(u)\le a(u)-1$. Since the case that $|A^-|=1$ can be dealt with by the same arguments as those used in Case 1, we further suppose that $|A^-|\ge 2$.

Next, we show that $\big(A\cup\{v\}\big)\setminus\{u\}$ has an a-nice subset. Then, this contradicts Claim 2(i) and completes the proof of Theorem 1.4.

First, we suppose that $N_{A=}(u)\neq\emptyset$. By Claim 2(i), $\big(A\cup\{v\}\big)\setminus\{u\}$ has no a-nice subsets. Then, every a-nice subset of $A\cup\{v\}$ must contain u which implies that $d_A(u)=a(u)-1$, $\mu_G(u,v)=\mu_G(u)$ and $\big(A\cup\{v\}\big)\setminus\{u\}$ is $(a-1)$-meager. Since $d_G(u)=a(u)+b(u)+2\mu_G(u)-3$, $e_G\big(u,B\setminus\{v\}\big)=b(u)+\mu_G(u)-2$, and so $\big(B\cup\{u\}\big)\setminus\{v\}$ is $(b-1)$-meager. As defined in the proof of Claim 7, we denote by $\big(A_3,B_3\big)=\big((A\cup\{v\})\setminus\{u\},(B\cup\{u\})\setminus\{v\}\big)$. By Claim 3(i), $\big(A_3,B_3\big)$ is also a maximum (a,b)-partition with $v\in A_3^-$ and $u\in B_3^-$. Let u_1 be a vertex in $N_{A=}(u)$. Since $u_1v,uv_1\notin E(G)$, $u_1\in A_3^-$ and $v_1\in B_3^-$. Now, $\min\big\{|A_3^-|,\ |B_3^-|\big\}\ge 2$ as $v\in A_3^-$ and $u\in B_3^-$, contradicting Claim 5.

So, we suppose that $N_{A^=}(u) = \emptyset$. In this case, we may suppose that $N_A(W) \subseteq A^+$ by symmetry.

If $N_A(x) \cap N_A(y) = \emptyset$ for each pair of vertices x and y of W, then $A \setminus W$ has an a-feasible subset. On the other hand, $B \cup W$ is not $(b-1)$-meager by Claim 2(ii), and hence $B \cup W$ contains a b-nice subset, which leads to an (a, b)-feasible pair, contradicting (2.2). So, there must exist distinct vertices $x, y \in W$, and a vertex $z \in N_A(x) \cap N_A(y)$ such that $a(z) + \mu_G(z) \le d_A(z) \le a(z) - 1 + \mu_G(x, z) + \mu_G(y, z)$. Now, we have the quadrangle

$$vxyzv.$$

By applying Claim 7 to $\{v, x, y, z\}$ (here, $\{x, y\}$ takes the role of $\{u, w\}$ in Claim 7), we conclude that (C1) holds, i.e., $v_2 \in N_{B^=}(v_1)$. Let $\big(A_5, B_5\big) = \big((A \cup \{v\}) \setminus \{x\}, (B \cup \{x\}) \setminus \{v\}\big)$. By Claim 2(i) and (ii), every a-nice subset of $A \cup \{v\}$ must contain x and y, and every b-nice subset of $B \cup \{x\}$ must contain v. Hence, $d_{A_5}(y) = a(y) + \mu_G(y) - 1$, as $d_A(y) \le a(y) - 1$ and $xy \notin E(G)$. By Claim 3(i), $\big(A_5, B_5\big)$ is also a maximum (a, b)-partition with $d_{A_5}(v) = a(v) + \mu_G(v) - 1 - \mu_G(x, v) \le a(v) + \mu_G(v) - 2$. This implies that $y \in N_{A_5^=}(v)$ and $v \in A_5^-$. Since $v_2 \in N_{B_5^=}(v_1)$ and $v_1 \in B_5^-$ as $d_{B_5}(v_1) = b(v_1) - 1$ by Claim 6, we have $yv_2 \in E(G)$ by Claim 4. But now, vy is contained in two quadrangles $vxzyv$ and yvv_1v_2y, a contradiction.

This completes the proof of Theorem 1.4. ■

Proof of Theorem 1.6. We may suppose that $d_G(v) = a(v) + b(v) + 2\mu_G(v) - 1$ holds for every $v \in V(G)$. Otherwise, if $d_G(v_0) < a(v_0) + b(v_0) + 2\mu_G(v_0) - 1$ for some vertex $v_0 \in V(G)$, then we may reset $a'(v_0)$ and $b'(v_0)$ such that $a'(v_0) + b'(v_0) + 2\mu_G(v_0) - 1 = d_G(v_0) \ge 2\mu_G(v_0) - 1$, $0 \le a'(v_0) \le a(v_0)$ and $0 \le b'(v_0) \le b(v_0)$, and let $a'(w) = a(w)$ and $b'(w) = b(w)$ for any vertex w other than v_0. If we can show the existence of an (a', b')-suitable partition of G, then this partition is also an (a, b)-suitable partition of G.

Let (A, B) be a partition of G with minimum weight. We claim that (A, B) is an (a, b)-suitable partition. If it is not the case, we may suppose, by symmetry, that A has a vertex, say x with $d_A(x) \ge a(x) + \mu_G(x)$. Consequently, $e_G(x, B) \le b(x) + \mu_G(x) - 1$ and $|A| \ge 2$, as G contains no loop. In this case, by (2.1) we have

$$\begin{aligned}\omega\big(A \setminus \{x\}, B \cup \{x\}\big) - \omega\big(A, B\big) &= e_G(x, B) - d_A(x) + a(x) - b(x)\\ &\le \big(b(x) + \mu_G(x) - 1\big) - \big(a(x) + \mu_G(x)\big) + a(x) - b(x)\\ &= -1,\end{aligned}$$

a contradiction. This contradiction implies the existence of an (a, b)-suitable partition. ■

3. Remark

Our Theorem 1.4 confirms Conjecture 1.2 (and certainly Conjecture 1.1 as well), and also generalizes Theorem 1.6 of [9] from simple graphs to graphs.

In [11], Ma and Yang strengthened the result of Diwan [5], and proved that if G is a simple graph without quadrangles, then for each pair of integral functions $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0, 1\}$ with $d_G(v) \ge a(v) + b(v) - 1$ for every vertex v, G has an (a, b)-feasible partition. Recently, Song and Xu [13] generalized Ma and Yang's conclusion in [11] to graphs, and proved that for each graph G without quadrangles, and for any two functions $a, b : V(G) \longrightarrow \mathbb{N} \setminus \{0, 1\}$ such that $d_G(v) \ge a(v) + b(v) + 2\mu_G(v) - 3$ for every vertex v, G has an (a, b)-feasible partition.

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Spectral characterization of the complete graph removing a path: Completing the proof of Cámara–Haemers Conjecture



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ABSTRACT

A graph G is $A-DS$ if every A-cospectral graph of G is isomorphic to G. Denote by $K_n \setminus P_k$ the graph obtained from the complete graph K_n with n vertices by deleting all edges of a path P_k with k vertices. In 2014, Cámara and Haemers conjectured that $K_n \setminus P_k$ is $A-DS$ for every $2 \leq k \leq n$. The conjecture has been confirmed for $k = n$ (Doob and Haemers, 2002), $2 \leq k \leq 6$ (Cámara and Haemers, 2014), $7 \leq k \leq 9$ (Mao et al., 2019) and $k \geq 20$ (Liu et al., 2020). In this paper, we completely settle the conjecture by proving the remaining cases.

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1. Introduction

Throughout this paper, G is a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $v \in V(G)$, the degree of v is denoted by $d_G(v)$, or $d(v)$ for short if no confusion occurs. We assume that $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$, where $d_i(G) = d_G(v_i)$ for $1 \leq i \leq n$, and we use $\Delta(G)$ to denote the maximum degree of G. A t-vertex is a vertex with degree t. In particular, a 1-vertex is called a *pendant vertex*. When t is a non-negative integer, we denote by tG the union of t vertex-disjoint copies of graph G. As usual, let K_n, C_n, P_n and $K_{1,n-1}$ be the complete graph, cycle, path and star with n vertices, respectively.

Let $A(G)$ be the adjacency matrix of G, and let $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$ be the eigenvalues of $A(G)$. Denote by $S_A(G)$ the multiset of these eigenvalues, that is, $S_A(G) = \{\rho_1(G), \rho_2(G), \ldots, \rho_n(G)\}$. Two graphs G and H are said to be *A-cospectral* if they have equal adjacency spectrum. A graph G is said to be $A - DS$ if every A-cospectral graph of G is isomorphic to G.

In 2014, Cámara and Haemers [1] proposed the following conjecture.

Conjecture 1.1 (*Cámara and Haemers [1]*). *For any $2 \leq k \leq n$, $K_n \setminus P_k$ is $A - DS$.*

Theorem 1.1. *Conjecture 1.1 has been confirmed for the following cases:*
(*i*) *(Doob and Haemers [2])* $k = n$.
(*ii*) *(Cámara and Haemers [1])* $2 \leq k \leq 6$.
(*iii*) *(Mao, Cioabă and Wang [3])* $7 \leq k \leq 9$.
(*iv*) *(Liu, Shan and Gu [4])* $k \geq 20$.

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In this paper, we will complete the proof of Conjecture 1.1.

Theorem 1.2. *For any $2 \le k \le n$, $K_n \setminus P_k$ is $A-DS$.*

Here is the outline of our proof. By Theorem 1.1, it suffices to assume that $10 \le k \le 19$ and $k \le n-1$. Let $\overline{G}$ denote the complement graph of G. Suppose that Γ is A-cospectral with $K_n \setminus P_k$, and we will show that $\overline{\Gamma} = P_k \cup (n-k)K_1$ for $10 \le k \le 19$. We will be using the following structure of $\overline{\Gamma}$ developed in [4] (see Remark 4.4, Corollary 4.8 and Theorem 5.5 of [4]). Let $Z_{s_1,s_2,\ldots,s_t}$ be the tree with maximum degree t (≥ 3) obtained by attaching t paths $P_{s_1}, P_{s_2}, \ldots, P_{s_t}$ to a single vertex. If $T \in \{Z_{p,1,1},\ Z_{2,2,1},\ Z_{3,2,1},\ Z_{4,2,1}\}$ for $p \ge 1$, then T is called a **first-type tree**.

Proposition 1.3 ([4]). *$\overline{\Gamma} = \Gamma_1 \cup F \cup \big(n - |V(F)| - |V(\Gamma_1)|\big)K_1$, where Γ_1 is either a unicyclic graph with $\Delta(\Gamma_1) \ge 3$ or a tree and F is a forest with $\Delta(F) \le 3$ such that each tree of F with maximum degree three is a first-type tree.*

By Proposition 1.3, we can write $\overline{\Gamma}$ in the form of $\Gamma_1 \cup F \cup \big(n - |V(F)| - |V(\Gamma_1)|\big)K_1$. We will show that Γ_1 is the path P_k and F is empty, and thus $\overline{\Gamma} = P_k \cup (n-k)K_1$. This paper is organized as follows: In Section 2, we list some known properties for $\overline{\Gamma}$ and Γ, via which we first show in Section 3 that Γ_1 is a tree. In Section 4, we further show that Γ_1 is P_k and F is empty, completing the proof of Theorem 1.2.

2. Some known properties of $\overline{\Gamma}$ and Γ

In this section, we list some properties of $\overline{\Gamma}$ and Γ that will be used in our proof.

Lemma 2.1. *Each of the following holds:*
(i) ([3]) Except for -1, every eigenvalue of graph Γ has multiplicity one.
(ii) ([3]) No two non-trivial trees of $\overline{\Gamma}$ are paths of the same nonzero length except for P_3.
(iii) ([4]) At most two non-trivial trees of $\overline{\Gamma}$ are isomorphic, and

$$2\cos\left(\frac{3\pi}{k+1}\right) \le \rho_2(\overline{\Gamma}) \le 2\cos\left(\frac{\pi}{k+1}\right).$$

Lemma 2.2 ([4]). *Let H be an induced subgraph of $\overline{\Gamma}$.*
(i) H is not a cycle with even length.
(ii) If $|V(H)| = s \ge 2$, then

$$-3 < -2\cos\left(\frac{\pi}{k+1}\right) - 1 \le \rho_s\big(K_s \setminus H\big) \le \rho_2\big(K_s \setminus H\big) \le 2\cos\left(\frac{\pi}{k+1}\right) - 1 < 1.$$

Definition 2.3 ([4]). (i) If $d_{\Gamma_1}(v) \ge 3$, then v is called a **special-vertex** of Γ_1. Let $q(\Gamma_1)$ and $\tau(\Gamma_1)$ be **the number of special-vertices and triangles** of Γ_1, respectively.
(ii) Let $\eta(\overline{\Gamma})$ be **the number of non-trivial components** of $\overline{\Gamma}$, and let $\varepsilon(F)$ be **the number of non-trivial paths** of the forest F.

Lemma 2.4 (*Corollary 4.11 of [4]*). *If Γ_1 is a unicyclic graph, then*

$$\sum_{i=1}^{|V(\Gamma_1)|} d_i(\Gamma_1)\big(d_i(\Gamma_1) - 2\big) = 2\big(\tau(\Gamma_1) + \varepsilon(F) - 1\big), \ \text{and}\ \varepsilon(F) \ge q(\Gamma_1) - \tau(\Gamma_1) + 1, \tag{2.1}$$

where the second equality holds if and only if each special-vertex of Γ_1 is a 3-vertex.

Lemma 2.5 ([4]). *(i) If $k \ge 13$ and Γ_1 is a tree, then $\Gamma = K_n \setminus P_k$.*
(ii) If Γ_1 is a tree, then

$$\sum_{i=1}^{|V(\Gamma_1)|} d_i(\Gamma_1)\big(d_i(\Gamma_1) - 2\big) = 2\big(\varepsilon(F) - 1\big) \ge 2\big(q(\Gamma_1) - 1\big), \tag{2.2}$$

where the second equality holds if and only if every special-vertex of Γ_1 is a 3-vertex.
(iii) Denote by $m_0(G)$ the multiplicity of 0 as an eigenvalue of $A(G)$. Then

$$n - k - 2 \le m_0(\Gamma_1) + m_0(F) + n - |V(\Gamma_1)| - |V(F)| = m_0(\overline{\Gamma}) \le n - k + 1, \tag{2.3}$$

where the right (resp., left) equality holds implies that k is odd (resp., even).

Table 1
Symbols and definitions.

$q(\Gamma_1)$	Number of special vertices (degree ≥ 3)
$\tau(\Gamma_1)$	Number of triangles of Γ_1
$\eta(\overline{\Gamma})$	Number of nontrivial components of $\overline{\Gamma}$
$\varepsilon(F)$	Number of nontrivial paths of the forest F
$m_0(G)$	Multiplicity of eigenvalue 0 of G
$m_1(G)$	Number of P_3 in G
$m_2(G)$	Number of $2P_2$ in G
$m_3(G)$	Number of P_4 in G
$s_1(G)$	Number of C_3 in G
$s_2(G)$	Number of $P_3 \cup P_2$ in G
$s_3(G)$	Number of $K_{1,3}$ in G
$s_4(G)$	Number of P_5 in G
$s_5(G)$	Number of G_a in G
$s_6(G)$	Number of C_5 in G
$\Phi(G)$	$(8n-20)m_1(G)+16m_2(G)-8m_3(G)$
$\Psi(G)$	$n(n-2)m_1(G)+4(n-3)m_2(G)-(n-2)m_3(G)$ $-3(n-2)s_1(G)-2s_2(G)-3s_3(G)+s_4(G)+s_5(G)-s_6(G)$

Lemma 2.6 ([5]). *Let $r(G)$ be the rank of $A(G)$.*
(i) If q is odd, then $r(P_q) = q-1$.
(ii) If q is even, then $r(P_q) = q$.
(iii) If $q \geq 3$, then $r(K_{1,q-1}) = 2$.

3. The graph Γ_1 is a tree

Since Γ is A-cospectral with $K_n \setminus P_k$, Γ and $K_n \setminus P_k$ contain the same number of edges, that is, $\overline{\Gamma}$ contains exactly $k-1$ edges. Hereafter, we always use this fact straightly. Theorem 3.15 is the main result of this section, in which we will show that if $10 \leq k \leq 19$, then Γ_1 is a tree.

We present some useful lemmas first. Denote by $m_1(G)$, $m_2(G)$, $m_3(G)$, $s_1(G)$, $s_2(G)$, $s_3(G)$, $s_4(G)$, $s_5(G)$ and $s_6(G)$ the numbers of distinct (not necessarily induced) subgraphs in G isomorphic to P_3, $2P_2$, P_4, C_3, $P_3 \cup P_2$, $K_{1,3}$, P_5, G_a and C_5, respectively, where G_a is the graph obtained from a triangle by adding a pendant edge to one of its vertices.

In what follows, we define $\Phi(G) = (8n-20)m_1(G)+16m_2(G)-8m_3(G)$, and $\Psi(G) = n(n-2)m_1(G)+4(n-3)m_2(G)-(n-2)m_3(G)-3(n-2)s_1(G)-2s_2(G)-3s_3(G)+s_4(G)+s_5(G)-s_6(G)$.

Lemma 3.1 ([3]). *If G is a graph with n vertices and e edges, then the number of 5-walks of $\overline{G}$ is equal to $120\binom{n}{5}+30(n-2)\binom{n}{3}-(10n^3-50n^2+90n-60)e+10n(n-2)m_1(G)+40(n-3)m_2(G)-10(n-2)m_3(G)-30(n-2)s_1(G)-20s_2(G)-30s_3(G)+10s_4(G)+10s_5(G)-10s_6(G)$.*

When Γ_1 is either a tree or a unicyclic graph, it has been shown that (in Corollary 6.2 of [4])

$$\Phi(\overline{\Gamma}) = \Phi\big(P_k \cup (n-k)K_1\big) = (8n-20)(k-2)+8(k-3)^2.$$

For $k \geq 4$, we have $m_1\big(P_k\big) = k-2$, $m_2\big(P_k\big) = \frac{1}{2}(k-2)(k-3)$, $m_3\big(P_k\big) = k-3$, $s_1(P_k) = s_3(P_k) = s_5(P_k) = s_6(P_k) = 0$, $s_2(P_k) = (k-3)(k-4)$ and $s_4(P_k) = k-4$. Since Γ is A-cospectral with $K_n \setminus P_k$, they have the same number of 5-walks. Combining this with $|V(\overline{\Gamma})| = |V(P_k \cup (n-k)K_1)| = n$, $|E(\overline{\Gamma})| = |E(P_k \cup (n-k)K_1)| = k-1$ and Lemma 3.1 we have

$$\Psi(\overline{\Gamma}) = \Psi(P_k \cup (n-k)K_1) = (nk-2n-3k+7)(2k+n-6)-(2k-7)(k-4).$$

Thus, we have the following lemma:

Lemma 3.2. *If Γ_1 is either a tree or a unicyclic graph, then $\Phi(\overline{\Gamma}) = \Phi(P_k \cup (n-k)K_1) = (8n-20)(k-2)+8(k-3)^2$ and $\Psi(\overline{\Gamma}) = \Psi(P_k \cup (n-k)K_1) = (nk-2n-3k+7)(2k+n-6)-(2k-7)(k-4)$.*

Definition 3.3 ([4]). *(i)* Let W_q the tree on q vertices obtained from the path $P_{q-2} = u_1u_2\cdots u_{q-2}$ and two isolated vertices u_{q-1} and u_q by adding two pendant edges u_2u_{q-1} and $u_{q-3}u_q$, where $q \geq 6$.
(ii) Denote by $U_{g;s,t}$ the unicyclic graph obtained from a cycle C_g by attaching one path P_s to the vertex u of C_g, and then attaching another path P_t to the vertex v of C_g, where $uv \in E(C_g)$.
(iii) Let $U^g_{s_1,s_2,\ldots,s_t}$ be the unicyclic graph obtained from a cycle C_g by attaching t paths P_{s_1}, P_{s_2}, …, P_{s_t} to one common vertex of C_g.

As an illustrated example, the graphs W_8, $U_{3;2,1}$ and $U^3_{2,1}$ are shown in Fig. 1.

Next, we survey the symbols and definitions introduced before, which we will always use in the sequel (see Table 1).

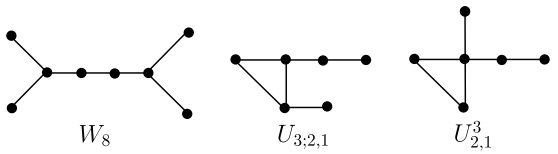


Fig. 1. The graphs W_8, $U_{3;2,1}$, and $U^3_{2,1}$.

Lemma 3.4 ([4]). *Let $G = U_1^7 \cup P_p \cup P_q$ and $t = p + q + 7$. If $q \geq 2$ and $p \geq 3$, then $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$, $m_2(G) = m_2(P_t)$ and $m_3(G) \leq m_3(P_t)$, where the inequality is strict if $q \geq 3$.*

Lemma 3.5 ([4]). *Let $G = Z_{p,q,1} \cup P_s$ and $t = p+q+s+1$, where $p \geq q \geq 1$ and $s \geq 2$. Then, $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$, $m_2(G) = m_2(P_t)$, and $m_3(G) \leq m_3(P_t)$. Furthermore, if either $s \geq 3$ or $q = 1$, then $m_3(G) < m_3(P_t)$.*

Lemma 3.6. *If $q \geq 3$ and $k = 9 + q$, then $\Psi\left(U_1^7 \cup P_2 \cup P_q \cup (n - 10 - q)K_1\right) > \Psi\left(P_k \cup (n - k)K_1\right)$.*

Proof. For short, we let G denote $U_1^7 \cup P_2 \cup P_q \cup (n - 10 - q)K_1$ here. From the definition, $m_1(G) = q + 7$, $m_2(G) = 18 + 9q + \frac{1}{2}(q - 2)(q - 3)$, $m_3(G) = q + 6$, $s_1(G) = 0 = s_5(G) = s_6(G)$, $s_2(G) = 15 + 18q + (q - 3)(q - 4)$, $s_3(G) = 1$, $s_4(G) = q + 5$ (if $q \geq 4$) and $s_4(G) = q + 6$ (if $q = 3$). Combining this with $k = 9 + q$, we have $\Psi(G) \geq (q + 7)n^2 + (2q^2 + 23q + 64)n - 8q^2 - 97q - 292 = \Psi\left(P_k \cup (n - k)K_1\right) + 3$, and thus the result follows. ■

Lemma 3.7. *Let $G = U_d^5 \cup P_p \cup P_q$, where $1 \leq d \leq 3 \leq p$ and $p \geq q \geq 2$. If $t = p + q + d + 4$, then $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$ and $m_2(G) = m_2(P_t)$.*
(i) If $d = 1$, then $m_3(G) \leq m_3(P_t)$, with equality if and only if $q = 2$.
(ii) If $2 \leq d \leq 3$, then $m_3(G) \geq m_3(P_t)$, with equality if and only if $q \geq 3$.

Proof. It is easy to see that $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t) = p + q + d + 2$ and $m_2(G) = 5d + 3 + \frac{1}{2}(d - 1)(d - 2) + (5 + d)(p + q - 2) + (p - 1)(q - 1) + \frac{1}{2}(p - 2)(p - 3) + \frac{1}{2}(q - 2)(q - 3) = \frac{1}{2}(t - 2)(t - 3) = m_2(P_t)$. If $d = 1$, then $m_3(G) \leq 7 + p - 3 + q - 2 = t - 3 = m_3(P_t)$, with first equality if and only if $q = 2$. If $2 \leq d \leq 3$, then $m_3(G) \geq d + 7 + p - 3 + q - 3 = t - 3 = m_3(P_t)$, with first equality if and only if $q \geq 3$. ■

A **special** C_q of G is a cycle C_q containing exactly one vertex with degree at least three. A path $P_s : u_1u_2 \cdots u_s$ with $s \geq 2$ is called a **pendant path** of G if $d_G(u_s) = 1 < d_G(u_{s-1}) = d_G(u_{s-2}) = \cdots = d_G(u_2) = 2 < d_G(u_1)$. Denote by J_n and I_n the **all-ones matrix** and **identity matrix** of order n, respectively. Let $q^{(s)}$ denote the s-tuple $(q, q, \ldots, q)$.

Lemma 3.8. *If $P_2 \in F$, then Γ_1 contains no special triangle, $P_5 \notin F$ and $\Gamma_1 \neq U_{3;3,t}$ for $t \geq 1$.*

Proof. Suppose that $V(\overline{\Gamma}) = \{u_1, u_2, \ldots, u_n\}$ and $V(P_2) = \{u_1, u_2\}$.

If Γ_1 contains a special triangle, then let $\{u_3, u_4\}$ be the two 2-vertices of C_3. Since $\left(1, -1, 0^{(n-2)}\right)$ and $\left(0^{(2)}, 1, -1, 0^{(n-4)}\right)$ are two orthogonal eigenvectors of -1 of $A(\overline{\Gamma})$ and $A(\Gamma) = J_n - A(\overline{\Gamma}) - I_n$, it is easy to see that $\left(1, -1, 0^{(n-2)}\right)$ and $\left(0^{(2)}, 1, -1, 0^{(n-4)}\right)$ are also two orthogonal eigenvectors of 0 of $A(\Gamma)$, which is contrary to Lemma 2.1(i).

We now assume that $\Gamma_1 = U_{3;3,t}$ or $P_5 \in F$. Then, let $P_5 = u_3u_4 \cdots u_7$ or $\{u_3, u_4, \ldots, u_7\}$ be five vertices of $U_{3;3,t}$ such that $P_4 = u_4u_5u_6u_7$ is the pendant path P_4 and u_3 is the unique 2-vertex of C_3 in $U_{3;3,t}$, where $d_{U_{3;3,t}}(u_4) = 3$. Since $\left(1, -1, 0^{(n-2)}\right)$ and $\left(0^{(2)}, 1, -1, 0, 1, -1, 0^{(n-7)}\right)$ are two orthogonal eigenvectors of -1 of $A(\overline{\Gamma})$ and $A(\Gamma) = J_n - A(\overline{\Gamma}) - I_n$, it is easy to see that $\left(1, -1, 0^{(n-2)}\right)$ and $\left(0^{(2)}, 1, -1, 0, 1, -1, 0^{(n-7)}\right)$ are also two orthogonal eigenvectors of 0 of $A(\Gamma)$, contrary to Lemma 2.1(i). ■

Lemma 3.9. *If C_5 is a special cycle of Γ_1, then $P_4 \notin F$.*

Proof. By contradiction, we assume that $P_4 \in F$. Suppose that $V(\overline{\Gamma}) = \{u_1, u_2, \ldots, u_n\}$, $\{u_1, u_2, u_3, u_4\}$ are the four 2-vertices of C_5 and $V(P_4) = \{u_5, u_6, u_7, u_8\}$. Since $\left(\sin(0.8\pi), \sin(1.6\pi), \sin(0.4\pi), \sin(1.2\pi), 0^{(n-4)}\right)$ and $\left(0^{(4)}, \sin(0.8\pi), \sin(1.6\pi), \sin(0.4\pi), \sin(1.2\pi), 0^{(n-8)}\right)$ are two orthogonal eigenvectors of $2\cos\left(\frac{4\pi}{5}\right)$ of $A(\overline{\Gamma})$, $\sin(0.8\pi) = -\sin(1.2\pi)$ and $\sin(1.6\pi) = -\sin(0.4\pi)$, we can conclude that $\left(\sin(0.8\pi), \sin(1.6\pi), \sin(0.4\pi), \sin(1.2\pi), 0^{(n-4)}\right)$ and $\left(0^{(4)}, \sin(0.8\pi), \sin(1.6\pi), \sin(0.4\pi), \sin(1.2\pi), 0^{(n-8)}\right)$ are two orthogonal eigenvectors of $-2\cos\left(\frac{\pi}{5}\right) - 1$ of $A(\Gamma)$, which contradicts Lemma 2.1(i). ■

Hereafter, let H_1, H_2, …, H_9 be the nine unicyclic graphs as shown in Fig. 2. For any vertex subset $S \subseteq V(G)$, we denote by $G[S]$ the subgraph of G induced by S. If $\overline{\Gamma}$ does not contain a graph H as an induced subgraph, then H is called **forbidden** in $\overline{\Gamma}$.

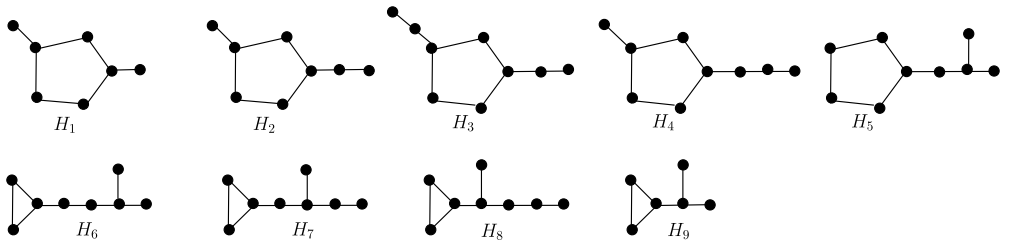


Fig. 2. The unicyclic graphs $H_1, H_2, \ldots, H_9$.

Lemma 3.10. *If $k \le 19$, then the following graphs are forbidden in $\overline{\Gamma}$:*
(i) $U_1^5 \cup Z_{2,1,1} \cup P_2 \cup P_3$, $U_1^5 \cup P_7$, $U_2^5 \cup 2K_{1,3} \cup P_3$, $U_2^5 \cup 2P_5$, $U_2^5 \cup K_{1,3} \cup P_2 \cup P_5$, $U_2^5 \cup P_3 \cup P_6$, $H_1 \cup K_{1,3} \cup P_2 \cup 2P_3$, $H_1 \cup P_6$, $H_1 \cup 2P_3 \cup P_5$, $U_{1,1}^3 \cup P_2 \cup P_4$, $U_{1,1}^3 \cup P_2 \cup 2P_3$, $U_6^3 \cup P_2 \cup P_3$, $U_{3,3}^3 \cup 2P_3$, $U_1^3 \cup P_5$, $U_1^3 \cup K_{1,3} \cup P_3$, $U_{3;1,1} \cup P_2 \cup 2P_3$, $U_{3;1,1} \cup P_2 \cup P_4$, $U_{3;5,1} \cup P_3 \cup K_1$, $U_{3;4,1} \cup 2P_3$, $U_1^3 \cup 2P_3 \cup P_4$, $U_4^3 \cup P_3 \cup P_4$,
(ii) $Z_{1,2,4} \cup K_1$, $Z_{2,2,1,1}$, W_6, $Z_{2,2,2}$, $Z_{1,3,3} \cup P_2 \cup 2P_3$, $Z_{2,1,1,1} \cup 2P_2 \cup P_3$, U_4^5, H_3, $H_4 \cup 2P_2 \cup P_3$, $H_5 \cup K_1$.

Proof. We suppose that H contains s vertices. If H is a graph of (i), by Lemma 2.2(ii), we have $-2\cos\left(\frac{\pi}{k+1}\right) - 1 \le \rho_s\left(K_s \setminus H\right) < -2.9754$ (see Appendix A), and thus $k \ge 20$, a contradiction. If H is a graph of (ii), by Lemma 2.2(ii), we have $0.978 < \rho_2\left(K_s \setminus H\right) \le 2\cos\left(\frac{\pi}{k+1}\right) - 1$ (see Appendix B), and thus $k \ge 20$, a contradiction. ■

Lemma 3.11. *If Γ_1 is a unicyclic graph with the unique cycle C_g, then $g \in \{3, 5\}$.*

Proof. For short, we use Δ to denote $\Delta(\Gamma_1)$ in this proof. Then, $\Delta \ge 3$ by Proposition 1.3, and thus $q(\Gamma_1) \ge 1$. By Lemma 2.2(i), g must be odd. Suppose to the contrary that $g \ge 7$. Since $q(\Gamma_1) \ge 1$ and in view of $\tau(\Gamma_1) = 0$, it follows from (2.1) that $\varepsilon(F) \ge 2$, with equality if and only if Γ_1 contains exact one special-vertex, which is a 3-vertex. As $Z_{1,2,4} \cup K_1$ is forbidden by Lemma 3.10(ii) and $\varepsilon(F) \ge 2$, we have $g = 7$. Also, since $\{Z_{2,2,1,1}, Z_{2,2,2}\}$ are forbidden by Lemma 3.10(ii), we conclude that $\Delta = 3$ and $\overline{\Gamma}$ does not contain U_2^7 as an induced subgraph.

If $q(\Gamma_1) \ge 2$, then since $Z_{1,2,4} \cup K_1$ is forbidden by Lemma 3.10(ii) and $\varepsilon(F) \ge 3$ by (2.1), $Z_{1,3,3} \cup P_2 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 2.1(ii), contrary to Lemma 3.10(ii). Thus, $\Gamma_1 = U_1^7$ and so $\varepsilon(F) = 2$ by (2.1).

Let P_q and P_p be two non-trivial paths of F, and let $t = 7 + p + q$, where $p \ge q \ge 2$ and $p \ge 3$ by Lemma 2.1(ii). Then, $t \ge 12$. Denote by F_1 the forest consisting of all first-type trees (if any) of F. By Lemmas 3.4 and 3.5 we have $m_1(\overline{\Gamma}) = m_1\left(U_1^7 \cup P_q \cup P_p\right) + m_1(F_1) = m_1(P_t) + m_1(F_1) = m_1\left(P_t \cup F_1\right) = m_1(P_k)$, $m_2(\overline{\Gamma}) = m_2\left(U_1^7 \cup P_q \cup P_p\right) + m_2(F_1) + |E\left(U_1^7 \cup P_q \cup P_p\right)| \cdot |E(F_1)| = m_2(P_t) + m_2(F_1) + |E(P_t)| \cdot |E(F_1)| = m_2\left(P_t \cup F_1\right) = m_2(P_k)$, and $m_3(\overline{\Gamma}) = m_3\left(U_1^7 \cup P_q \cup P_p\right) + m_3(F_1) \le m_3\left(P_t\right) + m_3(F_1) = m_3\left(P_t \cup F_1\right) \le m_3(P_k)$.

If either $q \ge 3$ or $F_1 \ne \emptyset$, then $m_3(\overline{\Gamma}) < m_3(P_k)$ by Lemmas 3.4 and 3.5. Combining this with $m_1(\overline{\Gamma}) = m_1(P_k)$ and $m_2(\overline{\Gamma}) = m_2(P_k)$, it follows that $\Phi(\overline{\Gamma}) > \Phi\left(P_k \cup (n-k)K_1\right)$, contradicting Lemma 3.2. Therefore, $q = 2$ and $F_1 = \emptyset$. This implies that $F = P_p \cup P_2$, which is contrary to Lemmas 3.2 and 3.6. ■

We further show that the unique cycle of Γ_1 must be a triangle in the following lemma.

Lemma 3.12. *If Γ_1 is a unicyclic graph with the unique cycle C_g, then $g = 3$.*

Proof. By Lemma 3.11, we suppose to the contrary that $g = 5$. If $\Delta(\Gamma_1) \ge 4$, then $\varepsilon(F) \ge 3$ by (2.1), and thus $Z_{2,1,1,1} \cup 2P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 2.1(ii), contrary to Lemma 3.10(ii). Thus, $\Delta(\Gamma_1) = 3$. In this case, Γ_1 contains U_1^5 as an induced subgraph. By (2.1) and $\Delta(\Gamma_1) = 3$, it follows that

$$\varepsilon(F) = q(\Gamma_1) + 1 \ge 2 \quad \text{and} \quad \Delta(\Gamma_1) = 3.$$

Let P_s be a longest path of F, and let U_d^5 be an induced subgraph of Γ_1 such that d is as large as possible. Since U_4^5 and $U_1^5 \cup P_7$ are forbidden by Lemma 3.10, we have

$$3 \le s \le 6$$

by Lemma 2.1(ii) and $d \le 3$. Moreover, since $U_1^5 \cup Z_{2,1,1} \cup P_2 \cup P_3$ is forbidden by Lemma 3.10(i) and $\varepsilon(F) \ge 2$, if T is a first-type tree of F, that is, $\Delta(T) = 3$, then $T = K_{1,3}$. Note that $U_2^5 \cup 2K_{1,3} \cup P_3$ is forbidden by Lemma 3.10(i). Thus,

$$\overline{\Gamma} \text{ contains at most one copy of } K_{1,3} \text{ if } d \ge 2. \tag{3.1}$$

Case 1. $d = 3$.

If $q(\Gamma_1) \geq 2$, then either H_4 or H_5 is an induced subgraph of Γ_1, as W_6 is forbidden by Lemma 3.10(ii). By (2.1) and $\varepsilon(F) = q(\Gamma_1)+1 \geq 3$, we can conclude that either $H_4 \cup 2P_2 \cup P_3$ or $H_5 \cup K_1$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 2.1(ii), contradicting Lemma 3.10(ii). Thus, $q(\Gamma_1) = 1$ and so $\Gamma_1 = U_3^5$. Combining this with (2.1), $\varepsilon(F) = 2$ and C_5 is a special cycle of Γ_1. Suppose that $P_s \cup P_t$ are the two paths of F, where $s \geq t \geq 2$ and $s \geq 3$.

We first suppose that $t \geq 3$. By Lemmas 3.5 and 3.7(ii), we have $\Phi(\overline{\Gamma}) \geq \Phi(P_k \cup (n-k)K_1)$, with equality holds if and only if $\Delta(F) = 2$. Combining this with Lemma 3.2, we can conclude that $\Delta(F) = 2$. Thus, $k = |E(\Gamma_1)|+|E(F)|+1 = 7+s+t$. Now, since $U_3^5 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$, by Lemma 2.2(ii) and Appendix B, we have $0.9696 < \rho_2\big(K_{14} \setminus (U_3^5 \cup 2P_3)\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) - 1$, and thus $k = 7+s+t \geq 17$. Note that $s \leq 6$ and $t \neq 4$ by Lemma 3.9. Thus, Lemma 2.1(ii) implies that $t = 5 \leq s \leq 6$ and so $U_2^5 \cup 2P_5$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 3.10(i).

We now suppose that $t = 2$. By Lemmas 3.2 and 3.7(ii), we have $\Delta(F) = 3$ and thus $U_3^5 \cup P_2 \cup P_3 \cup K_{1,3}$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 2.1(ii). By Lemma 2.2(ii) and Appendix B, we have $0.973 < \rho_2\big(K_{17} \setminus (U_3^5 \cup P_2 \cup P_3 \cup K_{1,3})\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) - 1$, and so $k \geq 19$. However, since (3.1) and $s \leq 6$, we have $k = |E(\Gamma_1)| + |E(F)| + 1 = s + 12 \leq 18$, a contradiction.

Case 2. $d = 2$.

Subcase 2.1. $q(\Gamma_1) \geq 2$. Since W_6 is forbidden by Lemma 3.10(ii), either $\Gamma_1 = H_2$ or $\Gamma_1 = H_3$. Thus, $\varepsilon(F) = q(\Gamma_1) + 1 = 3$ by (2.1). Since $H_1 \cup K_{1,3} \cup P_2 \cup 2P_3$ and H_3 are forbidden by Lemma 3.10 and $\varepsilon(F) \geq 3$, we have $\Delta(F) = 2$ and $\Gamma_1 = H_2$ by Lemma 2.1(ii). Since $H_1 \cup P_6$ and $H_1 \cup 2P_3 \cup P_5$ are forbidden Lemma 3.10(i), and in view of Lemma 3.8, we have $3 \leq s \leq 4$.

Since $3 \leq s \leq 4$, $k = |E(\Gamma_1)| + |E(F)| + 1 \leq 16$ by Lemma 2.1(ii), where the last equality requires that $F = 2P_3 \cup P_4$. In this case, Lemma 2.1(ii) implies that $H_2 \cup 2P_3 \cup P_2$ is an induced subgraph of $\overline{\Gamma}$, and so we have $0.957 < \rho_2\big(K_{16} \setminus (H_2 \cup P_2 \cup 2P_3)\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) - 1$ by Lemma 2.2(ii) and Appendix B. This implies that $15 \leq k \leq 16$ and hence $s = 4$, as at most two non-trivial trees of $\overline{\Gamma}$ are isomorphic by Lemma 2.1(iii). Now, since $\rho_2(H_2) < \rho_1(P_4) < \rho_1(H_2)$ and $\Gamma_1 = H_2$, we have $\rho_2(\overline{\Gamma}) = \rho_1(P_4) = 2\cos\left(\frac{\pi}{5}\right) < 2\cos\left(\frac{3\pi}{16}\right)$, contradicting Lemma 2.1(iii).

Subcase 2.2. $q(\Gamma_1) = 1$. Then, $\Gamma_1 = U_2^5$ and $\varepsilon(F) = 2$ by (2.1). We suppose that $P_s \cup P_t$ are the two paths of F, where $s \geq t \geq 2$ and $s \geq 3$.

We first suppose that $t = 2$. By Lemmas 3.2 and 3.7(ii), we have $\Delta(F) = 3$. Since $U_2^5 \cup K_{1,3} \cup P_2 \cup P_5$ is forbidden by Lemma 3.10(i) and in view of Lemmas 3.8 and 3.9, we have $s = 3$. By (3.1), $k = |E(\Gamma_1)| + |E(F)| + 1 = 14$. In this case, $m_0(\overline{\Gamma}) = m_0(U_2^5) + m_0(P_3) + m_0(P_2) + m_0(K_{1,3}) + n - 16 = n - 13$ by Lemma 2.6 and Appendix C, contrary to (2.3).

We now suppose that $t \geq 3$. By Lemmas 3.2, 3.5 and 3.7(ii), we have $\Delta(F) = 2$, and thus $F = P_s \cup P_t$ and $k = s+t+6$. Since $U_2^5 \cup P_3 \cup P_6$ is forbidden by Lemma 3.10(i) and $t \geq 3$, we have $3 \leq s \leq 5$ and $4 \notin \{s, t\}$ by Lemma 3.9.

If $s = 5$, then $t = 3$ by Lemma 2.1(ii) and $t \neq 4$, and so $k = 14$. In this case, $m_0(\overline{\Gamma}) = m_0(U_2^5)+m_0(P_3)+m_0(P_5)+n-15 = n - 13$ by Lemma 2.6 and Appendix C, contrary to (2.3).

If $s = 3$, then $t = 3$, and so $k = 12$. In this case, $m_0(\overline{\Gamma}) = m_0(U_2^5) + m_0(2P_3) + n - 13 = n - 11$ by Lemma 2.6 and Appendix C, contrary to (2.3).

Case 3. $d = 1$.

Subcase 3.1. $q(\Gamma_1) \geq 2$. Since W_6 is forbidden by Lemma 3.10(ii), $\Gamma_1 = H_1$ and $\varepsilon(F) = 3$ by (2.1). Furthermore, since $H_1 \cup K_{1,3} \cup P_2 \cup 2P_3$ is forbidden by Lemma 3.10(i), Lemma 2.1(ii) implies that $F = P_s \cup P_t \cup P_q$ and $k = s+t+q+5$, where $s \geq t \geq q \geq 2$ and $3 \leq t \leq s \leq 6$.

Since $H_1 \cup 2P_3 \cup P_5$ is forbidden by Lemma 3.10(i), we have $s \leq 4$ by Lemma 3.8, and thus $F \in \big\{P_2 \cup 2P_3, 2P_3 \cup P_4, P_2 \cup P_3 \cup P_4\big\}$ by Lemma 2.1(ii).

In this case, $m_1(\overline{\Gamma}) = k-2 = m_1(P_k)$, $m_2(\overline{\Gamma}) = 12+7(s+t+q-3)+(s-1)(t+q-2)+\frac{1}{2}(s-2)(s-3)+\frac{1}{2}(t-2)(t-3)+\frac{1}{2}(q-2)(q-3)+(t-1)(q-1) = \frac{1}{2}(k-2)(k-3) = m_2(P_k)$ $m_3(\overline{\Gamma}) \leq 9+s+t+q-8 = s+t+q+1 = k-4 < m_3(P_k)$, which contradicts Lemma 3.2.

Subcase 3.2. $q(\Gamma_1) = 1$. Then, $\Gamma_1 = U_1^5$ and $\varepsilon(F) = 2$ by (2.1). We suppose that $P_s \cup P_t$ are the two paths of F, where $s \geq t \geq 2$.

If either $t \geq 3$ or $\Delta(F) = 3$, then by Lemmas 3.5 and 3.7, we have $\Phi(\overline{\Gamma}) > \Phi\big(P_k \cup (n-k)K_1\big)$, contrary to Lemma 3.2. Thus, $t = 2$ and $\Delta(F) = 2$. In this case, $F = P_s \cup P_2$ and $k = |E(\Gamma_1)|+|E(F)|+1 = s+7 \leq 13$, where $3 \leq s \leq 6$. Lemmas 3.8 and 3.9 imply that $s \notin \{4, 5\}$.

If $s = 6$, then by Lemma 2.2(ii) and Appendix A, we have $-2\cos\left(\frac{\pi}{k+1}\right) - 1 \leq \rho_{14}\big(K_{14} \setminus (U_1^5 \cup P_2 \cup P_6)\big) < -2.962$, and so $k \geq 16$, a contradiction. Thus $s = 3$ and so $k = 10$.

In this case, $m_1(\overline{\Gamma}) = 8$, $m_2(\overline{\Gamma}) = 28$, $m_3(\overline{\Gamma}) = 7$, $s_1(\overline{\Gamma}) = 0 = s_5(\overline{\Gamma})$, $s_2(\overline{\Gamma}) = 39$, $s_3(\overline{\Gamma}) = 1$, $s_4(\overline{\Gamma}) = 7$, and $s_6(\overline{\Gamma}) = 1$. Thus, $\Psi(\overline{\Gamma}) = 8n^2 + 89n - 397 > 8n^2 + 89n - 400 = \Psi\big(P_{10} \cup (n-10)K_1\big)$, contrary to Lemma 3.2. ■

By Lemma 3.12 and Proposition 1.3, in what follows, **we may suppose that C_3 is the unique cycle of $\overline{\Gamma}$ with $V(C_3) = \{w_1, w_2, w_3\}$, where $d_{\Gamma_1}(w_1) \geq d_{\Gamma_1}(w_2) \geq d_{\Gamma_1}(w_3) \geq 2$ and $d_{\Gamma_1}(w_1) \geq 3$.**

Lemma 3.13. $\eta(\overline{\Gamma}) \geq 3$.

Proof. Suppose to the contrary that $\eta(\overline{\Gamma}) = 2$ by (2.1), and thus $q(\Gamma_1) = 1 = \varepsilon(F)$. Then $|V(\Gamma_1)| = |E(\Gamma_1)| = k - |V(F)|$. Since $q(\Gamma_1) = 1 = \varepsilon(F)$, $\Gamma_1 = U_d^3$ and F is a path, say P_s, where $s \geq 3$ by Lemma 3.8. Thus, $d+3 = |E(\Gamma_1)| = k - |V(F)| = k - s$ and so $k = s + d + 3$.

In this case, $m_1(\overline{\Gamma}) = d + s + 2$, $m_2(\overline{\Gamma}) = \frac{1}{2}(d+s-1)(d+s+2)$ and either $m_3(\overline{\Gamma}) = d + s - 1$ for $d \geq 2$ or $m_3(\overline{\Gamma}) = d + s - 2$ for $d = 1$. Thus, $\Phi(\overline{\Gamma}) \geq 4(d+s+2)(2n+2d+2s-7) - 8(d+s-1) = \Phi\big(P_k \cup (n-k)K_1\big) + 4(2n-7)$, contrary to Lemma 3.2. ■

Lemma 3.14. *$d_{\overline{\Gamma}}(w_1) = 3$ and $d_{\overline{\Gamma}}(w_2) = 2$.*

Proof. To show that $d_{\overline{\Gamma}}(w_1) = 3$, suppose to the contrary that $d_{\overline{\Gamma}}(w_1) \geq 4$. Then, $U_{1,1}^3$ is an induced subgraph of $\overline{\Gamma}$. Since $\big\{U_{1,1}^3 \cup P_2 \cup P_4,\ U_{1,1}^3 \cup P_2 \cup 2P_3\big\}$ are forbidden by Lemma 3.10(i) and since $\varepsilon(F) \geq 2$ by (2.1), we have $F \in \big\{P_2 \cup P_3,\ 2P_3\big\}$ by Lemma 2.1(ii). Thus, $\varepsilon(F) = 2$ and so $q(\Gamma_1) = 1$ by (2.1). In view of Lemma 2.4, it follows that $d_{\overline{\Gamma}}(w_1)\big(d_{\overline{\Gamma}}(w_1) - 3\big) = 2$, contrary with $d_{\overline{\Gamma}}(w_1) \geq 4$. Thus, $d_{\overline{\Gamma}}(w_1) = 3$.

To show $d_{\overline{\Gamma}}(w_2) = 2$, we suppose to the contrary that $d_{\overline{\Gamma}}(w_2) = 3$. In this case, $q(\Gamma_1) \geq 2$ and so $\varepsilon(F) \geq 2$ by (2.1). Note that $\big\{U_1^3 \cup P_5,\ U_1^3 \cup K_{1,3} \cup P_3\big\}$ are forbidden by Lemma 3.10(i). Thus, each non-trivial tree of $\overline{\Gamma}$ is a path with at most four vertices by Lemma 2.1(ii) and $\varepsilon(F) \geq 2$. Since $\big\{U_{3;1,1} \cup P_2 \cup 2P_3,\ U_{3;1,1} \cup P_2 \cup P_4\big\}$ are forbidden by Lemma 3.10(i) and $\varepsilon(F) \geq 2$, we have

$$F \in \big\{P_2 \cup P_3,\ 2P_3\big\}.$$

In this case, $\varepsilon(F) = q(\Gamma_1) = 2$ and hence equality holds in (2.1). Therefore, Γ_1 contains exactly two special-vertices that are 3-vertices. Since $U_{3;5,1} \cup P_3 \cup K_1$ is forbidden by Lemma 3.10(i), we have $\Gamma_1 = U_{3;s,t}$, where $1 \leq t \leq s \leq 4$.

Case 1. $s = 4$. Since $U_{3;4,1} \cup 2P_3$ is forbidden by Lemma 3.10(i), we have $F = P_2 \cup P_3$ and $k = 11 + t$. By Lemma 3.8, since $P_2 \in F$, $U_{3;4,3} \neq \Gamma_1$ and thus $t \neq 3$.

If $t = 4$, then $k = 15$. By Lemma 2.2(ii) and Appendix A,

$$-2\cos\left(\frac{\pi}{k+1}\right) - 1 \leq \rho_{16}\big(K_{16} \setminus (U_{3;4,4} \cup P_2 \cup P_3)\big) < -2.97,$$

and thus $k \geq 18$, a contradiction.

If $t = 2$, then $k = 13$. When $n \geq 16$, Lemma 2.2(ii) and Appendix A imply that $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{16}\big(K_{16} \setminus (U_{3;4,2} \cup P_2 \cup P_3 \cup 2K_1)\big) < -2.952$, and thus $k \geq 14$, a contradiction. If $14 \leq n \leq 15$, then it is straight forward to check that $K_n \setminus P_{13}$ and $K_n \setminus \big(U_{3;4,2} \cup P_2 \cup P_3\big)$ are not A-cospectral.

If $t = 1$, then $k = 12$. When $n \geq 15$, Lemma 2.2(ii) and Appendix A imply that $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{15}\big(K_{15} \setminus (U_{3;4,1} \cup P_2 \cup P_3 \cup 2K_1)\big) < -2.949$, and thus $k \geq 13$, a contradiction. If $13 \leq n \leq 14$, then it is straight forward to check that $K_n \setminus P_{12}$ and $K_n \setminus \big(U_{3;4,1} \cup P_2 \cup P_3\big)$ are not A-cospectral.

Case 2. $s = 3$. By Lemma 3.8, since $U_{3;3,t} \cup P_2$ is forbidden, we have $F = 2P_3$. Then, $k = |E(\Gamma_1)| + |E(F)| + 1 = 11 + t$.

If $t = 3$, then $k = 14$. By Lemma 2.2(ii) and Appendix A, $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{15}\big(K_{15} \setminus (U_{3;3,3} \cup 2P_3)\big) < -2.96$, and thus $k \geq 15$, a contradiction. If $1 \leq t \leq 2$, then $k \leq 13$. By Lemma 2.2(ii) and Appendix A, $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{13}\big(K_{13} \setminus (U_{3;3,1} \cup 2P_3)\big) < -2.951$, and thus $k \geq 14$, a contradiction.

Case 3. $s = 2$. If $F = 2P_3$, then $k = |E(\Gamma_1)| + |E(F)| + 1 = 10 + t$ and thus $k \leq 12$. By Lemma 2.2(ii) and Appendix A, we have $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{12}\big(K_{12} \setminus (U_{3;2,1} \cup 2P_3)\big) < -2.9419$, and thus $k \geq 13$, a contradiction. Thus, $F = P_2 \cup P_3$.

Recall that $1 \leq t \leq s = 2$. We first suppose that $t = 2$. Then, $k = |E(\Gamma_1)| + |E(F)| + 1 = 11$. If $n \geq 18$, then $U_{3;2,2} \cup P_2 \cup P_3 \cup 6K_1$ is an induced subgraph of $\overline{\Gamma}$. By Lemma 2.2(ii) and Appendix A, we have $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{18}\big(K_{18} \setminus (U_{3;2,2} \cup P_2 \cup P_3 \cup 6K_1)\big) < -2.935$, and thus $k \geq 12$, a contradiction. If $12 \leq n \leq 17$, it is straight forward to check that $K_n \setminus P_{11}$ and $K_n \setminus \big(U_{3;2,2} \cup P_2 \cup P_3\big)$ are not A-cospectral.

Thus $t = 1$. Then, $k = |E(\Gamma_1)| + |E(F)| + 1 = 10$. If $n \geq 16$, then $U_{3;2,1} \cup P_2 \cup P_3 \cup 5K_1$ is an induced subgraph of $\overline{\Gamma}$. By Lemma 2.2(ii) and Appendix A, we have $-2\cos\big(\frac{\pi}{k+1}\big) - 1 \leq \rho_{16}\big(K_{16} \setminus (U_{3;2,1} \cup P_2 \cup P_3 \cup 5K_1)\big) < -2.923$, and thus $k \geq 11$, a contradiction. If $11 \leq n \leq 15$, it is straight forward to check that $K_n \setminus P_{10}$ and $K_n \setminus \big(U_{3;2,1} \cup P_2 \cup P_3\big)$ are not A-cospectral.

Case 4. $s = 1$. Then, $t = 1$ and thus $\Gamma_1 = U_{3;1,1}$. Since $10 \leq k = |E(\Gamma_1)| + |E(F)| + 1 = 6 + |E(F)| \leq 10$, we have $F = 2P_3$ and $k = 10$. In this case, $m_0(\overline{\Gamma}) = m_0(U_{3;1,1}) + 2m_0(P_3) + n - 11 = n - 8$ by Lemma 2.6 and Appendix C, contrary to (2.3). ■

Theorem 3.15. *If $10 \leq k \leq 19$, then Γ_1 is a tree.*

Proof. By Proposition 1.3, suppose to the contrary that Γ_1 is a unicyclic graph. By Lemmas 3.12 and 3.14, we may assume that C_3 is the unique cycle of $\overline{\Gamma}$ with $V(C_3) = \{w_1, w_2, w_3\}$, where $d_{\Gamma_1}(w_1) = 3$ and $d_{\Gamma_1}(w_2) = d_{\Gamma_1}(w_3) = 2$. Thus, C_3 is a special triangle of Γ_1, and so $P_2 \notin F$ by Lemma 3.8. Let P_s and P_t be a longest path and a shortest path of F respectively,

and let U_d^3 be an induced subgraph of Γ_1 such that d is as large as possible. Since $U_1^3 \cup P_5$ is forbidden by Lemma 3.10(i), we have

$$3 \le t \le s \le 4.$$

We first prove the following claims.

Claim A. *$\Delta(\Gamma_1) = 3$ and $\eta(\overline{\Gamma}) - 1 = \varepsilon(F) = q(\Gamma_1)$.*

Proof of Claim A. If $\Delta(\Gamma_1) \ge 4$, then since $d_{\overline{\Gamma}}(w_1) = 3 > d_{\overline{\Gamma}}(w_2) = d_{\overline{\Gamma}}(w_3) = 2$, from (2.1) it follows that $\varepsilon(F) \ge 3$. Combining this with $3 \le t \le s \le 4$, $U_1^3 \cup 2P_3 \cup P_4$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 2.1(iii), contrary to Lemma 3.10(i). Thus, $\Delta(\Gamma_1) = 3$, and so $\varepsilon(F) = q(\Gamma_1)$ by Lemma 2.4. Since $t \ge 3$ and $U_1^3 \cup K_{1,3} \cup P_3$ is forbidden by Lemma 3.10(i), we have $\Delta(F) = 2$, which implies that $\eta(\overline{\Gamma}) = \varepsilon(F) + 1$. This completes the proof of Claim A.

Claim B. *$\eta(\overline{\Gamma}) - 1 = \varepsilon(F) = q(\Gamma_1) = 2$* **and** *$2 \le d \le 5$.*

Proof of Claim B. Since $U_1^3 \cup P_5$ is forbidden by Lemma 3.10(i), we have $1 \le d \le 6$. Note that $U_1^3 \cup 2P_3 \cup P_4$ is forbidden by Lemma 3.10(i) and $\varepsilon(F) = q(\Gamma_1)$ by Claim A. Thus, Lemma 2.1(iii) and $t \ge 3$ imply that $q(\Gamma_1) \le 2$. Since $q(\Gamma_1) = \eta(\overline{\Gamma}) - 1 \ge 2$ by Lemma 3.13 and Claim A, we have $q(\Gamma_1) = 2$ and thus $d \ge 2$. If $d = 6$, then since $q(\Gamma_1) = 2$, $U_6^3 \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contradicting Lemma 3.10(i). Now, Claim B follows from Claim A.

Claim C. *$F = 2P_3$ and $k = 9 + d$.*

Proof of Claim C. By Claim B and since $3 \le t \le s \le 4$, we may assume that $F = P_3 \cup P_4$ by Lemma 2.1(ii). Since $Z_{2,2,2}$ is forbidden by Lemma 3.10(ii), $d \le 5$ by Claim B and $q(\Gamma_1) = 2 = \Delta(\Gamma_1) - 1$, we have $|E(\Gamma_1)| \le 9$. Combining this with $F = P_3 \cup P_4$, it follows that $k = |E(\Gamma_1)| + |E(F)| + 1 \le 15$. By Claim B, we have $d \ge 2$ and so $U_2^3 \cup P_3 \cup P_4$ is an induced subgraph of $\overline{\Gamma}$. By Lemma 2.2(ii) and Appendix A, $-2\cos\left(\frac{\pi}{k+1}\right) - 1 \le \rho_{12}\big(K_{12} \setminus (U_2^3 \cup P_3 \cup P_4)\big) < -2.966$, and thus $k \ge 16$, a contradiction. Thus, $F = 2P_3$.

Since $q(\Gamma_1) = 2 = \Delta(\Gamma_1) - 1$, $Z_{2,2,2}$ is forbidden by Lemma 3.10(ii) and $F = 2P_3$, we have $k = |E(\Gamma_1)| + |E(F)| + 1 = 9 + d$, completing the proof of Claim C.

Now we are ready to complete the proof of this theorem. We divide into three cases according to the value of d.

Case 1. $d \in \{3, 5\}$. By Claim C, $k = 9 + d$ is even. Since $F = 2P_3$ by Claim C, it follows that $m_0(\overline{\Gamma}) = m_0(\Gamma_1) + 2m_0(P_3) + n - 10 - d \ge n - 8 - d = n - k + 1$ by Lemma 2.6, contradicting (2.3).

Case 2. $d = 4$. In this case, $k = 13$ by Claim C. Since $q(\Gamma_1) = 2 = \Delta(\Gamma_1) - 1$ and $Z_{2,2,2}$ is forbidden by Lemma 3.10(ii), we have $\Gamma_1 \in \{H_6, H_7, H_8\}$. If $\Gamma_1 = H_6$, then Lemma 2.2(ii) and Appendix A imply that $-2\cos\left(\frac{\pi}{k+1}\right) - 1 \le \rho_{14}\big(K_{14} \setminus (H_6 \cup 2P_3)\big) < -2.96$, and thus $k \ge 15$, a contradiction. If $\Gamma_1 \in \{H_7, H_8\}$, then Lemma 2.2(ii) and Appendix B imply that $0.967 < \min\big\{\rho_2\big(K_{14} \setminus (H_7 \cup 2P_3)\big), \rho_2\big(K_{14} \setminus (H_8 \cup 2P_3)\big)\big\} \le 2\cos\left(\frac{\pi}{k+1}\right) - 1$, and thus $k \ge 17$, a contradiction.

Case 3. $d = 2$. Since $q(\Gamma_1) = 2 = \Delta(\Gamma_1) - 1$, we have $\Gamma_1 = H_9$ and thus $k = 11$. Since $F = 2P_3$, it follows that $m_0(\overline{\Gamma}) = m_0(H_9) + 2m_0(P_3) + n - 12 = n - 9 = n - k + 2$ by Appendix C, contrary to (2.3). ■

4. Completing the proof of Theorem 1.2

Theorem 3.15 implies that Γ_1 is a tree. By Lemma 2.5(i), if $k \ge 13$ and Γ_1 is a tree, then $\Gamma = K_n \setminus P_k$ as desired. Thus we may assume that $10 \le k \le 12$ in this section. By Theorem 4.1 and Proposition 1.3, we immediately have $\overline{\Gamma} = P_k \cup (n-k)K_1$, completing the proof of Theorem 1.2.

Theorem 4.1. *If $10 \le k \le 12$ and Γ_1 is a tree, then $\Gamma_1 = P_k$ and F is empty.*

In order to prove Theorem 4.1, we present two lemmas first.

Lemma 4.2 ([4]). *Let $G = W_q \cup P_{s_1} \cup P_{s_2}$ and $t = s_1 + s_2 + q - 2$, where $q \ge 7$. If $s_1 \ge s_2 \ge 2$ and $s_1 \ge 3$, then $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$, $m_2(G) = m_2(P_t)$, and $m_3(G) < m_3(P_t)$.*

Lemma 4.3. *If $k \le 12$, then $Z_{2,1,1,1} \cup 2P_2$, $K_{1,5} \cup 2P_2 \cup P_3$, and $Z_{1,2,3} \cup P_2$ are forbidden.*

Proof. Suppose that H contains s vertices. If $H \in \big\{Z_{2,1,1,1} \cup 2P_2, K_{1,5} \cup 2P_2 \cup P_3, Z_{1,2,3} \cup P_2\big\}$, then by Lemma 2.2(ii) and Appendix B, we have $0.942 < \rho_2\big(K_s \setminus H\big) \le 2\cos\left(\frac{\pi}{k+1}\right) - 1$, and thus $k \ge 13$, a contradiction. ■

In the remainder of this section, we present the proof of Theorem 4.1.

Proof of Theorem 4.1. Let P_s be the longest path of F. If all nontrivial trees of $\overline{\Gamma}$ are paths, then $\varepsilon(F) = 0$ by Lemma 2.5(ii), and thus $\overline{\Gamma} = P_k \cup (n-k)K_1$. This implies that the result already holds. In what follows, we may choose Γ_1 as a non-trivial tree of $\overline{\Gamma}$ such that $\Delta(\Gamma_1) = \Delta(\overline{\Gamma})$, and subject to this, $\rho_1(\Gamma_1)$ is as large as possible. By Proposition 1.3, we have $\Delta(\Gamma_1) \geq 3$, and thus it suffices to consider the following two cases:

Case 1. $\Delta(\Gamma_1) \geq 4$. If Γ_1 is not a star, then $\varepsilon(F) \geq 2$ by (2.2) and thus $Z_{2,1,1,1} \cup 2P_2$ is an induced subgraph of $\overline{\Gamma}$, contrary to Lemma 4.3. Thus, we may assume that $\Gamma_1 = K_{1,q}$, where $q \geq 4$. By Lemma 2.5(ii), we have

$$\varepsilon(F) = \frac{1}{2}\Delta(\Gamma_1)\big(\Delta(\Gamma_1) - 3\big) + 1 \geq 3. \tag{4.1}$$

Since $\varepsilon(F) \geq 3$ and $K_{1,5} \cup 2P_2 \cup P_3$ is forbidden by Lemma 4.3, Lemma 2.1(ii) implies that $q = 4$ and thus $\varepsilon(F) = 3$ by (4.1) and $10 \leq k = |E(K_{1,4})| + |E(F)| + 1 = 5 + |E(F)| \leq 12$, implying that $|E(F)| \leq 7$. Since $\varepsilon(F) = 3$ and $|E(F)| \leq 7$, we have $F = P_{q_1} \cup P_{q_2} \cup P_s$ and $\Gamma_1 = K_{1,4}$, where $2 \leq q_1 \leq q_2 \leq s \leq 5$ by Lemma 2.1(ii). If $s = 5$, then $|E(F)| \leq 7$ implies that $q_1 = 2$, contrary to Lemma 3.8. Thus, $s \leq 4$ and hence $F \in \{P_2 \cup 2P_3, P_2 \cup P_3 \cup P_4, 2P_3 \cup P_4\}$ by Lemma 2.1(ii).

If $F = 2P_3 \cup P_d$ for $d \in \{2, 4\}$, then $k = 8 + d$. In this case, $m_0(\overline{\Gamma}) = m_0(K_{1,4}) + 2m_0(P_3) + m_0(P_d) + n - 11 - d = n - 6 - d = n - k + 2$ by Lemma 2.6, contrary to (2.3). Thus, $F = P_2 \cup P_3 \cup P_4$ and $k = 11$. In the latter case, we have $m_1(\overline{\Gamma}) = 9 = m_1(P_{11})$, $m_2(\overline{\Gamma}) = 36 = m_2(P_{11})$, and $m_3(\overline{\Gamma}) = 1 < 8 = m_3(P_{11})$. Thus, $\Phi(\overline{\Gamma}) > \Phi\big(P_{11} \cup (n-11)K_1\big)$, contradicting Lemma 3.2.

Case 2. $\Delta(\Gamma_1) = 3$. Since $Z_{2,2,2,}$ is forbidden by Lemma 3.10(ii), we may assume that $Z_{p_1,p_2,1}$ is an induced subgraph of Γ_1 such that p_2 is as large as possible, and subject to this, $p_1 + p_2$ is as large as possible, where $p_1 \geq p_2 \geq 1$. Since $Z_{1,2,3} \cup P_2$ is forbidden by Lemma 4.3, $1 \leq p_2 \leq 2$.

Subcase 2.1. $q(\Gamma_1) \geq 2$. In this case, $\varepsilon(F) = q(\Gamma_1) \geq 2$ by (2.2). Recall that $1 \leq p_2 \leq 2$.

If $p_2 = 1$, then $\Gamma_1 = W_q$ by the choice of p_2. As W_6 is forbidden by Lemma 3.10(ii), we have $q \geq 7$. From Lemmas 3.5 and 4.2, we can deduce that $\Phi(\overline{\Gamma}) > \Phi\big(P_k \cup (n-k)K_1\big)$, contrary to Lemma 3.2. If $p_2 = 2$, then since $Z_{1,2,3} \cup P_2$ is forbidden by Lemma 4.3, we have $p_1 = 2$. Combining $p_1 = 2$ and $q(\Gamma_1) \geq 2$, W_6 is an induced subgraph of $\overline{\Gamma}$, which contradicts Lemma 3.10(ii).

Subcase 2.2. $q(\Gamma_1) = 1$. By (2.2), $\varepsilon(F) = q(\Gamma_1) = 1$ and thus $\overline{\Gamma}$ contains exactly $\eta(\overline{\Gamma}) - 1$ non-path trees (each of which has exactly one 3-vertex) and one path P_s, where $s \geq 2$. Combining this with $k = |E(\Gamma_1)| + |E(F)| + 1 \leq 12$, we have $\eta(\overline{\Gamma}) \leq 4$.

If $p_2 = 1$ or $s \geq 3$, then by applying Lemma 3.5, we can obtain another forest F_1 with exact $\eta(\overline{\Gamma}) - 2$ first-type trees and one path $P_{p_1+p_2+s+1}$ such that $\Phi(\overline{\Gamma}) > \Phi(F_1)$. With a similar method, by repeatedly applying Lemma 3.5 $\eta(\overline{\Gamma}) - 1$ (≤ 3) times, we can deduce that $\Phi(\overline{\Gamma}) > \Phi(P_k \cup (n-k)K_1)$, a contradiction. Thus, $p_2 = 2 = s$. Since $Z_{1,2,3} \cup P_2$ is forbidden by Lemma 4.3, we have $p_1 = p_2 = 2 = s$. Thus, $10 \leq k = |E(\Gamma_1)| + |E(F)| + 1 = 6 + |E(F)| \leq 12$, and so $4 \leq |E(F)| \leq 6$. Combining this with $P_2 \in F$ and $\varepsilon(F) = 1$, we can conclude that $\eta(\overline{\Gamma}) = 3$ and $\Delta(F) = 3$.

Since $\eta(\overline{\Gamma}) = 3$ and $s + p_1 + p_2 + 1 = 7$, from Lemma 3.5 we can obtain another forest F_2 with exactly one first-type tree and one path P_7 such that $\Phi(\overline{\Gamma}) = \Phi(F_2)$. Once again, from Lemma 3.5, we can deduce that $\Phi(\overline{\Gamma}) > \Phi(P_k \cup (n-k)K_1)$, a contradiction. ■

5. Concluding remark

Though Conjecture 1.1 was settled by combining [1–4] with the current paper, the complete proof seems too complicated. Thus, as pointed out at the end of [4], the authors would like to mention that it is still meaningful and interesting to find a simple proof of Conjecture 1.1.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. The graphs H and the values of $\rho_s(K_s \setminus H)$

H	$U_1^5 \cup Z_{2,1,1} \cup P_2 \cup P_3$	$U_1^5 \cup P_7$	$U_2^5 \cup 2K_{1,3} \cup P_3$
$\rho_s(K_s \setminus H)$	−2.98027	−2.98990	−2.97819
H	$U_2^5 \cup 2P_5$	$U_2^5 \cup K_{1,3} \cup P_2 \cup P_5$	$U_2^5 \cup P_3 \cup P_6$
$\rho_s(K_s \setminus H)$	−2.98468	−2.98003	−2.98059
H	$H_1 \cup K_{1,3} \cup P_2 \cup 2P_3$	$H_1 \cup P_6$	$H_1 \cup 2P_3 \cup P_5$
$\rho_s(K_s \setminus H)$	−2.97541	−2.98850	−2.98323
H	$U_{1,1}^3 \cup P_2 \cup P_4$	$U_{1,1}^3 \cup P_2 \cup 2P_3$	$U_6^3 \cup P_2 \cup P_3$
$\rho_s(K_s \setminus H)$	−3.00000	−3.00000	−2.97550
H	$U_{3,3}^3 \cup 2P_3$	$U_1^3 \cup P_5$	$U_1^3 \cup K_{1,3} \cup P_3$
$\rho_s(K_s \setminus H)$	−2.98190	−2.98125	−2.98919
H	$U_{3;1,1} \cup P_2 \cup 2P_3$	$U_{3;1,1} \cup P_2 \cup P_4$	$U_{3;5,1} \cup P_3 \cup K_1$
$\rho_s(K_s \setminus H)$	−2.97694	−2.98006	−2.97741
H	$U_{3;4,1} \cup 2P_3$	$U_1^3 \cup 2P_3 \cup P_4$	$U_4^3 \cup P_3 \cup P_4$
$\rho_s(K_s \setminus H)$	−2.98289	−2.99409	−2.97546
H	$U_1^5 \cup P_2 \cup P_6$	$U_{3;4,4} \cup P_2 \cup P_3$	$U_{3;4,2} \cup P_2 \cup P_3 \cup 2K_1$
$\rho_s(K_s \setminus H)$	−2.96224	−2.97065	−2.95259
H	$U_{3;4,1} \cup P_2 \cup P_3 \cup 2K_1$	$U_{3;3,3} \cup 2P_3$	$U_{3;3,1} \cup 2P_3$
$\rho_s(K_s \setminus H)$	−2.94995	−2.96063	−2.95165
H	$U_{3;2,1} \cup 2P_3$	$U_{3;2,2} \cup P_2 \cup P_3 \cup 6K_1$	$U_{3;2,1} \cup P_2 \cup P_3 \cup 5K_1$
$\rho_s(K_s \setminus H)$	−2.94197	−2.93523	−2.92363
H	$U_2^3 \cup P_3 \cup P_4$	$H_6 \cup 2P_3$	
$\rho_s(K_s \setminus H)$	−2.96686	−2.96028	

Appendix B. The graphs H and the values of $\rho_2(K_s \setminus H)$

H	$Z_{1,2,4} \cup K_1$	$Z_{2,2,1,1}$	W_6	$Z_{2,2,2}$
$\rho_2(K_s \setminus H)$	0.97883	1.00000	1.00000	1.00000
H	$Z_{1,3,3} \cup P_2 \cup 2P_3$	$Z_{2,1,1,1} \cup 2P_2 \cup P_3$	U_4^5	H_3
$\rho_2(K_s \setminus H)$	0.97845	0.98425	0.99006	0.98139
H	$H_4 \cup 2P_2 \cup P_3$	$H_5 \cup K_1$	$U_3^5 \cup 2P_3$	$U_3^5 \cup P_2 \cup P_3 \cup K_{1,3}$
$\rho_2(K_s \setminus H)$	0.97828	0.98642	0.96962	0.97398
H	$H_2 \cup P_2 \cup 2P_3$	$H_7 \cup 2P_3$	$H_8 \cup 2P_3$	$Z_{2,1,1,1} \cup 2P_2$
$\rho_2(K_s \setminus H)$	0.95735	0.96702	0.99291	0.94234
H	$K_{1,5} \cup 2P_2 \cup P_3$	$Z_{1,2,3} \cup P_2$		
$\rho_2(K_s \setminus H)$	0.94646	0.94233		

Appendix C. The graphs H and their adjacency spectra

G	$S_A(G)$
U_2^5	−1.94486, −1.61803, −0.89579, 0.42063, 0.61803, 1.26848, 2.15154
$U_{3;1,1}$	−1.61803, −1.30278, 0, 0.61803, 2.30278
H_9	−1.89122, −1, −0.70462, 0, 1.31743, 2.27841

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Unified extremal results for k-apex unicyclic graphs (trees)

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ABSTRACT

A k-cone c-cyclic graph is the join of the complete graph K_k and a c-cyclic graph (if $k = 0$, we get the usual connected graph). A k-apex tree (resp., k-apex unicyclic graph) is defined as a connected graph G with a k-subset $V_k \subseteq V(G)$ such that $G - V_k$ is a tree (resp., unicylic graph), but $G - X$ is not a tree (resp., unicylic graph) for any $X \subseteq V(G)$ with $|X| < k$. In this paper, we extend those extremal results and majorization theorems concerning connected graphs of Liu et al. (2019) to k-cone c-cyclic graphs. We also use a unified method to characterize the extremal maximum and minimum results of many topological indices in the class of k-apex trees and k-apex unicyclic graphs, respectively. The later results extend the main results of Javaid et al. (2019); Liu et al. (2020) and partially answer the open problem of Javaid et al. (2019). Except for the new majorization theorem, some new techniques are also established to deal with the minimum extremal results of this paper.

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1. Introduction

Throughout this paper, we are only concerned with simple connected graphs, unless specified otherwise. If $G = (V, E)$ is a connected graph with $|E(G)| = |V(G)| + c - 1$, then G is called a *c-cyclic graph*. Particularly, when $c = 0, 1, 2$ or 3, then G is called a *tree*, *unicyclic graph*, *bicyclic graph* or *tricyclic graph*, respectively. As usual, let $N_G(v)$ and $d_G(v)$ denote the neighbor set and degree of vertex v of G. A vertex with degree one will be referred as a *pendant vertex*. When there is no confusion, we simplify $N_G(v)$ and $d_G(v)$ as $N(v)$ and $d(v)$, respectively. The positive integer sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v_i)$ holds for $1 \le i \le n$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$. Throughout this paper, we use d_i to denote the ith largest degree of G and we suppose that $d(v_i) = d_i$, where $1 \le i \le n$.

Let $A(G)$ and $D(G)$ be, respectively, the adjacency matrix and diagonal matrix of a graph G. The signless Laplacian matrix and Laplacian matrix of G is defined as $Q(G) = D(G) + A(G)$ and $L(G) = D(G) - A(G)$, respectively. As in [28], we define $A(G) + \beta D(G)$ as the *general matrix* of G and denote its largest eigenvalue by $\Theta(G, \beta)$, that is, $\Theta(G, \beta)$ is the *general spectral radius* of G.

Among those vertex-degree-based graph invariants, the *Randić index* $R(G)$ [22] and *second Zagreb index* $M_2(G)$ [21] are two famous topological indices, where

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}}, \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} (d(u)d(v)).$$

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Bollobás and Erdős [2] generalized the concepts of Randić index and second Zagreb index to the *general Randić index* $W_\alpha(G)$, where

$$W_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^\alpha .$$

The *general sum-connectivity index* [37] $\chi_\alpha(G)$ of G is also an extension of many known topological indices, where

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u)+d(v))^\alpha .$$

As a special case, $\chi_{-\frac{1}{2}}(G)$ is known as the *sum-connectivity index* of G [36], $\chi_2(G)$ is also called the *Hyper-Zagreb index* of G [23], while $2\chi_{-1}(G)$ is equal to the *Harmonic index* of G [5].

The *first reformulated Zagreb index* $Z_2(G)$ of G [20] is a slight modification to $\chi_2(G)$, where

$$Z_2(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^2 .$$

Another famous vertex-degree-based graph invariant, called the *Atom–Bond connectivity index* of G [4], is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

As a generalization of $Z_2(G)$, $Z_\alpha(G)$ is defined as [18]:

$$Z_\alpha(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^\alpha . \tag{1.1}$$

The zeroth-order general Randić index $R^0_\alpha(G)$ [11] is an extension of the first Zagreb index, where

$$R^0_\alpha(G) = \sum_{u\in V(G)} (d(u))^\alpha .$$

In order to study on such graph invariants based on adjacent vertex degree, Wang [25] recently proposed a new symmetric function:

A symmetric bivariate function $f(x,y)$ defined on positive real numbers is called **escalating** (resp. **de-escalating**) if

$$f(x_1,x_2)+f(y_1,y_2) \geq f(x_2,y_1)+f(x_1,y_2) \ \big(resp. f(x_1,x_2)+f(y_1,y_2) \leq f(x_2,y_1)+f(x_1,y_2)\big) \tag{1.2}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (1.2) is strict if $x_1 > y_1$ and $x_2 > y_2$.

In what follows we suppose that $f(x,y)$ is twice differentiable.

Definition 1.1. A non-negative escalating function $f(x,y)$ is called a **good escalating function,** if $f(x,y)$ satisfies

$$\frac{\partial f(x,y)}{\partial x} > 0, \quad \frac{\partial^2 f(x,y)}{\partial x^2} \geq 0, \ \text{and}$$

$$f(x_1+1,x_2)+f(x_1+1,y_2)+f(x_1+1,y_1-1) > f(x_1,x_2)+f(y_1,y_2)+f(x_1,y_1)$$

holds for any $x_1 \geq y_1 \geq 2$ and $x_2 \geq y_2 \geq 1$.

Remark 1.1. Here, the notation of good escalating function is different from that of [18], where it requires that $f(x_1+1,y_2)+f(x_1+1,y_1-1) \geq f(y_1,y_2)+f(x_1,y_1)$ instead of $f(x_1+1,x_2)+f(x_1+1,y_2)+f(x_1+1,y_1-1) > f(x_1,x_2)+f(y_1,y_2)+f(x_1,y_1)$. Since $\frac{\partial f(x,y)}{\partial x} > 0$, our definition is more general than that of [18].

Gutman [6], and later Wang [25] independently, defined a graph invariant of a connected graph G associated with a symmetric bivariate function $f(x,y)$ to be

$$M_f(G) = \sum_{uv\in E(G)} f\,(d(u),d(v)), \tag{1.3}$$

where $M_f(G)$ was called the *connectivity function* of G by Wang [25].

For a connected graph G, the first Zagreb index $M_1(G)$ and the second multiplicative Zagreb index $\prod_2(G)$ of G are defined as

$$M_1(G) = \sum_{v\in V(G)} (d(v))^2, \quad \text{and} \quad \prod_2(G) = \prod_{u\in V(G)} (d(u))^{d(u)}.$$

Then, $M_1(G)$ and $\prod_2(G)$ are two topological indices related with the degree of vertices of G. Actually, they can be generalized to *the degree-function index* $H_f(G)$ of G [28]. Here,

$$H_f(G) = \sum_{v \in V(G)} f(d(v)),$$

where $f(x)$ is a function defined on positive real numbers.

Let G_1 and G_2 be two vertex disjoint graphs. By $G_1 \vee G_2$ we denote the *join* of G_1 and G_2, which is obtained by joining each vertex of G_1 to each vertex of G_2. Let H be a connected c-cyclic graph on $n-k$ vertices, then $K_k \vee H$ is called a *k-cone c-cyclic graph*. It is worth to observe that for $k = 0$, $K_0 \vee H = H$, therefore any connected graph can be seen as a 0-cone graph.

Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π. Similarly, $\Gamma(\pi, k; c)$ denotes the class of k-cone c-cyclic graphs with π as their degree sequence. Clearly, $\Gamma(\pi, k; c) \subseteq \Gamma(\pi)$. For simplification, $\Gamma(\pi, k; 0)$, $\Gamma(\pi, k; 1)$, and $\Gamma(\pi, k; 2)$ are also denoted by $\mathscr{T}(\pi, k)$, $\mathscr{U}(\pi, k)$, and $\mathscr{B}(\pi, k)$, respectively.

For a subset V_1 of $V(G)$ and an induced subgraph H of G with $V(H) \cap V_1 = \emptyset$, $G - V_1$ denotes the graph which is obtained from G by deleting the vertices of V_1 and all edges incident to any of them, and $H + V_1$ is the subgraph of G induced by vertex set $V(H) \cup V_1$. Particularly, $H - \{v\}$ and $H + \{v\}$ are always abbreviated to $H - v$ and $H + v$, respectively.

Definition 1.2 ([26]). A *k-**apex tree*** (resp., *k-**apex unicyclic graph*** [14]) is defined as a connected graph G with a k-subset $V_k \subseteq V(G)$ such that $G - V_k$ is a tree (resp., unicyclic graph) but $G - X$ is not a tree (resp., unicyclic graph) for any subset $X \subseteq V(G)$ with $|X| < k$.

The rest of this paper is organized as follows. In Section 2, we are concerned with the extremal graphs and majorization theorems of connectivity function $M_f(G)$ in the class of k-cone c-cyclic graphs. In Section 3, we use a unified method to determine the unique extremal maximum graph for $\Theta(G, \beta)$, $Z_\alpha(G)$, $\chi_\alpha(G)$, $H_f(G)$, $\prod_2(G)$ and $M_2(G)$, in the class of k-apex unicyclic graphs and k-apex trees with n vertices, respectively. In the last section, we obtain a unified method to determine the extremal minimum graph for $H_f(G)$, $\prod_2(G)$ and $M_2(G)$ in the class of k-apex unicyclic graphs and k-apex trees with n vertices, respectively.

2. Extremal graphs and majorization theorems of $M_f(G)$

This section is dedicated to the extremal graphs and majorization theorems of $M_f(G)$.

2.1. Extremal graphs of $M_f(G)$

In what follows, we call G an *extremal graph of $M_f(G)$* in some graph category $\mathcal{G}$ if either $M_f(G)$ is maximized when $f(x, y)$ is escalating or $M_f(G)$ is minimized when $f(x, y)$ is de-escalating among all graphs of $\mathcal{G}$.

Let $G = K_k \vee H$ be a k-cone c-cyclic graph with n vertices, where $k \geq 0$. Denote by

$$M_{f^*}(G) = \sum_{uv \in E(H)} f(d_H(u) + k, d_H(v) + k).$$

Lemma 2.1. *Let $G = K_k \vee H$ be a graph of $\Gamma(\pi, k; c)$, where $\min\{k, c\} \geq 0$. If either $M_{f^*}(G)$ is maximized when $f(x, y)$ is escalating or $M_{f^*}(G)$ is minimized when $f(x, y)$ is de-escalating, then G is an extremal graph of $M_f(G)$ in $\Gamma(\pi, k; c)$.*

Proof. Since the degree sequence of G is $\pi = \left((n-1)^k, d_{k+1}, d_{k+2}, \ldots, d_n\right)$, we have

$$M_f(G) = \binom{k}{2} f(n-1, n-1) + k \sum_{i=1}^{n-k} f(n-1, d_{k+i}) + \sum_{uv \in E(H)} f(d_H(u) + k, d_H(v) + k).$$

If $G_1 = K_k \vee H_1$ and $G_2 = K_k \vee H_2$ are two graphs of $\Gamma(\pi, k; c)$, then

$$M_f(G_1) - M_f(G_2) = M_{f^*}(G_1) - M_{f^*}(G_2). \tag{2.1}$$

Thus, the result follows. ■

In what follows, let $\pi = \left((n-1)^k, d_{k+1}, d_{k+2}, \ldots, d_n\right)$ be the degree sequence of a k-cone c-cyclic graph with n vertices, and define by $\pi^* = \left(d_1^*, d_2^*, \ldots, d_{n-k}^*\right)$, where $d_j^* = d_{k+j} - k$ for $j \in \left\{1, 2, \ldots, n-k\right\}$. For the sake of readability, we simplify writing $v_j^* = v_{k+j}$ for $j \in \{1, 2, \ldots, n-k\}$. For a connected graph G and two vertices $\{u, v\}$ of G, denote by $dist_G(u, v)$ the distance between u and v in G.

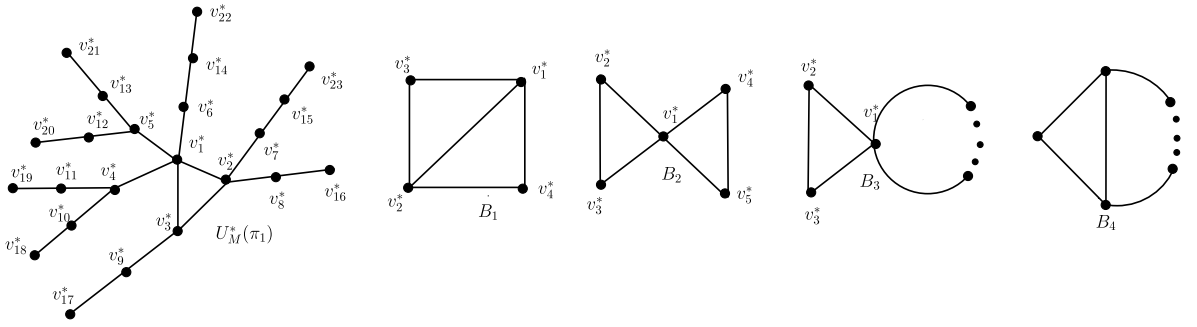


Fig. 2.1. The graphs $U_M^*(\pi_1)$, B_1, B_2, B_3 and B_4.

Definition 2.1. Let $G = K_k \vee H$ be a k-cone graph with $V(H) = \{v_1^*, v_2^*, \ldots, v_{n-k}^*\}$, where $k \geq 0$. If a well-ordering $v_1^* \prec v_2^* \prec \cdots \prec v_{n-k}^*$ of $V(H)$ satisfies the following (i) and (ii), then $\prec$ is called a **BFS-ordering** of $V(H)$, and G is called a k-**cone BFS-graph**.

(i) $d_H(v_1^*) \geq d_H(v_2^*) \geq \cdots \geq d_H(v_{n-k}^*)$, and $h_H(v_1^*) \leq h_H(v_2^*) \leq \cdots \leq h_H(v_{n-k}^*)$, where $h_H(v_i^*) = dist_H(v_i^*, v_1^*)$ for $i = 1, 2, \ldots, n-k$;

(ii) Let $v \in N_H(u) \backslash N_H(w)$, and $z \in N_H(w) \backslash N_H(u)$ such that $h_H(u) = h_H(w) = h_H(v) - 1 = h_H(z) - 1$. If $u \prec w$, then $v \prec z$.

A 0-cone BFS-graph is always simply called a *BFS-graph*. In Theorem 2.1 of [18], the authors proved that

Theorem 2.1 (*[18]*). *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a c-cyclic degree sequence. If $d_n = 1$, then there exists an extremal graph $G \in \Gamma(\pi)$ such that G is a BFS-graph. Furthermore, $\{v_1, v_2, v_3\}$ forms a triangle of G when $c \geq 1$.*

According to Lemma 2.1 and Eq. (2.1), with the similar argument as in the proof of Theorem 2.1 in [18], we can deduce that the following result holds. Here, due to the length restriction of this paper, we omit its detailed proof.

Theorem 2.2. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a k-cone c-cyclic degree sequence, where $\min\{k, c\} \geq 0$. If $d_{n-k}^* = 1$, then in the class of $\Gamma(\pi, k; c)$, there exists an extremal graph G of $M_f(G)$ such that G is a k-cone BFS-graph, and $\{v_1^*, v_2^*, v_3^*\}$ forms a triangle of G when $c \geq 1$.*

We use the symbol $p^{(q)}$ to define q copies of the real number p. It is well-known that the *BFS*-tree is unique for any given tree degree sequence π [30], and in what follows we use $T_M^*(\pi)$ to denote the unique *BFS*-tree with tree degree sequence π^*. When $\pi^* = (d_1^*, d_2^*, \ldots, d_{n-k}^*)$ is a unicyclic degree sequence and $d_{n-k}^* = 1$, we can construct a unique k-cone *BFS*-unicyclic graph $U_M(\pi) = K_k \vee U_M^*(\pi)$ with $V(U_M(\pi)) = \{v_1, v_2, \ldots, v_n\}$ by the following breadth-first-search method: The unique cycle of $U_M^*(\pi)$ is a triangle with $V(C_3) = \{v_1^*, v_2^*, v_3^*\}$. Select the vertex v_1^* as the root vertex and begin with v_1^* of the zeroth layer. Select the vertices $v_2^*, v_3^*, v_4^*, v_5^*, \ldots, v_{d_1^*+1}^*$ as the first layer such that $N_{U_M^*(\pi)}(v_1^*) = \{v_2^*, v_3^*, v_4^*, v_5^*, \ldots, v_{d_1^*+1}^*\}$. Let $N_{U_M^*(\pi)}(v_2^*) = \{v_1^*, v_3^*, v_{d_1^*+2}^*, v_{d_1^*+3}^*, \ldots, v_{d_1^*+d_2^*-1}^*\}$ and $N_{U_M^*(\pi)}(v_3^*) = \{v_1^*, v_2^*, v_{d_1^*+d_2^*}^*, \ldots, v_{d_1^*+d_2^*+d_3^*-3}^*\}$. Then, append $d_4^* - 1$ vertices to v_4^* such that $N_{U_M^*(\pi)}(v_4^*) = \{v_1^*, v_{d_1^*+d_2^*+d_3^*-2}^*, \ldots, v_{d_1^*+d_2^*+d_3^*+d_4^*-4}^*\}$, and so on. Informally, consider the 2-cone unicyclic degree sequence $\pi_1 = (24^{(2)}, 7, 6, 5^{(3)}, 4^{(10)}, 3^{(8)})$. Then, $n = 25$, $k = 2$ and $U_M^*(\pi_1)$ is depicted in Fig. 2.1.

When $c \in \{0, 1\}$, by Theorem 2.2 it follows that

Corollary 2.1. *Let $\pi^* = (d_1^*, d_2^*, \ldots, d_{n-k}^*)$ be a c-cyclic degree sequence, where $d_{n-k}^* = 1$. (i) If $k \geq 0$, then $K_k \vee T_M^*(\pi)$ is an extremal graph of $M_f(G)$ in $\mathscr{T}(\pi, k)$. (ii) If $k \geq 0$, then $K_k \vee U_M^*(\pi)$ is an extremal graph of $M_f(G)$ in $\mathscr{U}(\pi, k)$.*

When G is a connected graph with at least one cycle, we use $\mathcal{R}(G)$ to define the *base graph* obtained from G by recursively deleting pendant vertices to the resultant graph until no pendant vertices remain. Let B_1, B_2, B_3 and B_4 be the four bicyclic graphs as shown in Fig. 2.1. Paths $P_{s_1}, P_{s_2}, \ldots, P_{s_q}$ are said to *have almost equal lengths* if $s_1, s_2, \ldots, s_q$ satisfy $|s_i - s_j| \leq 1$ for $1 \leq i \leq j \leq q$. If $\pi^* = (d_1^*, d_2^*, \ldots, d_{n-k}^*)$ is a bicyclic degree sequence, then $\sum_{i=1}^{n} d_i^* = 2(n-k+1)$, which implies that π^* should be one of the following four cases. Moreover, we construct a special bicyclic graph $B_M^*(\pi)$ of $\Gamma(\pi^*)$ as follows:

(i) If $d_{n-k}^* = 1$ and $d_1^* \geq d_2^* \geq 3$, then let $B_M^*(\pi)$ be a *BFS*-graph such that $\mathcal{R}(B_M^*(\pi)) \cong B_1$ and the remaining vertices appear in a *BFS*-ordering.

(ii) If $d_1^* \geq 5 > d_2^* = 2$ and $d_{n-k}^* = 1$, then let $B_M^*(\pi)$ be the bicyclic graph with $n-k$ vertices obtained from B_2 by attaching $d_1^* - 4$ paths of almost equal lengths to the maximum degree vertex of B_2, namely, v_1^*.

(iii) If $\pi^* = (4, 2^{(n-k-1)})$, then let $B_M^*(\pi) \cong B_3$.
(iv) If $\pi^* = (3^{(2)}, 2^{(n-k-2)})$, then let $B_M^*(\pi) \cong B_4$.

Similarly with the proof of Theorem 2.2 of [18], we can deduce that

Theorem 2.3. *If $k \geq 0$ and π^* is a bicyclic degree sequence, then $K_k \vee B_M^*(\pi)$ is an extremal graph of $M_f(G)$ in $\mathscr{B}(\pi, k)$.*

2.2. Majorization theorems of $M_f(G)$

Definition 2.2 (*[19]*)**.** Let $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ be two non-increasing sequences of real numbers. We write $(x) \trianglelefteq (y)$ if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, \ldots, n$. Furthermore, we write $(x) \triangleleft (y)$ if and only if $(x) \trianglelefteq (y)$ and $(x) \neq (y)$. The ordering $\pi \trianglelefteq \pi'$ is called **majorization**.

As early as in 2008, Bıyıkoğlu et al. [1] considered the relation between the maximum spectral radii in two classes of trees with given degree sequences, and Zhang [30] considered the similar problem for the Laplacian spectral radii (i.e., the signless Laplacian spectral radii since $L(G)$ and $Q(G)$ share the same spectra when G is a simple bipartite graph), and they showed that

Theorem 2.4. *Let π and π' be two different non-increasing degree sequences of trees with $\pi \triangleleft \pi'$. Suppose T and T' are the maximal extremal trees in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then (i) [1] $\Theta(T, 0) < \Theta(T', 0)$, and (ii) [30] $\Theta(T, 1) < \Theta(T', 1)$.*

Similar result of Theorem 2.4 is called majorization theorem. In the sequel, the majorization theorems of (signless Laplacian) spectral radii for unicyclic and bicyclic graphs were also proved [8,10,16,31]. However, the majorization theorem of (signless Laplacian) spectral radius does not hold for all c-cyclic graphs [17].

By an observation to Theorem 2.4, the main idea of the majorization theorem is to transfer the comparison of spectral invariants of two graphs to the comparison of their degree sequences in the majorization ordering $\triangleleft$. Zhang et al. [33] first applied the majorization theorem to topological index theory, they proved the majorization theorem for the Wiener index. After that, more and more majorization theorems of topological indices or spectral invariants were discovered [12,15,24,29,35]. For instance, we have

Theorem 2.5 (*[7]*)**.** *Let π_1 and π_2 be two different non-increasing k-cone c-cyclic degree sequences with $\pi_1 \triangleleft \pi_2$ and $k \geq 0$. Let $G_1 = K_k \vee H_1$ and $G_2 = K_k \vee H_2$ be an extremal maximum k-cone c-cyclic graph of $\Theta(G, \beta)$ in $\Gamma(\pi_1, k; c)$ and $\Gamma(\pi_2, k; c)$, respectively. For $c \in \{0, 1\}$, if $\beta \geq 0$, then $\Theta(G_1, \beta) < \Theta(G_2, \beta)$.*

Theorem 2.6 (*[28]*)**.** *Let π_1 and π_2 be two different non-increasing degree sequences, and G_1 and G_2 be two graphs with $G_1 \in \Gamma(\pi_1)$ and $G_2 \in \Gamma(\pi_2)$. If $\pi_1 \triangleleft \pi_2$, then $\prod_2(G_1) < \prod_2(G_2)$ and $H_f(G_1) < H_f(G_2)$ for any strictly convex function $f(x)$ defined on $x \geq 1$.*

For more results on the majorization theorem and their application, one can refer to two surveys [17,32] and some recent papers [7,18,28].

In what follows, we will prove the majorization theorem of $M_f(G)$, which improves the corresponding results of [18]. For this purpose, we need to list more lemmas as follows.

Let $G - uv$ denote the graph obtained from G by deleting the edge $uv \in E(G)$. Similarly, denote by $G + uv$ the graph obtained from G by adding an edge $uv \notin E(G)$.

Lemma 2.2. *Let u, v be two vertices of a connected graph H with $d_H(u) \geq d_H(v) \geq 2$ and w be some vertex of $N_H(v) \setminus \big(V(P_{uv}) \cup N_H(u) \cup \{u\}\big)$, where P_{uv} is a path connecting u and v in H. Let $G = K_k \vee H$ and $G' = G + wu - wv$. Suppose that $N_H(v)\setminus\{u\} = \{z_1', z_2', \ldots, z_{|N_H(v)\setminus\{u\}|}'\}$, and there exists $\{z_1, z_2, \ldots, z_{|N_H(v)\setminus\{u\}|}\} \subseteq N_H(u) \setminus \{v\}$ such that $d_H(z_i) \geq d_H(z_i')$ for $1 \leq i \leq |N_H(v)\setminus\{u\}|$. If $f(x, y)$ is a good escalating function, then $M_f(G') > M_f(G)$.*

Proof. We may suppose that $w = z_1'$ and $|V(G)| = n$. Since $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$, $f(x, y)$ is a convex function on x. Combining this with $d_H(u) \geq d_H(v) \geq 2$ and $f(x, y)$ being a bivariate function, we have

$$\begin{aligned} &f(n-1, d_G(u)+1) + f(n-1, d_G(v)-1) - f(n-1, d_G(u)) - f(n-1, d_G(v)) \\ =&f(d_G(u)+1, n-1) + f(d_G(v)-1, n-1) - f(d_G(u), n-1) - f(d_G(v), n-1) \geq 0. \end{aligned} \tag{2.2}$$

Case 1. $uv \notin E(G)$. Then, $|N_H(v)\setminus\{u\}| = d_H(v)$. Since $\frac{\partial f(x,y)}{\partial x} > 0$ and (2.2),

$$\begin{aligned} &M_f(G') - M_f(G) \\ \geq &k\big(f(n-1, d_G(u)+1) + f(n-1, d_G(v)-1) - f(n-1, d_G(u)) - f(n-1, d_G(v))\big) \end{aligned}$$

$$+\sum_{i=2}^{d_H(v)}\big(f(d_G(u)+1,d_G(z_i))+f(d_G(v)-1,d_G(z_i'))-f(d_G(u),d_G(z_i))-f(d_G(v),d_G(z_i'))\big)$$
$$+f(d_G(u)+1,d_G(z_1))-f(d_G(u),d_G(z_1))+f(d_G(u)+1,d_G(w))-f(d_G(v),d_G(w)).$$

Since $d_H(u)\geq d_H(v)$, $d_H(z_i)\geq d_H(z_i')$, $\frac{\partial^2 f(x,y)}{\partial x^2}\geq 0$ and $f(x,y)$ is escalating,

$$\begin{aligned}&f(d_G(u)+1,d_G(z_i))+f(d_G(v)-1,d_G(z_i'))-f(d_G(u),d_G(z_i))-f(d_G(v),d_G(z_i'))\\ =&f(d_G(u)+1,d_G(z_i))+f(d_G(v)-1,d_G(z_i))-f(d_G(u),d_G(z_i))-f(d_G(v),d_G(z_i))\\ &+f(d_G(v),d_G(z_i))+f(d_G(v)-1,d_G(z_i'))-f(d_G(v)-1,d_G(z_i))-f(d_G(v),d_G(z_i'))\\ \geq&f(d_G(u)+1,d_G(z_i))+f(d_G(v)-1,d_G(z_i))-f(d_G(u),d_G(z_i))-f(d_G(v),d_G(z_i))\geq 0.\end{aligned}$$

Combining this with $\frac{\partial f(x,y)}{\partial x}>0$ and $d_G(u)\geq d_G(v)$, we have

$$M_f(G')-M_f(G)>f(d_G(u)+1,d_G(w))-f(d_G(v),d_G(w))>0.$$

Case 2. $uv\in E(G)$. In this case, $|N_H(v)\backslash\{u\}|=d_H(v)-1$ and thus

$$\begin{aligned}&M_f(G')-M_f(G)\\ \geq&\sum_{i=2}^{d_H(v)-1}\big(f(d_G(u)+1,d_G(z_i))+f(d_G(v)-1,d_G(z_i'))-f(d_G(u),d_G(z_i))-f(d_G(v),d_G(z_i'))\big)\\ &+f(d_G(u)+1,d_G(z_1))-f(d_G(u),d_G(z_1))+f(d_G(u)+1,d_G(w))-f(d_G(v),d_G(w))\\ &+f(d_G(u)+1,d_G(v)-1)-f(d_G(u),d_G(v))\\ \geq&f(d_G(u)+1,d_G(z_1))+f(d_G(u)+1,d_G(w))+f(d_G(u)+1,d_G(v)-1)\\ &-f(d_G(u),d_G(z_1))-f(d_G(v),d_G(w))-f(d_G(u),d_G(v)).\end{aligned}$$

Since $f(x,y)$ is good escalating, we have $M_f(G')-M_f(G)>0$. ■

If $\pi=(d_1,d_2,\ldots,d_n)$ is a non-increasing integer sequence and $d_i\geq d_j+2$ holds for some integers $1\leq i<j\leq n$, then the following operation is called a *unit transformation* from i to j on π: subtract 1 from d_i and add 1 to d_j. The following famous lemma about majorization for integer sequences is due to Muirhead (see [19]).

Lemma 2.3 (*Muirhead Lemma*). *If π and π' are two non-increasing integer sequences and $\pi\lhd\pi'$, then π can be obtained from π' by a finite sequence of unit transformations.*

Suppose that $\pi=((n-1)^{(k)},d_{k+1},d_{k+2},\ldots,d_n)$ and $\pi'=((n-1)^{(k)},d'_{k+1},d'_{k+2},\ldots,d'_n)$ are two k-cone c-cyclic degree sequences. If $\pi\lhd\pi'$, by Lemma 2.3, we may suppose that π and π' differ only in two positions where the difference is 1, that is,

$$d_i=d'_i,\ \ d'_p=d_p+1,\ \text{ and } d'_q=d_q-1,\ \text{ where } k+1\leq p<q\leq n \text{ and } i\notin\{p,q\}. \tag{2.3}$$

Let $G_1=K_k\vee H_1$ and $G_2=K_k\vee H_2$ be an extremal k-cone c-cyclic graph of $\Gamma(\pi_1,k;c)$ and $\Gamma(\pi_2,k;c)$, respectively. If w is a vertex of H_1 as described in Lemma 2.2 such that $u=v_p$ and $v=v_q$, then we call w as a *surprising vertex* of G.

If $f(x,y)$ is good escalating and G_1 contains some surprising vertex w, then let $G'_2=G_1+v_pw-v_qw$. Thus, $G'_2\in\Gamma(\pi_2,k;c)$. Since $p<q$ and Theorem 2.2, we may suppose that $d_{H_1}(v_p)\geq d_{H_1}(v_q)$, thus Lemma 2.2 implies that $M_f(G_1)<M_f(G'_2)\leq M_f(G_2)$. Therefore, we can conclude that

$$\text{if } G_1 \text{ contains a surprising vertex, then } M_f(G_1)<M_f(G_2). \tag{2.4}$$

Theorem 2.7. *Let π_1 and π_2 be two different non-increasing k-cone c-cyclic degree sequences with $\pi_1\lhd\pi_2$ and $k\geq 0$. Let $G_1=K_k\vee H_1$ and $G_2=K_k\vee H_2$ be a maximum extremal k-cone c-cyclic graph of $M_f(G)$ in $\Gamma(\pi_1,k;c)$ and $\Gamma(\pi_2,k;c)$, respectively. For $c\in\{0,1,2\}$, if $f(x,y)$ is a good escalating function, then $M_f(G_1)<M_f(G_2)$.*

Proof. We will prove for the case $c=2$ only, as the case of $c\in\{0,1\}$ can be proved similarly. By Theorem 2.3, it suffices to show that $M_f\big(K_k\vee B_M^*(\pi_1)\big)<M_f\big(K_k\vee B_M^*(\pi_2)\big)$. Suppose that $\pi_1^*=(d_1^*,d_2^*,\ldots,d_{n-k}^*)$ and $\pi_2^*=(d'_1,d'_2,\ldots,d'_{n-k})$.

Assume first $d_{n-k}^*\geq 2$. In this case, either $\pi_1^*=(4,2^{(n-k-1)})$ or $\pi_1^*=(3^{(2)},2^{(n-k-2)})$.

If $\pi_1^*=(4,2^{(n-k-1)})$, then either $\pi_2^*=(5,2^{(n-k-2)},1)$ or $\pi_2^*=(4,3,2^{(n-k-3)},1)$. If $\pi_1^*=(3^{(2)},2^{(n-k-2)})$, then $\pi_2^*=(4,2^{(n-k-1)})$ or $\pi_2^*=(3^{(3)},2^{(n-k-4)},1)$ or $\pi_2^*=(4,3,2^{(n-k-3)},1)$. In all cases, by Theorem 2.3, $B_M^*(\pi_1)$ contains a surprising vertex, and so the result follows from (2.4).

Now, suppose that $d^*_{n-k} = 1$.

Case 1. $d^*_{n-k} = 1$ and $d^*_2 = 2$.

In this case, $\pi^*_1 = \left(t+4, 2^{(n-k-t-1)}, 1^{(t)}\right)$, where $t \geq 1$. Then, either $\pi^*_2 = \left(t+5, 2^{(n-k-t-2)}, 1^{(t+1)}\right)$ or $\pi^*_2 = \left(t+4, 3, 2^{(n-k-t-3)}, 1^{(t+1)}\right)$. By Theorem 2.3, $\mathcal{R}(B^*_M(\pi_1)) \cong B_2$.

If $\pi^*_2 = (t+4, 3, 2^{(n-k-t-3)}, 1^{(t+1)})$, since $v^*_5 \in N_{B^*_M(\pi_1)}(v^*_4) \setminus \left(N_{B^*_M(\pi_1)}v^*_2 \cup \{v^*_2\}\right)$ and $v^*_5 \notin V(P_{v^*_2 v^*_4})$, it is easy to see that v^*_5 is a surprising vertex of $B^*_M(\pi_1)$.

If $\pi^*_2 = (t+5, 2^{(n-k-t-2)}, 1^{(t+1)})$, then $p = 1$, $q \geq 6$ and $d^*_q = 2$. By the structure of $B^*_M(\pi_1)$, there exists a vertex v^*_t $(t > q)$ such that $v^*_t \in N_{B^*_M(\pi_1)}(v^*_q) \setminus \left(N_{B^*_M(\pi_1)}(v^*_p) \cup \{v^*_p\}\right)$ and $v^*_t \notin V(P_{v^*_p v^*_q})$. In this case, v^*_t is also a surprising vertex of $B^*_M(\pi_1)$.

In both cases, the result follows from (2.4).

Case 2. $d^*_{n-k} = 1$ and $d^*_1 \geq d^*_2 \geq 3$.

By Theorem 2.3, $\mathcal{R}(B^*_M(\pi_1)) \cong B_1$. If $q \geq 5$, then $d^*_q = (d'_q)^* + 1 \geq 2$. If $3 \leq q \leq 4$, since $B^*_M(\pi_2)$ is a bicyclic graph, $d^*_q = (d'_q)^* + 1 \geq 3$. In both cases, by the structure of $B^*_M(\pi_1)$, there exists vertex v^*_t $(t > q)$ such that $v^*_t \in N_{B^*_M(\pi_1)}(v^*_q) \setminus \left(N_{B^*_M(\pi_1)}(v^*_p) \cup \{v^*_p\}\right)$ and $v^*_t \notin V(P_{v^*_p v^*_q})$, namely, v^*_t is a surprising vertex of $B^*_M(\pi_1)$. By (2.4), the result follows. Thus, we may suppose that $q = 2$, and hence $p = 1$ in the sequel.

If $q = 2$ and $d^*_2 \geq 4$, since $\mathcal{R}(B^*_M(\pi_1)) \cong B_1$, $B^*_M(\pi_1)$ also contains a surprising vertex. Otherwise, $q = 2$ and $d^*_2 = 3$, and hence $(d'_2)^* = 2$. In this case, $\pi^*_1 = (t+3, 3, 2^{(n-k-t-2)}, 1^{(t)})$ and $\pi^*_2 = (t+4, 2^{(n-k-t-1)}, 1^{(t)})$, where $t \geq 1$. By Theorem 2.3, $\mathcal{R}(B^*_M(\pi_1)) \cong B_1$ and $\mathcal{R}(B^*_M(\pi_2)) \cong B_2$. Then, $\mathcal{R}(B^*_M(\pi_1))$ is obtained from B_1 by attaching t paths, say P_{s_1}, P_{s_2}, ..., P_{s_t}, of almost equal lengths to one vertex of degree three of B_1, where $s_1 \geq s_2 \geq \cdots \geq s_t \geq 1$ and $s_1 \geq 2$.

If $s_1 \geq 3$, since $t \geq 1$, $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$ and $f(x,y)$ is good escalating, we have

$$\begin{aligned}
&M_f\left(K_k \vee B^*_M(\pi_2)\right) - M_f\left(K_k \vee B^*_M(\pi_1)\right)\\
&= k\big(f(n-1,t+4) + f(n-1,2) - f(n-1,t+3) - f(n-1,3)\big) + (t+4)f(t+4+k,2+k)\\
&\quad + f(2+k,2+k) - (t+2)f(t+3+k,2+k) - f(t+3+k,3+k) - 2f(3+k,2+k)\\
&> (t+1)f(t+4+k,2+k) + f(t+3+k,2+k) + f(3+k,2+k) + f(t+3+k,3+k)\\
&\quad + f(2+k,2+k) - (t+2)f(t+3+k,2+k) - f(t+3+k,3+k) - 2f(3+k,2+k)\\
&= (t+1)f(t+4+k,2+k) + f(2+k,2+k) - (t+1)f(t+3+k,2+k) - f(3+k,2+k)\\
&> f(t+4+k,2+k) + f(2+k,2+k) - f(t+3+k,2+k) - f(3+k,2+k) \geq 0.
\end{aligned}$$

Otherwise, $s_1 = 2$. We may suppose that $(s_1, s_2, \ldots, s_t) = (2^{(m)}, 1^{(t-m)})$, where $1 \leq m \leq t$. In this case, since $m \geq 1$, $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$ and $f(x,y)$ is good escalating, we have

$$\begin{aligned}
&M_f\left(K_k \vee B^*_M(\pi_2)\right) - M_f\left(K_k \vee B^*_M(\pi_1)\right)\\
&= k\big(f(n-1,t+4) + f(n-1,2) - f(n-1,t+3) - f(n-1,3)\big) + (m+3)f(t+k+4,k+2)\\
&\quad + (t+1-m)f(t+k+4,k+1) + 2f(k+2,k+2) - (m+2)f(t+k+3,k+2) - f(t+k+3,k+3)\\
&\quad - 2f(k+3,k+2) - (t-m)f(t+k+3,k+1) - f(k+2,k+1)\\
&> (m+1)f(t+k+4,k+2) + (t-m)f(t+k+4,k+1) + f(t+k+3,k+2) + f(t+k+3,k+3)\\
&\quad + f(k+3,k+1) + 2f(k+2,k+2) - (m+2)f(t+k+3,k+2) - f(t+k+3,k+3)\\
&\quad - 2f(k+3,k+2) - (t-m)f(t+k+3,k+1) - f(k+2,k+1)\\
&= (m+1)f(t+k+4,k+2) + (t-m)f(t+k+4,k+1) + f(k+3,k+1) + 2f(k+2,k+2)\\
&\quad - (m+1)f(t+k+3,k+2) - 2f(k+3,k+2) - (t-m)f(t+k+3,k+1) - f(k+2,k+1)\\
&> (m+1)\big(f(t+k+4,k+2) - f(t+k+3,k+2)\big) + (t-m)\big(f(t+k+4,k+1) - f(t+k+3,k+1)\big)\\
&\quad - 2\big(f(k+3,k+2) - f(k+2,k+2)\big)\\
&\geq 2\big(f(t+k+4,k+2) + f(k+2,k+2) - f(t+k+3,k+2) - f(k+3,k+2)\big) \geq 0. \quad \blacksquare
\end{aligned}$$

2.3. Some applications

The majorization theorem has important application in dealing with extremal ordering problem of topological and spectral invariants (see [8,18,28–30]). In this subsection, we list some known topological indices that satisfy our new results.

Proposition 2.1. *If $\alpha > 1$, then $Z_\alpha(G)$ and $\chi_\alpha(G)$ are good escalating.*

Proof. Here, we only prove $Z_\alpha(G)$, as $\chi_\alpha(G)$ can be proved similarly. By (1.1), we may define $f(x,y) = (x+y-2)^\alpha$ with $\min\{x,y\} \geq 1$ and $\max\{x,y\} \geq 2$.

Since $\alpha > 1, f(x,y) = (x+y-2)^{\alpha}$ is escalating by Remark 1.1. Moreover, since $x+y \geq 3$, $\frac{\partial f(x,y)}{\partial x} = \alpha(x+y-2)^{\alpha-1} > 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} = \alpha(\alpha-1)(x+y-2)^{\alpha-2} \geq 0$.

When $x_1 \geq y_1 \geq 2$ and $x_2 \geq y_2 \geq 1$, it is easy to see that $f(x_1+1,x_2)+f(x_1+1,y_2)+f(x_1+1,y_1-1)-f(x_1,x_2)-f(y_1,y_2)-f(x_1,y_1) > f(x_1+1,y_2)-f(y_1,y_2) > 0$, and thus $Z_\alpha(G)$ is a good escalating function for $\alpha > 1$. ■

Similarly with Proposition 2.1, we can show the following:

Proposition 2.2. *$M_2(G)$ is good escalating.*

The following topological indices satisfy our new results.
(*i*) If either $\alpha > 1$ or $\alpha < 0$, then $Z_\alpha(G)$ and $\chi_\alpha(G)$ are escalating [18], which implies that the extremal graphs with maximum $Z_\alpha(G)$ (resp., $\chi_\alpha(G)$) satisfy Theorems 2.2 and 2.3 and Corollary 2.1;
(*ii*) If $\alpha \neq 0$, then $W_\alpha(G)$ is escalating [18], and so the extremal graphs with maximum $W_\alpha(G)$ satisfy Theorems 2.2 and 2.3 and Corollary 2.1;
(*iii*) If $0 < \alpha < 1$, then $Z_\alpha(G)$ and $\chi_\alpha(G)$ are de-escalating [18]. This implies that the extremal graphs with minimum $Z_\alpha(G)$ (resp., $\chi_\alpha(G)$) satisfy Theorems 2.2 and 2.3 and Corollary 2.1;
(*iv*) It has been shown that the Atom–Bond connectivity index of G is de-escalating [34], and thus the extremal graphs with minimum Atom–Bond connectivity index satisfy Theorems 2.2 and 2.3 and Corollary 2.1.
(*v*) By Proposition 2.1, $Z_\alpha(G)$ and $\chi_\alpha(G)$ are good escalating for $\alpha > 1$. Thus, if $\alpha > 1$, then $Z_\alpha(G)$ and $\chi_\alpha(G)$ satisfy Theorem 2.7.
(*vi*) By Proposition 2.2, $M_2(G)$ is good escalating, and thus $M_2(G)$ satisfy Theorem 2.7.
(*vii*) If $\alpha > 1$, then $R^0_\alpha(G)$ is a strictly increasing convex function on $x \geq 1$ [28], and thus $R^0_\alpha(G)$ satisfy Theorem 2.6.

3. Unified extremal maximum graph of k-apex unicyclic graphs and k-apex trees

In this section, we will determine the unique unified extremal maximum graph of k-apex unicyclic graphs and k-apex trees with n vertices, respectively, for $k \geq 1$ and $n \geq k+3$ (See Remark 3.2). For this aim, we will introduce the following concepts:

Definition 3.1. For a graph category $\mathcal{G}$, we say that G is an **extremal maximum graph** of $\mathcal{G}$, if G satisfies all of the following items:

(i) $\Theta(G,\beta)$ is largest in $\mathcal{G}$ for $\beta \geq 0$;
(ii) $Z_\alpha(G)$ and $\chi_\alpha(G)$ are largest in $\mathcal{G}$ for $\alpha > 1$;
(iii) $H_f(G)$ is largest in $\mathcal{G}$, where $f(x)$ is a strictly increasing convex function on $x \geq 1$;
(iv) $\prod_2(G)$ and $M_2(G)$ are largest in $\mathcal{G}$.

Definition 3.2. For $k \geq 1$, a connected graph G is called a k-**generalized quasi** c-**cyclic graph**, if there exists a subset $V_k \subseteq V(G)$ with cardinality k such that $G - V_k$ is a c-cyclic graph but for every subset V_{k-1} of cardinality $k-1$ of $V(G)$, the graph $G - V_{k-1}$ is not c-cyclic. The vertex set V_k will be called a k-**quasi vertex set** of G.

Denote by $\mathcal{Z}_{n,c;k}$ the class of k-generalized quasi c-cyclic graphs with n vertices. A k-generalized quasi 0-cyclic (resp., 1-cyclic) graph is also called k-generalized quasi-tree [27] (resp., quasi-unicyclic graph [9]). Two of the present authors and their cooperator [14] pointed out that it allows for a graph to be k-generalized quasi-unicyclic graph for several values of k. Hereafter, let $\mathbb{T}^k_n$ (resp., $\mathbb{U}^k_n$) be the class of k-apex trees (resp., k-apex unicyclic graphs) with n vertices, and let $\mathcal{U}^k_n$ and $\mathcal{T}^k_n$ be the class of k-generalized quasi-unicyclic graphs and k-generalized quasi-trees with n vertices, respectively. It is not difficult to check that k-generalized quasi-trees and k-apex trees are two equivalent concepts. Thus, $\mathbb{U}^k_n \subseteq \mathcal{U}^k_n = \mathcal{Z}_{n,1;k}$ and $\mathbb{T}^k_n = \mathcal{T}^k_n = \mathcal{Z}_{n,0;k}$.

In what follows, we will prove that the unique extremal maximum graph of $\mathcal{U}^k_n$ (resp., $\mathcal{T}^k_n$) is also a k-apex unicyclic graph (resp., k-apex tree), and thus it is also the unique extremal maximum graph of k-apex unicyclic graphs (resp., k-apex trees).

Lemma 3.1. *Let H be a unicyclic graph (resp., tree) with $n-k$ vertices. Then $K_k \vee H$ is a k-apex unicyclic graph (resp. k-apex tree) with n vertices, where $k \geq 1$ and $n \geq k+3$.*

Proof. Here, we only prove the case of H being a tree, as the case of H being unicyclic has been shown in Proposition 1.1 of [14]. Denote by $G = K_k \vee H$. Then, $|V(H)| = n-k \geq 3$. By contradiction, we assume that $G \notin \mathbb{T}^k_n$. According to Definition 1.2 and H being a tree, there exists $W \subset V(G)$ such that $H_1 = G - W$ is a tree, where $0 \leq |W| = s \leq k-1$. For convenience, we suppose that $|W \cap V(K_k)| = s_1$ and $S_2 = W \cap V(H)$. Then, $s = s_1 + |S_2|$ and $H_1 = K_{k-s_1} \vee (H - S_2)$. Since $K_{k-s_1} \subseteq H_1$ and H_1 is a tree, we have $k-2 \leq s_1 \leq k-1$.

If $s_1 = k-2$, then $0 \leq |S_2| \leq 1$ and so $H - S_2$ has at least one vertex. Combining this with $K_{k-s_1} = K_2$, we can conclude that $K_3 \subseteq H_1$, a contradiction. Otherwise, $s_1 = k-1$. Then $|S_2| = 0$ and so $K_1 \vee H = H_1$, contrary with the fact that both H and H_1 are trees. ■

Suppose that $k \geq 1$ and $G \in \mathcal{Z}_{n,c;k}$. Then, there exists a k-quasi vertex set V_k of G such that $H = G - V_k$ is a c-cyclic graph. Let $G_1 = K_k \vee H$. Let $\Phi(G)$ be a graph invariant defined on connected G such that $\Phi(G) > \Phi(G')$ holds for each proper connected subgraph G' of G. If $d_G(z) < n-1$ for some vertex z of V_k, then $G \subset G_1$ and so $\Phi(G) < \Phi(G_1)$. Combining this with Lemma 3.1, we obtain

Lemma 3.2. *Let $G \in \mathcal{Z}_{n,c;k}$, and z be a vertex in a k-quasi vertex set of G, where $k \geq 1$ and $n \geq k+3$. Let $\Phi(G)$ be a graph invariant defined on connected graphs such that $\Phi(G) > \Phi(G')$ holds for each proper connected subgraph G' of G. If $c \in \{0, 1\}$ and $\Phi(G)$ is maximum, then $d_G(z) = n-1$.*

Let $S_n^{(0)}$ be the star with n vertices, and $S_n^{(1)}$ be the unicyclic graph obtained by adding an edge between two pendant vertices of $S_n^{(0)}$.

Theorem 3.1. *For $c \in \{0, 1\}$, $K_k \vee S_{n-k}^{(c)}$ is the unique extremal maximum graph among all k-generalized c-cyclic graphs with n vertices, where $k \geq 1$ and $n \geq k+3$.*

Proof. Let G be an extremal maximum graph among all k-generalized c-cyclic graphs with n vertices. If $\Phi(G)$ belongs to those graph invariants specified in Definition 3.1, then $\Phi(G) > \Phi(G')$ holds for each proper connected subgraph G' of G. By Lemma 3.2, G is a k-cone c-cyclic graph.

Denote by $\pi_1 = \left((n-1)^{(k+1)}, (k+1)^{(n-k-1)}\right)$ and $\pi_2 = \left((n-1)^{(k+1)}, (k+2)^{(2)}, (k+1)^{(n-k-3)}\right)$. Then, $\mathscr{T}(\pi_1, k) = \left\{K_k \vee S_{n-k}^{(0)}\right\}$ and $\mathscr{U}(\pi_2, k) = \left\{K_k \vee S_{n-k}^{(1)}\right\}$. Since π_{1+c} uniquely maximizes in the majorization relation $\trianglelefteq$ among all those degree sequences of $\Gamma(\pi_{1+c}, k; c)$ for $c \in \{0, 1\}$, the result follows from Theorems 2.5–2.7 and Proposition 2.1. ■

Remark 3.1. By Theorems 2.6 and 3.1, $K_k \vee S_{n-k}^{(c)}$ is the unique extremal maximum graph of $R_\alpha^0(G)$ for $\alpha > 1$.

Remark 3.2. By Lemma 3.1, $K_k \vee S_{n-k}^{(0)} \in \mathbb{T}_n^k$ and $K_k \vee S_{n-k}^{(1)} \in \mathbb{U}_n^k$. Since $\mathbb{T}_n^k = \mathcal{T}_n^k$ and $\mathbb{U}_n^k \subseteq \mathcal{U}_n^k$, $K_k \vee S_{n-k}^{(0)}$ (resp., $K_k \vee S_{n-k}^{(1)}$) is also the unique extremal graph of $\mathbb{T}_n^k$ (resp., $\mathbb{U}_n^k$) for $k \geq 1$ and $n \geq k+3$.

4. Unified extremal minimum graphs of k-apex unicyclic graphs and k-apex trees

Throughout this section, we define $\Phi(G)$ as a graph invariant of $\left\{M_2(G), H_f(G), \prod_2(G)\right\}$, where $f(x)$ is a strictly increasing convex function on $x \geq 1$. Let $G[V_1]$ be a subgraph of G induced by the vertex set V_1. Our goal in this section is to determine the unified extremal minimum graphs of k-apex unicyclic graphs and k-apex trees with n vertices, respectively (See Remarks 4.2–4.5).

Definition 4.1. For a graph category $\mathcal{G}$, we say that G is an **extremal minimum graph** of $\mathcal{G}$, if G satisfies all of the following items:

(i) $H_f(G)$ is smallest in $\mathcal{G}$ when $f(x)$ is a strictly increasing convex function on $x \geq 1$;
(ii) $\prod_2(G)$ and $M_2(G)$ are smallest in $\mathcal{G}$.

If G is a connected graph with at least one cycle, then $\mathcal{R}(G)$ is unique and G is obtained from $\mathcal{R}(G)$ by attaching some rooted trees to the vertices of $\mathcal{R}(G)$. In the coming discussion, we use the notation T_v to denote a rooted tree with root $v \in V(\mathcal{R}(G))$, and we agree that T_v includes the root v. Furthermore, if $|V(T_v)| \geq 2$, then T_v is called a *nontrivial rooted* tree.

Lemma 4.1. *Let $G \in \mathcal{Z}_{n,c;k}$, where $c \in \{0, 1\}$ and $k \geq 2$. If V_k is a k-quasi vertex set of G, then for any nontrivial rooted tree T_{v_0}, either $V(T_{v_0}) \cap V_k = \emptyset$ or $V(T_{v_0}) \subseteq V_k$.*

Proof. Let $H = G - V_k$. Then, H is a c-cyclic graph. Suppose that $V(T_{v_0}) \cap V_k \neq \emptyset$. If $v_0 \notin V_k$, then $v_0 \in V(H)$ and hence there exists W such that $G - W$ is also a c-cyclic graph and $|W| = k-1$, where $|W \cap V(T_{v_0})| = |V_k \cap V(T_{v_0})| - 1$. This is contrary to $G \in \mathcal{Z}_{n,c;k}$, so $v_0 \in V_k$. Combining this with H being a c-cyclic graph, we can conclude that $V(T_{v_0}) \subseteq V_k$, as each vertex of $T_{v_0} - v_0$ is disconnected with any vertex of $G - V(T_{v_0})$. ■

A *pendant path* is a path with exactly one pendant vertex.

Lemma 4.2. *Let w_0 be a vertex of a rooted tree T_{v_0}, $P = w_0 w_{11} w_{12} \cdots w_{1j_1}$ and $P' = w_0 w_{21} w_{22} \cdots w_{2j_2}$ be two pendant paths of G, where $v_0 = w_0$ is permitted and $j_1 \geq j_2 \geq 1$. If $G^* = G - w_0 w_{21} + w_{1j_1} w_{21}$, then $\Phi(G) > \Phi(G^*)$. Furthermore, if $G \in \mathcal{Z}_{n,c;k}$ and $k \geq 2$, then $G^* \in \mathcal{Z}_{n,c;k}$.*

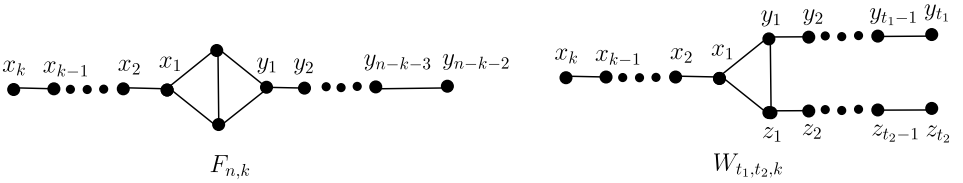


Fig. 4.1. The graphs $F_{n,k}$ and $W_{t_1,t_2,k}$.

Proof. By the definition, $v_0 \in \mathcal{R}(G)$, $d_G(w_0) \geq 3$ and $\{w_{1j_1}, w_{2j_2}\}$ are two pendant vertices of G. From the definition of G and G^*, the difference between degree sequences of G and G^* is $(d_G(w_0), 1)$ and $(d_G(w_0)-1, 2)$, and thus the degree sequence of G^* is majorized by that of G. By Theorem 2.6, we have $\prod_2(G) > \prod_2(G^*)$ and $H_f(G) > H_f(G^*)$.

Due to the choice of w_0, there exists $u_0 \in N_G(w_0) \setminus \{w_{21}, w_{11}\}$ such that $d_G(u_0) \geq 2$ and thus

$$\sum_{u\in N_G(w_0)\setminus\{w_{21},w_{11}\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) \geq d_G(w_0) - 1. \tag{4.1}$$

If $j_2 \geq 2$, then $M_2(G) - M_2(G^*) = \sum_{u\in N_G(w_0)\setminus\{w_{21},w_{11}\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) + 2d_G(w_0) - 4 \geq 3d_G(w_0) - 5 > 0$ by (4.1).

If $j_1 \geq 2$ and $j_2 = 1$, then $M_2(G) - M_2(G^*) = \sum_{u\in N_G(w_0)\setminus\{w_{21},w_{11}\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) + d_G(w_0) - 2 \geq 2d_G(w_0) - 3 > 0$ by (4.1).

If $j_1 = 1 = j_2$, then $M_2(G) - M_2(G^*) = \sum_{u\in N_G(w_0)\setminus\{w_{21},w_{11}\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) \geq d_G(w_0) - 1 > 0$ by (4.1).

It remains to prove the 'Furthermore' part. By Lemma 4.1, either $V(T_{v_0}) \subseteq V_k$ or $V(T_{v_0}) \cap V_k = \emptyset$. In both cases, $G^* - V_k$ is also a c-cyclic graph. We assume that $G^* - W$ is a c-cyclic graph for some vertex set W with $|W| = k-1$. No matter $V(T_{v_0}) \cap W = \emptyset$ or $V(T_{v_0}) \cap W \neq \emptyset$, $G - W$ is also a c-cyclic graph, contrary to $G \in \mathcal{Z}_{n,c;k}$. Thus, $G^* \in \mathcal{Z}_{n,c;k}$. ■

Lemma 4.3. *Suppose that $T_{w_0} = w_0w_1w_2\cdots w_q$ is a pendant path of G and $v_0w_0 \in E(\mathcal{R}(G))$. If $G^* = G - v_0w_0 + w_qv_0$ and $q \geq 1$, then $\Phi(G) > \Phi(G^*)$.*

Proof. Since T_{w_0} is a rooted tree, $w_0 \in V(\mathcal{R}(G))$ and thus $d_G(w_0) \geq 3$. From the definition of G and G^*, the difference between degree sequences of G and G^* is $(d_G(w_0), 1)$ and $(d_G(w_0)-1, 2)$, and thus the degree sequence of G^* is majorized by that of G. By Theorem 2.6, we have $\prod_2(G) > \prod_2(G^*)$ and $H_f(G) > H_f(G^*)$.

Recall that $w_0 \in V(\mathcal{R}(G))$. Thus, there exists $x_0 \in \big(N_G(w_0) \cap V(\mathcal{R}(G))\big) \setminus \{v_0\}$, and so

$$\sum_{u\in N_G(w_0)\setminus\{w_1,v_0\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) \geq d_G(w_0) - 1. \tag{4.2}$$

If $q \geq 2$, then $M_2(G) - M_2(G^*) = \sum_{u\in N_G(w_0)\setminus\{w_1,v_0\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) + (d_G(w_0)-2)d_G(v_0) \geq (d_G(w_0)-2)d_G(v_0) + d_G(w_0) - 1 > 0$ by (4.2).

If $q = 1$, then $M_2(G) - M_2(G^*) = \sum_{u\in N_G(w_0)\setminus\{w_1,v_0\}} \big(d_G(w_0)d_G(u) - (d_G(w_0)-1)d_G(u)\big) + \big(d_G(w_0)-2\big)\big(d_G(v_0)-1\big) \geq \big(d_G(w_0)-2\big)\big(d_G(v_0)-1\big) + d_G(w_0) - 1 > 0$ by (4.2). ■

Corollary 4.1. *Let G be a c-cyclic graph with n vertices and p pendant vertices. If $p \geq 1$ and $c \geq 1$, then there exists a c-cyclic graph G^* with n vertices and $p-1$ pendant vertices such that $\Phi(G) > \Phi(G^*)$.*

Proof. Since $c \geq 1$ and $p \geq 1$, G contains at least one rooted tree. Now, the result follows from Lemmas 4.2 and 4.3. ■

Hereafter, denote by $F_{n,k}$ and $W_{t_1,t_2,k}$ the graphs as shown in Fig. 4.1. Let

$$\mathbb{W}_{n,k} = \big\{W_{t_1,t_2,k} : \text{ where } t_1 \geq t_2 \geq k, \text{ and } t_1 + t_2 = n - k\big\}. \tag{4.3}$$

When $k \geq 2$ and $n \geq 2k+2$, it is easily checked that $F_{n,k} \in \mathcal{U}_n^k$ and

$$\prod_2(F_{n,k}) = 3^{12}4^{n-6},\ H_f(F_{n,k}) = 4f(3) + 2f(1) + (n-6)f(2), \text{ and } M_2(F_{n,k}) \leq 4n + 29. \tag{4.4}$$

Lemma 4.4. *Let G be a tricyclic graph with $n \geq 2k+2$ vertices. If $k \geq 2$ and G contains no pendant vertex, then $\Phi(G) > \Phi(F_{n,k})$.*

Proof. Suppose that G contains exactly p pendant vertices and the degree sequence of G is $\pi = (d_1, d_2, \ldots, d_n)$, where $d_G(v_i) = d_i$ for $1 \leq i \leq n$. Since $d_n \geq 2$, by Proposition 17 of [13] we have

$$\pi \in \big\{(6, 2^{(n-1)}), (5, 3, 2^{(n-2)}), (4^{(2)}, 2^{(n-2)}), (4, 3^{(2)}, 2^{(n-3)}), (3^{(4)}, 2^{(n-4)})\big\}.$$

Denote by $\pi_1 = (3^{(4)}, 2^{(n-4)})$. Then, $\pi_1 \lhd \pi$, and thus

$$H_f(G) \geq 4f(3) + (n-4)f(2) > H_f(F_{n,k}) \quad \text{and} \quad \prod\nolimits_2(G) \geq 3^{12}4^{n-4} > \prod\nolimits_2(F_{n,k})$$

by Theorem 2.6 and (4.4).

If $\pi \in \left\{(6, 2^{(n-1)}), (5, 3, 2^{(n-2)}), (4^{(2)}, 2^{(n-2)})\right\}$, then no matter $v_1v_2 \in E(G)$ or not, it is easily checked that $M_2(G) \geq 4n + 40 > M_2(F_{n,k})$ by (4.4).

If $\pi = (4, 3^{(2)}, 2^{(n-3)})$, then $3K_1 \subseteq G[\{v_1, v_2, v_3\}] \subseteq K_3$, and so $M_2(G) \geq 4n + 36 > M_2(F_{n,k})$.

If $\pi = \pi_1$, then $4K_1 \subseteq G[\{v_1, v_2, v_3, v_4\}] \subset K_4$, and thus $M_2(G) \geq 4n + 32 > M_2(F_{n,k})$. ■

Lemma 4.5. *Let G be a c-cyclic graph with n vertices. If $c \geq 3$, $n \geq 2k+2$ and $k \geq 2$, then $\Phi(G) > \Phi(F_{n,k})$.*

Proof. Since $c \geq 3$, there exists one edge uv of some cycle of G such that $G - uv$ is a $(c-1)$-cyclic graph with n vertices. Recall that $\Phi(G)$ is a graph invariant of $\left\{M_2(G), H_f(G), \prod\nolimits_2(G)\right\}$, where $f(x)$ is a strictly increasing convex function on $x \geq 1$. Thus, $\Phi(G) > \Phi(G - uv)$. This implies that it suffices to show that $\Phi(G) > \Phi(F_{n,k})$ in the case $c = 3$. Now, the result follows from Lemma 4.4 and Corollary 4.1. ■

4.1. Extremal minimum graph of $\mathcal{U}_n^k$

Throughout this subsection, we may suppose that G_0 **is an extremal minimum graph** of $\mathcal{U}_n^k$, where $k \geq 2$ and $n \geq 2k+2$.

Lemma 4.6. *If $k \geq 2$, then G_0 is a bicyclic graph which satisfies the following items:*

(i) Each nontrivial rooted tree of G_0 is a pendant path;

(ii) For any k-quasi vertex set V_k of G_0, $G_0[V_k]$ is a nontrivial pendant path of G_0;

(iii) If $\mathcal{R}(G_0) - v_0$ is a unicyclic graph, then T_{v_0} is a nontrivial pendant path with $|V(T_{v_0})| \geq k$.

Proof. Since $F_{n,k} \in \mathcal{U}_n^k$ and $k \geq 2$, by Lemma 4.5, G_0 is either unicyclic or bicyclic. We assume that G_0 is a unicyclic graph with unique cycle C_g. Then, G_0 is obtained from C_g by attaching some rooted trees to these vertices of C_g, and $U = G_0 - V_k$ is also a unicyclic graph with the unique cycle C_g. This implies that V_k comes from these rooted trees and so there exists W with $|W| = k-1$ (as $k \geq 2$) such that $G - W$ is also a unicyclic graph, contrary with $G_0 \in \mathcal{U}_n^k$. Thus, G_0 is a bicyclic graph.

Now, we assume that T_{v_0} is a nontrivial rooted tree with at least two pendant vertices. By Lemma 4.2, there exists another $G^* \in \mathcal{U}_n^k$ such that $\Phi(G_0) > \Phi(G^*)$, contrary to the choice of G_0. Thus, each rooted tree of G_0 is a pendant path, and so (i) holds.

Let V_k be a k-quasi vertex set of G_0, and let $S = V_k \cap V(\mathcal{R}(G_0))$. Since $U = G_0 - V_k$ is a unicyclic graph and G_0 is a bicyclic graph, $S \neq \emptyset$ and $G_0[S]$ is a path. If $|S| \geq 2$, then there exists W with $|W| = k-1$ such that $G_0 - W$ is also a unicyclic graph, where $|W \cap V(\mathcal{R}(G_0))| = |S| - 1$, contrary to $G_0 \in \mathcal{U}_n^k$. Thus, $|S| = 1$ and so $G_0[V_k]$ is a nontrivial rooted tree of G_0, as $k \geq 2$. Combining this with (i), we get (ii).

Now, we turn to prove (iii). Let T_{v_0} be a rooted tree of G_0, where $G_0 - v_0$ is a unicyclic graph. We assume that $t = |V(T_{v_0})|$ and $t \leq k-1$. Since $G_0 \in \mathcal{U}_n^k$ and $G_0 - v_0$ is a unicyclic graph, we have $t \leq k-2$. Since $G_0[V_k]$ is a nontrivial pendant path by (ii), by Lemma 4.1 we may suppose that $V(T_{v_0}) \cap V_k = \emptyset$, as $v_0 \in V(\mathcal{R}(G_0))$. Thus, there exists $W \subseteq V(G_0)$ with $|W| = k-1$, $V(T_{v_0}) \subseteq W$ and $|W \cap V_k| = k - 1 - t$ such that $G_0 - W$ is a unicyclic graph, which contradicts $G_0 \in \mathcal{U}_n^k$. Thus, (iii) holds. ■

Theorem 4.1. *If $k \geq 2$ and $n \geq 2k+2$, then $F_{n,k}$ is the extremal minimum graph of $\mathcal{U}_n^k$.*

Proof. It is sufficient to prove $G_0 = F_{n,k}$. By Lemma 4.6, $\mathcal{R}(G_0)$ is also a bicyclic graph, and thus $\mathcal{R}(G_0) \in \left\{W_1, W_2, W_3\right\}$ (See Fig. 4.2). Denote by $\pi_0 = \left(3^{(4)}, 2^{(n-6)}, 1^{(2)}\right)$. By contradiction, we assume that $G_0 \neq F_{n,k}$. In what follows, we shall show that $\Phi(G_0) > \Phi(F_{n,k})$ to get a contradiction to the choice of G_0 and $F_{n,k} \in \mathcal{U}_n^k$.

Case 1. $\mathcal{R}(G_0) = W_1$. By Lemma 4.6(iii), G_0 contains at least $s + t - 2$ rooted trees, where each rooted tree is a pendant path with at least k vertices. Since each rooted tree of G_0 is a path, via repeated application of Lemma 4.3, there exists a bicyclic graph G_1 with degree sequence $\pi_1 = (4, 3^{(s+t-2)}, 2^{(n+3-2s-2t)}, 1^{(s+t-2)})$ such that $\Phi(G_0) \geq \Phi(G_1)$, where the equality holds if and only if $d_{G_0}(v_1) = 4$ (see Fig. 4.2). Since $s + t \geq 6$, we have $\pi_0 \lhd \pi_1$ and thus $H_f(G_1) > H_f(F_{n,k})$ and $\prod\nolimits_2(G_1) > \prod\nolimits_2(F_{n,k})$ by Theorem 2.6.

If $k \geq 3$, since $s + t \geq 6$ and Lemma 4.6(iii), then

$M_2(G_1) \geq 4\times3\times3+3\times3\times(s+t-4)+4\times2+3\times2+2\times3\times(s+t-2)+2\times(s+t-2)+2\times2\times\left(n+1-s-t-1-2(s+t-2)\right) = 4n + 5(s+t) + 14 \geq 4n + 44 > M_2(F_{n,k})$ by (4.4).

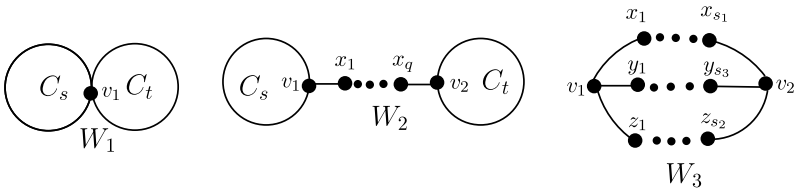


Fig. 4.2. The bicyclic graphs W_1, W_2 and W_3.

If $k = 2$, since $s + t \geq 6$ and Lemma 4.6(iii), then

$M_2(G_1) \geq 4 \times 3 \times 3 + 3 \times 3 \times (s+t-4) + 4 \times 2 + 3 \times 2 + 3 \times (s+t-2) + 2 \times 2 \times \big(n+1-s-t-1-(s+t-2)\big) = 4(n+s+t+4) \geq 4n+40 > M_2(F_{n,k})$ by (4.4).

Case 2. $\mathcal{R}(G_0) = W_2$. By Lemma 4.6(iii), G_0 contains at least $s+t-2$ rooted trees, where each rooted tree is a pendant path with at least k vertices. By applying several times of Lemma 4.3, there exists a bicyclic graph G_2 with degree sequence $\pi_2 = \big(3^{(s+t)}, 2^{(n+2-2s-2t)}, 1^{(s+t-2)}\big)$ such that $\Phi(G_0) \geq \Phi(G_2)$, where the equality holds if and only if $d_{G_0}(v_1) = d_{G_0}(v_2) = 3$ and either $d_{G_0}(x_1) = d_{G_0}(x_2) = \cdots = d_{G_0}(x_q) = 2$ or $q = 0$ (see Fig. 4.2). Since $s + t \geq 6$, we have $\pi_0 \lhd \pi_2$. Thus $H_f(G_2) > H_f(F_{n,k})$ and $\prod_2(G_2) > \prod_2(F_{n,k})$ by Theorem 2.6.

If $k \geq 3$, since $s + t \geq 6$ and Lemma 4.6(iii), then

$M_2(G_2) \geq 3 \times 3 \times (s+t) + 3 \times 2 \times 2 + 3 \times 2 \times (s+t-2) + 2 \times (s+t-2) + 2 \times 2 \times (n+1-s-t-2-2(s+t-2)) = 4n + 5(s+t) + 8 \geq 4n + 38 > M_2(F_{n,k})$ by (4.4).

If $k = 2$, since $s + t \geq 6$ and Lemma 4.6(iii), then $M_2(G_2) \geq 3 \times 3 \times (s+t) + 3 \times 2 \times 2 + 3 \times (s+t-2) + 2 \times 2 \times (n+1-s-t-2-(s+t-2)) = 4(n+s+t) + 10 \geq 4n + 34 > M_2(F_{n,k})$ by (4.4).

Case 3. $\mathcal{R}(G_0) = W_3$. By Lemma 4.6, G_0 contains at least $s_1 + s_2 + s_3$ rooted trees, where each rooted tree is a pendant path with at least k vertices. Suppose that $s_1 \geq s_2 \geq s_3$ and $\pi_3 = (3^{(s_1+s_2+s_3+2)}, 2^{(n-2-2s_1-2s_2-2s_3)}, 1^{(s_1+s_2+s_3)})$. By repeated application of Lemma 4.3, there exists a bicyclic graph G_3 with degree sequence π_3 such that $\Phi(G_0) \geq \Phi(G_3)$, where the equality holds if and only if $d_{G_0}(v_1) = d_{G_0}(v_2) = 3$ (see Fig. 4.2). If $\pi_3 = \pi_0$, then $s_1 = s_2 = 1$ and $s_3 = 0$, and so $\mathcal{R}(G_3) \cong B_1$ (see Fig. 2.1). By Lemma 4.6 and $\pi_3 = \pi_0$, $G_0 = F_{n,k}$ and hence the result already holds. Thus, we may suppose that $\pi_3 \neq \pi_0$. Since $s_1 + s_2 + s_3 \geq 2$ and $\pi_3 \neq \pi_0$, we have $\pi_0 \lhd \pi_3$ and thus $H_f(G_3) > H_f(F_{n,k})$ and $\prod_2(G_3) > \prod_2(F_{n,k})$ by Theorem 2.6.

Let v_1 and v_2 be the two vertices with degree three in W_3 (see Fig. 4.2), where $d_{G_0}(v_1) \geq d_{G_0}(v_2) \geq 3$. By Lemma 4.6(i), $3 \leq d_{G_0}(v_1) \leq 4$.

Subcase 3.1. $d_{G_0}(v_1) = 4$. Let x_1 be the vertex as shown in Fig. 4.2. Since $d_{G_0}(x_1) = 3$ by Lemma 4.6(iii), by the proof of Lemma 4.3, we have

$$M_2(G_0) \geq M_2(G_3) + \big(d_{G_0}(v_1) - 2\big)\big(d_{G_0}(x_1) - 1\big) + d_{G_0}(v_1) - 1 = M_2(G_3) + 7. \tag{4.5}$$

If $k \geq 3$, then since $s_1 + s_2 + s_3 \geq 2$, $M_2(G_3) \geq 3 \times 3 \times (s_1+s_2+s_3+1) + 3 \times 2 \times 4 + 3 \times 2 \times (s_1+s_2+s_3) + 2 \times (s_1+s_2+s_3) + 2 \times 2 \times \big(n+1-3(s_1+s_2+s_3)-5\big) = 4n + 17 + 5(s_1+s_2+s_3) \geq 4n+27$. Combining this with (4.4) and (4.5), we have $M_2(G_0) \geq 4n + 34 > M_2(F_{n,k})$.

Otherwise, $k = 2$. Since $s_1+s_2+s_3 \geq 2$, $M_2(G_3) \geq 3 \times 3 \times (s_1+s_2+s_3+1) + 3 \times 2 \times 4 + 3 \times (s_1+s_2+s_3) + 2 \times 2 \times (n+1-2(s_1+s_2+s_3)-5) = 4n+17+4(s_1+s_2+s_3) \geq 4n+25$. Combining this with (4.4) and (4.5), $M_2(G_0) \geq 4n+32 > M_2(F_{n,k})$.

Subcase 3.2. $d_{G_0}(v_1) = 3$. Then, $d_{G_0}(v_1) = 3 = d_{G_0}(v_2)$. Since $G_0 \neq F_{n,k}$ and Lemma 4.6(iii), we have $s_1 + s_2 + s_3 \geq 3$.

If $k \geq 3$, since $s_1 + s_2 + s_3 \geq 3$ and (4.4), $M_2(G_0) \geq 3 \times 3 \times (s_1+s_2+s_3+3) + 3 \times 2 \times (s_1+s_2+s_3) + 2 \times (s_1+s_2+s_3) + 2 \times 2 \times (n+1-3(s_1+s_2+s_3+1)) = 4n + 19 + 5(s_1+s_2+s_3) \geq 4n+34 > M_2(F_{n,k})$.

If $k = 2$, since $s_1 + s_2 + s_3 \geq 3$ and (4.4), $M_2(G_0) \geq 3 \times 3 \times (s_1+s_2+s_3+3) + 3 \times (s_1+s_2+s_3) + 2 \times 2 \times (n+1-2(s_1+s_2+s_3)-3) = 4n + 19 + 4(s_1+s_2+s_3) \geq 4n+31 > M_2(F_{n,k})$. ■

4.2. Extremal minimum graph of $\mathcal{T}_n^k$

Throughout this subsection, we may suppose that H_0 **is an extremal minimum graph of** $\mathcal{T}_n^k$, where $k \geq 2$ and $n \geq 3k$. Suppose that $R_0 \in \mathbb{W}_{n,k}$ (See (4.3)). By an elementary computation, it follows that

$$\prod_2(R_0) = 3^9 4^{n-6},\ H_f(R_0) = 3f(3) + 3f(1) + (n-6)f(2),\ \text{and}\ M_2(R_0) \leq 4n + 15. \tag{4.6}$$

Lemma 4.7 ([3]). *If G is a bicyclic graph with $n \geq 7$ vertices, then $M_2(G) \geq 4n + 16$, with equality if and only if G has two vertices of degree three and $n-2$ vertices of degree two, where the two vertices of degree three are not adjacent.*

Lemma 4.8. *Let G be a bicyclic graph with n vertices, where $n \geq 3k$. If G contains at least one pendant vertex and $k \geq 2$, then $\Phi(G) > \Phi(R_0)$.*

Proof. Since G is a bicyclic graph with $p \geq 1$ pendant vertices, by Corollary 4.1, it suffices to show the following claim:

Claim 1. *If G is a bicyclic graph with exactly one pendant vertex, then $\Phi(G) > \Phi(R_0)$.*

Proof of Claim 1. Suppose the degree sequence of G is π. Since G is a bicyclic graph, then $\mathcal{R}(G) \in \{W_1, W_2, W_3\}$ (see Fig. 4.2). By (4.6) and Lemma 4.7, we have $M_2(G) > M_2(R_0)$. Denote by $\pi_0 = (3^{(3)}, 2^{(n-6)}, 1^{(3)})$. Then, $R_0 \in \Gamma(\pi_0)$.

If $\mathcal{R}(G) = W_1$, then either $\pi = \pi_1 = (5, 2^{(n-2)}, 1)$ or $\pi = \pi_2 = (4, 3, 2^{(n-3)}, 1)$. Note that $\pi_2 \lhd \pi_1$ and $\pi_0 \lhd (4, 3, 2^{(n-5)}, 1^{(3)})$. Thus, by (4.6) and Theorem 2.6, we have $\prod_2(G) \geq 27 \times 4^{n+1} > \prod_2(R_0)$ and $H_f(G) \geq f(4) + f(3) + f(1) + (n-3)f(2) > f(4) + f(3) + 3f(1) + (n-5)f(2) > H_f(R_0)$, as $f(x)$ is a strictly increasing convex function on $x \geq 1$.

If $\mathcal{R}(G) = W_2$ or $\mathcal{R}(G) = W_3$, then either $\pi = \pi_3 = (4, 3, 2^{(n-3)}, 1)$ or $\pi = \pi_4 = (3^{(3)}, 2^{(n-4)}, 1)$. Note that $\pi_4 \lhd \pi_3$. Thus, by (4.6) and Theorem 2.6, we have $\prod_2(G) \geq 3^9 \times 4^{n-4} > \prod_2(R_0)$ and $H_f(G) \geq 3f(3) + f(1) + (n-4)f(2) > H_f(R_0)$. ■

Lemma 4.9. *If $k \geq 2$, $n \geq 3k$ and H_0 is a unicyclic graph, then*

(i) Each nontrivial rooted tree of H_0 is a path;

(ii) For any k-quasi vertex set V_k of H_0, $H_0[V_k]$ is a nontrivial pendant path of H_0;

(iii) For each vertex $v_0 \in \mathcal{R}(H_0)$, T_{v_0} is a nontrivial pendant path with $|V(T_{v_0})| \geq k$.

Proof. By Lemma 4.2, each nontrivial rooted tree of H_0 is a pendant path. Thus, (i) holds. We may suppose that C_q is the unique cycle of H_0.

Let V_k be a k-quasi vertex set of H_0, and let $S = V_k \cap V(C_q)$. Since $T = H_0 - V_k$ is a tree and H_0 is a unicyclic graph, $S \neq \emptyset$ and $H_0[S]$ is a path. If $|S| \geq 2$, then there exists W with $|W| = k-1$ such that $H_0 - W$ is also a unicyclic graph, where $|W \cap V(C_q)| = |S| - 1$, contrary to $H_0 \in \mathcal{T}_n^k$. Thus, $|S| = 1$ and so (i) implies that $H_0[V_k]$ is a nontrivial pendant path of H_0. Thus, (ii) holds.

We turn to prove (iii). Let T_{v_0} be a rooted tree of H_0. By (ii), we may suppose that $V(T_{v_0})$ is not a k-quasi vertex set of H_0. We assume that $|V(T_{v_0})| = t \leq k-1$. If $t = k-1$, then $H_0 - V(T_{v_0})$ is a tree, contrary with $H_0 \in \mathcal{T}_n^k$. Otherwise, $t \leq k-2$. By Lemma 4.1 and (ii), we may suppose that $V_k \cap V(T_{v_0}) = \emptyset$. Thus, there exists $W \subseteq V(H_0)$ with $|W| = k-1$, $V(T_{v_0}) \subseteq W$ and $|W \cap V_k| = k - 1 - t$ such that $H_0 - W$ is a tree, which contradicts $H_0 \in \mathcal{T}_n^k$. Thus, (iii) holds. ■

Lemma 4.10. *If $k \geq 2$, $n \geq 3k$ and H_0 is a unicyclic graph, then $H_0 \in \mathbb{W}_{n,k}$.*

Proof. We suppose that the unique cycle of H_0 is C_q. Lemma 4.9(ii) and (iii) imply that H_0 is obtained from C_q by attaching exactly one path to each vertex of C_q such that each pendant path contains at least k vertices and at least one pendant path has exactly k vertices. This implies that the degree sequence of H_0 is $\pi = (3^{(q)}, 2^{(n-2q)}, 1^{(q)})$. Recall that R_0 is a graph of $\mathbb{W}_{n,k}$ and the degree sequence of R_0 is $\pi_0 = (3^{(3)}, 2^{(n-6)}, 1^{(3)})$.

First assume that $q \geq 4$. Then, $\pi_0 \lhd \pi$. By Theorem 2.6, $\prod_2(H_0) > \prod_2(R_0)$ and $H_f(G) > H_f(R_0)$. If $k \geq 3$, then $M_2(H_0) = 4n + 5q \geq 4n + 20 > M_2(R_0)$ by (4.6), which contradicts $R_0 \in \mathcal{T}_n^k$. Thus, $k = 2$. In the later case, $M_2(H_0) \geq 4(n-2q) + 9q + 3q = 4n + 4q \geq 4n + 16 > 4n + 14 \geq M_2(R_0)$, which contradicts $R_0 \in \mathcal{T}_n^k$.

Thus, $q = 3$ and so $H_0 \in \mathbb{W}_{n,k}$ by Lemma 4.9(ii) and (iii). ■

Theorem 4.2. *Let $G \in \mathcal{T}_n^k$ and $R_0 \in \mathbb{W}_{n,k}$. If $k \geq 3$ and $n \geq 3k$, then $\Phi(G) \geq \Phi(R_0)$, with equality if and only if $G \in \mathbb{W}_{n,k}$.*

Proof. By Lemma 4.10, it suffices to show that H_0 is a unicyclic graph. Firstly, Definition 3.2 implies that H_0 is not a tree. By (4.4) and (4.6), $\prod_2(F_{n,k}) > \prod_2(R_0)$ and $H_f(F_{n,k}) > H_f(R_0)$, as $f(x)$ is a strictly increasing convex function on $x \geq 1$. Since $F_{n,k}$ is a bicyclic graph, we have $M_2(F_{n,k}) > M_2(R_0)$ by (4.6) and Lemma 4.7. By combining with $R_0 \in \mathbb{W}_{n,k} \subset \mathcal{T}_n^k$ and Lemma 4.5, we can deduce that H_0 is unicyclic or bicyclic. Now, we assume that H_0 is a bicyclic graph with p pendant vertices and a k-quasi vertex set V_k.

By Lemma 4.8, we have $p = 0$ and thus $H_0 \in \{W_1, W_2, W_3\}$ (See Fig. 4.2). Since $H_0 \in \mathcal{T}_n^k$ and $k \geq 3$, $H_0[V_k]$ is equal to one path or two separate paths, the longest containing at least two vertices. This implies the existence of vertex set W of G with $|W| = k-1$ such that $H_0 - W$ is a tree, contrary to $H_0 \in \mathcal{T}_n^k$. Thus, H_0 is a unicyclic graph. ■

Let $\pi = (3^{(2k-2)}, 2^{(n+2-2k)})$, and let $L_{n,k}$ be a k-cyclic graph of $\Gamma(\pi)$ such that $L_{n,k}$ contains exactly k quadrilaterals, and any two vertices with degree three are not adjacent to each other. When $k \geq 3$ and $n \geq 5k-1$, $L_{n,k}$ is a $(k-1)$-generalized quasi-unicyclic graph and a k-generalized quasi-tree.

Remark 4.1. By comparing Theorems 3.1, 4.1 and 4.2, it is natural for us to consider the problem: Whether the extremal graphs of Theorems 4.1 and 4.2 are also these extremal graphs of $Z_\alpha(G)$ and/or $\chi_\alpha(G)$. Unfortunately, the answers are negative. For instance, when α is large enough, $n \geq 5k-1$ and $k \geq 3$, we have

$$\chi_\alpha(L_{n,k+1}) = 5^\alpha \times 6k + 4^\alpha(n-5k) < 6^\alpha \times 5 + 5^\alpha \times 2 + 3^\alpha \times 2 + 4^\alpha(n-8) = \chi_\alpha(F_{n,k}),$$
$$Z_\alpha(L_{n,k+1}) = 3^\alpha \times 6k + 2^\alpha(n-5k) < 4^\alpha \times 5 + 3^\alpha \times 2 + 2 + 2^\alpha(n-8) = Z_\alpha(F_{n,k}),$$
$$\chi_\alpha(L_{n,k}) = 5^\alpha \times 6(k-1) + 4^\alpha\big(n-5(k-1)\big) < 6^\alpha \times 3 + 5^\alpha \times 3 + 3^\alpha \times 3 + 4^\alpha(n-9) = \chi_\alpha(R_0),$$
$$Z_\alpha(L_{n,k}) = 3^\alpha \times 6(k-1) + 2^\alpha\big(n-5(k-1)\big) < 4^\alpha \times 3 + 3^\alpha \times 3 + 3 + 2^\alpha(n-9) = Z_\alpha(R_0).$$

Remark 4.2. When $k \geq 2$, it is easy to see that $F_{n,k} \in \mathbb{U}_n^k \subseteq \mathcal{U}_n^k$. Thus, $F_{n,k}$ is also the corresponding extremal minimum graph of $\mathbb{U}_n^k$. Similarly, Theorem 4.2 also holds for $\mathbb{T}_n^k$.

Remark 4.3. Since the degree sequence of W_2 and W_3 is majorized by that of W_1, $\Phi(W_1) > \min\{\Phi(W_2), \Phi(W_3)\}$ by Theorem 2.6 and Lemma 4.7. When $k=2$ and $n \geq 3k$, since $\Phi(F_{n,k}) > \Phi(R_0)$, and in view of Lemmas 4.5, 4.8, 4.10, the extremal minimum graphs of $\mathcal{T}_n^k$ (that is, $\mathbb{T}_n^k$) are either the graphs of $\mathbb{W}_{n,k}$ or some bicyclic graphs with degree sequence $(3^{(2)}, 2^{(n-2)})$.

Remark 4.4. When $k=1$, by Definition 3.2 with $k=1$, any graph of $\mathcal{T}_n^k$ is not a tree. Since C_n is a graph of $\mathcal{T}_n^1$ and $\big(2^{(n)}\big)$ is minimum among all degree sequences of unicyclic graphs with n vertices (see Lemma 3.4 of [14]), Corollary 4.1 implies that C_n is the unique extremal minimum graph of $\mathcal{T}_n^1$ (resp., $\mathbb{T}_n^1$).

Remark 4.5. When $k=1$, by Definition 3.2 with $k=1$, any graph of $\mathcal{U}_n^k$ is not unicyclic. Since $\big(3^{(2)}, 2^{(n-2)}\big)$ is minimum among all degree sequences of bicyclic graphs with n vertices (see Lemma 3.4 of [14]), from Corollary 4.1, Theorem 2.6 and Lemma 4.7, we can deduce that the extremal minimum graphs of $\mathcal{U}_n^1$ (resp., $\mathbb{U}_n^1$) are some bicyclic graphs with degree sequence $\big(3^{(2)}, 2^{(n-2)}\big)$.

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On graphs whose second largest eigenvalue is at most 1[☆]



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ABSTRACT

We determine all connected $\{K_{1,3}, K_5 - e\}$-free graphs whose second largest eigenvalue does not exceed 1. Our result includes all connected line graphs with the same spectral property, and therefore strengthens the result of Petrović and Milekić (1998).
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1. Introduction

For a finite simple undirected graph we use λ_2 to denote its second largest eigenvalue, that is the second largest eigenvalue of its adjacency matrix. The problem of characterizing graphs whose second largest eigenvalue does not exceed a comparatively small constant has attracted a great deal of attention in the last decades. Many results are surveyed in [12]. We note that graphs with $\lambda_2 \leq 1$ are not fully determined, but it is worth mentioning that bipartite graphs with $\lambda_2 \leq 1$ have been determined by Petrović [7]. In particular, Neumaier [6] investigated trees with the same spectral property and he also described an algorithm for deciding whether λ_2 of a tree does not exceed an arbitrary bound. Later, line graphs and generalized line graphs with $\lambda_2 \leq 1$ have been completely characterized by Petrović and Milekić [8,9], while threshold graphs (also known as nested split graphs) with $\lambda_2 \leq 1$ have been determined by Stanić [10]. Recently, Cheng, Greaves and Koolen [2] identified all graphs which have exactly three distinct eigenvalues and whose second largest eigenvalue does not exceed 1. Some other results can be found in [3,5,11].

The result of [8] concerning line graphs with $\lambda_2 \leq 1$ is a starting point for our investigation. We know from [1,4] that G is a line graph if and only if it does not contain any of the graphs $K_{1,3}$, $K_5 - e$, W_1, W_2, ..., W_7 as an induced subgraph, where the first two graphs are the star with 3 pendant

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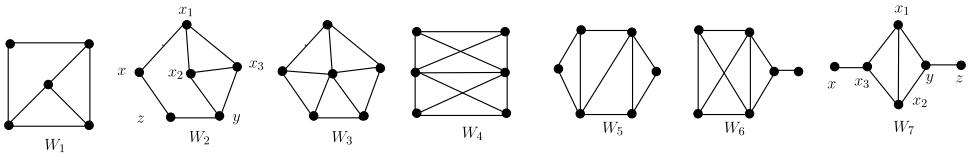


Fig. 1. The graphs $W_1, W_2, \ldots, W_7$.

vertices and the graph obtained by removing an edge from the complete graph with 5 vertices respectively, while the remaining 7 graphs are illustrated in Fig. 1. In this study we determine all connected graphs that do not contain the first two graphs as induced subgraphs and whose second largest eigenvalue does not exceed 1. In other words, we include the possibility that some of the remaining 7 graphs are induced subgraphs of graphs under consideration. Therefore, our result is an evident strengthening of the result of [8].

In Section 2 we formulate our main theorem and give some related remarks. The considerably long proof is given in Section 3.

2. Main result

Our main result deals with connected graphs which have no $K_{1,3}$ or $K_5 - e$ as an induced subgraph (in short, these are $\{K_{1,3}, K_5 - e\}$-free graphs) and whose second largest eigenvalue is at most 1. To formulate the result and some consequences we need to introduce some graphs. As usual, by P_q and C_q we denote the path and the cycle with q vertices, respectively. Let $D_1, D_2, \ldots, D_{16}$ be the graphs illustrated in Fig. 2, and let $\mathcal{D}$ be the class of graphs obtained by taking a complete graph K_q with at least 5 vertices and a set of isolated vertices, and then inserting edges between the vertices of K_q and the vertices out of it, in such a way that every vertex of K_q is adjacent to at most one additional vertex and every vertex out of K_q is adjacent to exactly two vertices of K_q.

Our main contribution reads as follows.

Theorem 2.1. *For a connected $\{K_{1,3}, K_5 - e\}$-free graph G, $\lambda_2 \leq 1$ holds if and only if G is an induced subgraph of a graph belonging to $\{C_5, D_3, D_4, \ldots, D_{16}\} \cup \mathcal{D}$.*

This result implies the following corollary that is of particular interest if we restrict ourselves to graphs with at least 9 vertices.

Corollary 2.2. *For a connected $\{K_{1,3}, K_5 - e\}$-free graph G with at least 9 vertices, $\lambda_2 \leq 1$ holds if and only if G is an induced subgraph of a graph belonging to $\{D_6, D_7\} \cup \mathcal{D}$.*

Theorem 2.1 also improves the result of [8] originally formulated as follows.

Theorem 2.3. *A connected line graph G has the property $\lambda_2(G) \leq 1$ if and only if G is an induced subgraph of some graph of $\{P_5, C_5, C_6, D_1, D_2, \ldots, D_7\} \cup \mathcal{D}$.*

Moreover, we observe that P_5, C_6 are induced subgraphs of D_6 and D_1, D_2 are induced subgraphs of D_7. Therefore, the previous theorem can be reformulated as follows.

Theorem 2.4. *A connected line graph G has the property $\lambda_2(G) \leq 1$ if and only if G is an induced subgraph of some graph of $\{C_5, D_3, D_4, \ldots, D_7\} \cup \mathcal{D}$.*

3. Proof

The proof of Theorem 2.1 is separated into two subsections. In the first one we fix some terminology and notation, and prove some initial results. The second subsection contains deeper results along with their proofs.

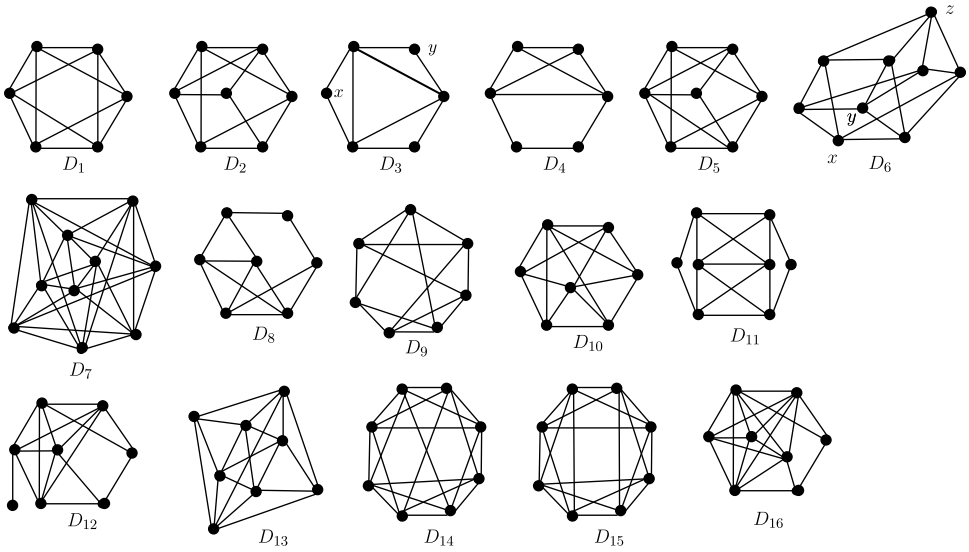


Fig. 2. The graphs $D_1, D_2, \ldots, D_{16}$.

3.1. Terminology, notation and preliminary results

We first introduce some graphs. Let $H_1, H_2, \ldots, H_{40}$ be the graphs illustrated in Fig. 3, and $G_1, G_2, \ldots, G_{14}$ be the graphs illustrated in Fig. 4. Some vertices are labelled so we can refer to them in the forthcoming text. Throughout this section we suppose that G has n vertices and denote its set of vertices by $V = V(G)$. We designate that a graph H is an induced subgraph of G by writing $H \subset G$.

By direct computation we get the following lemma.

Lemma 3.1. *If $G \in \{P_6,\ G_1,\ G_2,\ \ldots,\ G_{14}\}$, then $\lambda_2(G) > 1$.*

Note that $\lambda_2 \leq 1$ is a hereditary property in the sense that if it holds for G then it holds for every induced subgraph of G. We say that H is *forbidden* for $\lambda_2 \leq 1$ if H is not an induced subgraph of any graph with second largest eigenvalue being at most 1. Evidently, every graph with $\lambda_2 > 1$ is forbidden; this in particular holds for graphs of Lemma 3.1. We employ this fact straightly in the later discussion.

Throughout the remainder of the paper we denote by $\mathcal{G}$ the set of connected $\{K_{1,3}, K_5 - e\}$-free graphs with $\lambda_2 \leq 1$.

Lemma 3.2. *If $G \in \mathcal{G}$ is triangle-free, then G is an induced subgraph of C_5, D_4 or D_6.*

Proof. If G contains no triangle, then the degree of each vertex of G is at most 2; for otherwise, we would have $K_{1,3} \subset G$ or $K_3 \subset G$, which is disallowed. It follows that G is a cycle C_q with $q \geq 4$ or a path P_k with $k \geq 2$. Since P_6 is forbidden, we have $q \leq 6$ and $k \leq 5$. Thus, G is an induced subgraph of some of C_5, D_4, D_6, as $C_4 \subset D_4$ and $C_6 \subset D_6$. ■

The *clique number* ω of G is the number of vertices of a maximal clique (i.e., an induced complete graph) contained in G. Let further K_q be a *maximal clique* of G, where $G \in \mathcal{G}$ and $q \geq 3$, and let $V(K_q) = \{x_1, x_2, \ldots, x_q\}$. Denote by T the set $V(G) \backslash V(K_q)$. Every vertex of T is adjacent to at most two vertices of K_q. For $q = 3$ this comes from the maximality of q; for $q \geq 4$ it depends on the absence of $K_5 - e$ among the induced subgraphs of G. Thus, $T = T_0 \cup T_1 \cup T_2$, where T_i is the set of vertices of T which are adjacent to exactly i vertices of K_q. Also, we may suppose that $T_1 = T_{x_1} \cup T_{x_2} \cup \cdots \cup T_{x_q}$

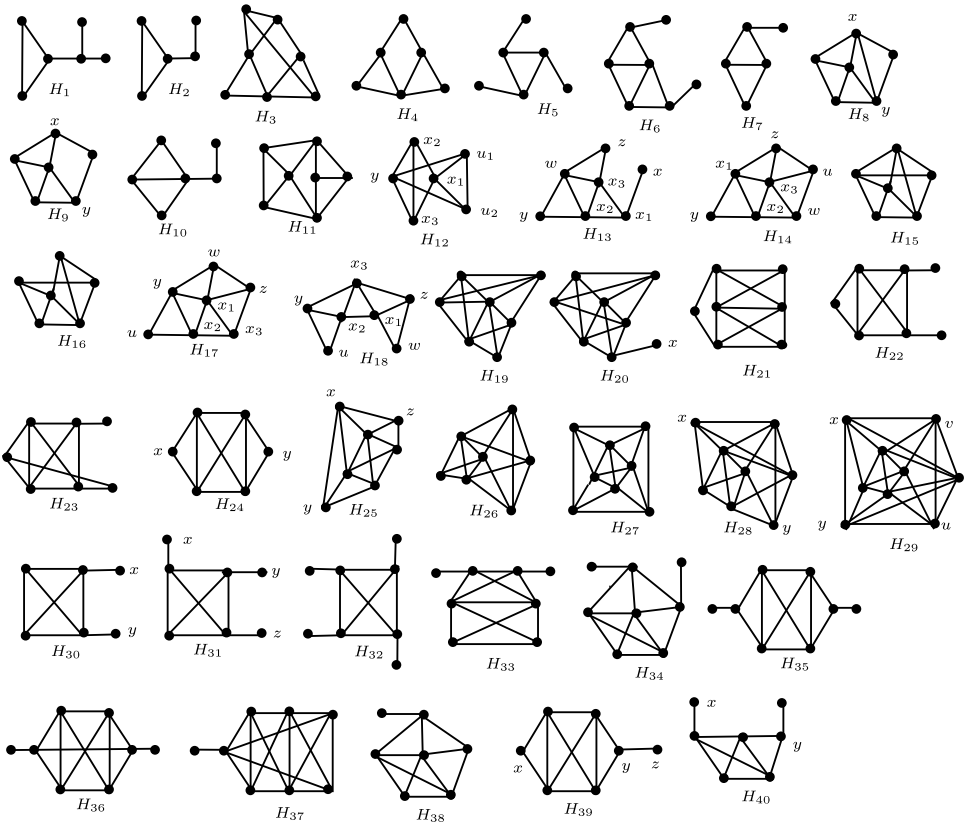


Fig. 3. The graphs $H_1, H_2, \ldots, H_{40}$.

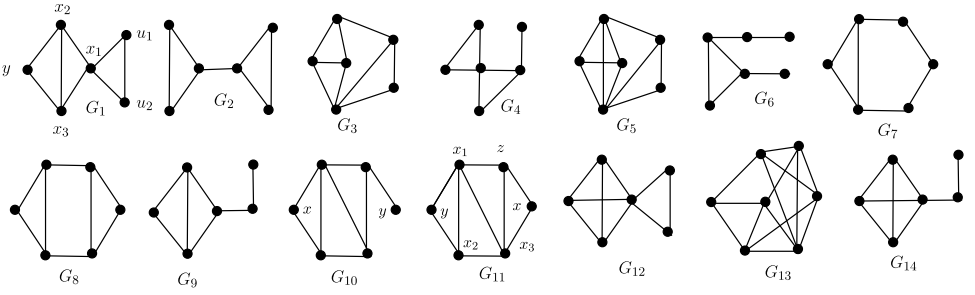


Fig. 4. The forbidden graphs $G_1, G_2, \ldots, G_{14}$.

and $T_2 = T_{x_1x_2} \cup T_{x_1x_3} \cup \cdots \cup T_{x_{q-1}x_q}$, where T_{x_i} is the set of vertices which are adjacent precisely to the vertex x_i of K_q, and $T_{x_ix_j}$ is the set of vertices which are adjacent precisely to the vertices x_i, x_j of K_q.

We proceed with the following lemma.

Lemma 3.3. *Let K_q be a maximal clique of $G \in \mathcal{G}$, and let i, j, k be different positive integers. If $q \geq 3$, then the following statements hold:*

(1) T_{x_i} and $T_{x_ix_j}$ induce complete graphs;

(2) *Every vertex of* $T_1 \cup T_2$ *is adjacent to at most one vertex of* T_0*;*
(3) *Every vertex of* T_{x_i} *is adjacent to at most one vertex of* T_{x_j}*. Moreover, every vertex of* T_{x_i} *is non-adjacent to at most one vertex of* T_{x_j}*;*
(4) *If the vertices* $x \in T_{x_i}$ *and* $y \in T_{x_j}$ *are adjacent, then every vertex* $z \in T_{x_k}$ *is either adjacent to both* x *and* y *or non-adjacent to both;*
(5) *If in addition* $q \geq 4$*, then every vertex of* $T_{x_ix_j}$ *is adjacent to every vertex of* $T_{x_ix_k}$*. Moreover, if* $T_{x_ix_j} \neq \emptyset$*, then every vertex of* T_1 *is non-adjacent to* x_i, x_j*;*
(6) *If* $|T_{x_i}| \geq 2$*, then* $T_{x_ix_j} = \emptyset$*. Moreover, if* $T_{x_jx_k} \neq \emptyset$*, then every vertex of* $T_{x_jx_k}$ *is adjacent to every vertex of* T_{x_i}*.*

Proof. Since $K_{1,3}$ is forbidden and $q \geq 3$, we get that each of T_{x_i} and $T_{x_ix_j}$ induce a complete graph, which completes (1).

To show (2), we assume that u is a vertex of $T_1 \cup T_2$ adjacent to at least two vertices of T_0. Then G contains H_1 as a subgraph, where the pendant vertices of H_1 belong to T_0. If $u \in T_2$, then $K_{1,3}$ or G_1 is an induced subgraph of G, a contradiction. For otherwise, $K_{1,3}$ or G_2 is an induced subgraph of G, a contradiction. Thus, (2) holds.

We proceed with (3). If a vertex of T_{x_i} is adjacent to at least two vertices of T_{x_j}, then G contains G_3 as induced subgraph by (1), a contradiction. If a vertex of T_{x_i} is non-adjacent to at least two vertices of T_{x_j}, then G contains G_4 as induced subgraph by (1), a contradiction. This completes (3).

If under the assumption of (4) there is a vertex $z \in T_{x_k}$ adjacent to x, but non-adjacent to y, then $K_{1,3}$ is an induced subgraph of G. Thus, (4) holds.

Next, we show (5). Since $K_{1,3}$ is forbidden, every vertex of $T_{x_ix_j}$ is adjacent to every vertex of $T_{x_ix_k}$. We assume that for $T_{x_ix_j} \neq \emptyset$, a vertex u of T_1 is adjacent to x_i or x_j. Since $K_{1,3}$ is forbidden, u is adjacent to the vertices of $T_{x_ix_j}$, and then G_5 is an induced subgraph of G, a contradiction.

Finally, we show (6). If $x, y \in T_{x_i}$, then $xy \in E(G)$ by (1). If there exists a vertex $u \in T_{x_ix_j}$, then u is adjacent to both x and y, as $K_{1,3}$ is forbidden, but in this case, $G_5 \subset G$, a contradiction. Thus, $T_{x_ix_j} = \emptyset$. Next, if $v \in T_{x_jx_k}$, then since G_1 and G_3 are forbidden, v is adjacent to both x and y, and thus (6) follows. ■

3.2. The remainder of the proof

We divide our considerations into the three parts depending on the clique number $\omega(G)$. Precisely, the case $\omega(G) = 3$ is considered in Lemma 3.4, $\omega(G) = 4$ is considered in Lemma 3.6 and $\omega(G) \geq 5$ is considered in Lemma 3.7.

Lemma 3.4. *If* $G \in \mathcal{G}$ *and* $\omega(G) = 3$*, then* G *is an induced subgraph of some of graphs of* $\{D_h, D_{12}, D_{14}, D_{15} \mid 3 \leq h \leq 10\} \cup \mathcal{D}$*.*

Proof. Let K_3 be a fixed induced complete graph of G. By virtue of Lemma 3.3(1), we immediately get the following fact.

Fact 1. *We have* $|T_{x_ix_j}| \leq 1$ *and* $|T_{x_i}| \leq 2$*, where* $|T_{x_i}| = 2$ *implies that two vertices of* T_{x_i} *are adjacent.*

We now distinguish cases depending on the structure outside a fixed maximal clique.

Case 1: $T_1 \neq \emptyset$ **and** $T_2 = \emptyset$. If $|T_1| = 1$, then $|T_0| \leq 1$ by Lemma 3.3(2), as $T_2 = \emptyset$. Thus, G is an induced subgraph of H_2 and so $G \subset D_4$. Hence, we may assume that $|T_1| \geq 2$.

We first suppose that $T_0 \neq \emptyset$. Then G contains H_2 as an induced subgraph, as $T_0 \neq \emptyset$ and $T_2 = \emptyset$. If G contains G_6 as a subgraph, then one of $K_{1,3}, G_6, G_7, G_8$ is an induced subgraph of G, which is impossible. On the other hand, since G_6 is not a subgraph of G, from Fact 1 we get that G_4 must be a subgraph of G (as $|T_1| \geq 2$). But then either $G_1 \subset G$ or $G_4 \subset G$, a contradiction.

We now suppose that $T_0 = \emptyset$. Combining this with $T_2 = \emptyset$ and Fact 1, we obtain $n \leq 9$. Without loss of generality, we may suppose that $|T_{x_3}| \leq |T_{x_2}| \leq |T_{x_1}| \leq 2$.

If $|T_{x_1}| = |T_{x_2}| = 2$, then $H_3 \subset G$, by Lemma 3.3(3) and Fact 1, which together with Lemma 3.3(3)–(4) implies $G \subset D_6$. If $|T_{x_1}| = 2$ and $|T_{x_2}| = 1$, then $H_4 \subset G$, by Lemma 3.3(3) and Fact 1, which as before implies $G \subset D_6$. If $|T_{x_1}| = 2$ and $|T_{x_2}| = 0$, we also have $G \subset D_6$ by Fact 1.

Since $|T_1| \geq 2$, we may suppose that $|T_{x_1}| = |T_{x_2}| = 1$, and thus $|T_{x_3}| \leq 1$. If there is at least one edge between T_{x_i} and T_{x_j}, then $G \subset D_6$, by Lemma 3.3(3)–(4). For otherwise, we get $G \subset H_5 \subset \mathcal{D}$.

Case 2: $T_1 = \emptyset$ **and** $T_2 \neq \emptyset$. We first eliminate the possibility that H_6 is a subgraph of G (where pendant vertices of H_6 belong to T_0). If these pendant vertices are adjacent, then $G_9 \subset G$, by Lemma 3.3(2), a contradiction. For otherwise, since G_6 is forbidden, we see that two vertices of H_6 pertaining to T_2 must be adjacent, but this implies $K_{1,3} \subset G$, by Lemma 3.3(2). Therefore, we further assume that H_6 is not a subgraph of G.

On the basis of Fact 1, Lemma 3.3(2) and the previous assumption, we conclude that $|T_2| \leq 3$ and $|T_0| \leq 1$. If $|T_2| = 1$, then $G \subset H_7 \subset D_2 \subset D_7$, so in what follows we take that $|T_2| \geq 2$.

Subcase 2.1: $|T_0| = 1$. Let first $|T_2| = 2$ with $T_2 = \{x, y\}$. Then G_{10} is a subgraph of G. Since $K_{1,3}$ and G_{10} are forbidden, we get either $G = H_8 \subset D_5$ (for $xy \in E(G)$, see Fig. 4) or $G = H_9 \subset D_2 \subset D_7$ (for $xy \notin E(G)$).

Let now $|T_2| = 3$ with $T_2 = \{x, y, z\}$. Since $|T_0| = 1$, we have either $H_8 \subset G$ or $H_9 \subset G$. In the former case (so, $H_8 \subset G$), since $K_{1,3}, G_{10}$ are forbidden and $\omega(G) = 3$, we have either $G = D_2$ (if z is non-adjacent to x, y, see Fig. 4) or $G = D_5$ (if z is adjacent to exactly one of x, y). In the latter case, the unique vertex of T_0 is adjacent to all vertices of T_2, as $K_{1,3}, G_{10}$ are forbidden. But since H_8 is not an induced subgraph of G, these three vertices induce an empty graph, and thus $K_{1,3} \subset G$, a contradiction.

Subcase 2.2: $|T_0| = 0$. As before, we first let $|T_2| = 2$. Then either $G \subset D_7$ (if the vertices of T_2 are adjacent) or $G \subset D_2 \subset D_7$ (otherwise).

Let now $|T_2| = 3$. If the vertices of T_2 induce a triangle (resp. an empty graph), then $G = D_1 \subset D_7$ ($G = D_3$). For otherwise, the vertices of T_2 induce $K_1 \cup K_2$ or P_3, which yields $G \subset D_2 \subset D_7$ or $G \subset D_5$.

Case 3: $T_1 \neq \emptyset$ **and** $T_2 \neq \emptyset$.

Subcase 3.1: $T_0 \neq \emptyset$. We denote a vertex of T_0 by z.

Subsubcase 3.1.1: z **is adjacent to a vertex of** T_1. Here, H_2 is a subgraph of G and, since $T_2 \neq \emptyset$, either G_9 or H_{10} is a subgraph of G.

If H_{10} is a subgraph of G, then G_{10} is a subgraph of G, as $K_{1,3}$ is forbidden and a neighbour of z belongs to T_1. Since G_{10} is forbidden, z is adjacent to the vertex of $T_2 \in V(G_{10})$. This implies $G_{11} \subset G$, which is impossible. Thus, H_{10} is not a subgraph of G, and so G_9 is a subgraph of G. Since $K_{1,3}, G_3, G_9$ are forbidden, we have $W_2 \subset G$. Let $V(W_2) = \{x_1, x_2, x_3, x, y, z\}$, where x_1, x_2, x_3 are the vertices of K_3 as in Fig. 1. Since H_{10} is not a subgraph, we have $|T_2| = 1$ and $T_2 = \{y\}$, by Fact 1.

If some vertex, say u, of T_1 is adjacent to x_2 or x_3, then u is also adjacent to y, as $K_{1,3}$ is forbidden. Then, z is non-adjacent to any of u, x_1, x_2, x_3, as G_{11} is forbidden and $z \in T_0$. If $ux_3 \in E(G)$, then u, y, x_2, z induce $K_{1,3}$, and similarly for $ux_2 \in E(G)$. Hence, there are no edges between T_1 and x_2, x_3.

If, apart from x, there is another vertex, say v, of T_1 and $vx_1 \in E(G)$, then $vx \in E(G)$ by Fact 1. In this case, since G_1 is forbidden and W_2 is an induced subgraph of G, v must be adjacent to y. Moreover, since $K_{1,3}$ is forbidden, v is adjacent to z, as well. Thus, G contains H_{11} as an induced subgraph, which implies $G_3 \subset G$, a contradiction. Consequently, we have $T_1 = \{x\}$, $T_2 = \{y\}$ and (from before) $W_2 \subset G$.

If $|T_0| = 1$, then $G = W_2 \subset D_8$. If $|T_0| \geq 2$, then we let w be another vertex of T_0. By Lemma 3.3(2), w is non-adjacent to x, y, and so it is adjacent to z, but then w, z, y, x_1, x_2, x_3 induce G_9, a contradiction.

Subsubcase 3.1.2: z **is non-adjacent to any vertex of** T_1. Then z is adjacent to a vertex of T_2. In this case, $W_7 \subset G$ with $V(W_7) = \{x_1, x_2, x_3, y, z, x\}$ as in Fig. 1, since $K_{1,3}$ is forbidden.

We first show that $T_2 = \{y\}$. Assume by way of contradiction that $|T_2| \geq 2$. Since $K_{1,3}$ is forbidden, another vertex, say v, of T_2 is adjacent to both x and x_3, by Fact 1. Observe that v is non-adjacent to z (because of the non-existence of $K_{1,3}$), and hence v is non-adjacent to y. Combining this with $W_7 \subset G$, we get $G_9 \subset G$, a contradiction. This confirms that $|T_2| = 1$, and then necessarily $T_2 = \{y\}$.

In a similar way we show that $T_1 = \{x\}$. Namely, as before, we let w be another vertex of T_1. By a very similar reasoning, we get that w is non-adjacent to x_1, x_2, and then $wx_3, wx \in E(G)$, by Fact 1. But in this case either $K_{1,3}$ (if y is adjacent to w) or G_1 (if y is non-adjacent to w) is an induced subgraph of G, a contradiction.

We proceed with showing that $T_0 = \{z\}$. Assume that z' is another vertex of T_0. Since $T_1 = \{x\}$, $T_2 = \{y\}$, by Lemma 3.3(2), we get that z' is adjacent to z and z' is non-adjacent to y, which implies $G_9 \subset G$, a contradiction. Thus, $T_0 = \{z\}$, and so $G = W_7 \subset D_{12}$.

Subcase 3.2: $T_0 = \emptyset$. We first suppose that $|T_{x_i}| = 2$ for some vertex x_i. Then, T_{x_i} induces an edge by Fact 1. Since $T_2 \neq \emptyset$, T_2 contains exactly one vertex by Lemma 3.3(6) and Fact 1, which is adjacent to $V(K_3) \setminus \{x_i\}$ and two vertices of T_{x_i}. Hence, $H_{12} \subset G$. We may suppose that $V(H_{12}) = \{u_1, u_2, x_1, x_2, x_3, y\}$ and $T_2 = \{y\}$ (as in Fig. 3). We claim that $G = H_{12}$. For otherwise, there exists $x \in T_1$, as $T_2 = \{y\}$ and $T_0 = \emptyset$. By Fact 1, x is adjacent to either x_2 or x_3. Since $K_{1,3}$ is forbidden, x is also adjacent to y, u_1, u_2, but then x, y, u_1, u_2 induce K_4, a contradiction. Thus, $G = H_{12} \subset D_{15}$.

We secondly suppose that $|T_{x_i}| \leq 1$ for each vertex x_i of K_3. Since $|T_{x_ix_j}| \leq 1$ for each edge x_ix_j of K_3 (by Fact 1), it follows that $1 \leq |T_1|, |T_2| \leq 3$. We proceed with the following claim.

Claim 1. *If $|T_1| = 3$, then $G = D_2 \subset D_7$.*

Proof. Since $K_{1,3}$ is forbidden and $T_2 \neq \emptyset$, H_{13} is a subgraph of G. Let $V(H_{13}) = \{x, y, z, w, x_1, x_2, x_3\}$ as in Fig. 3.

We first suppose that $yz \in E(G)$. Since $\omega(G) = 3$, x is not adjacent to w, by Lemma 3.3(4). Since G_{10} is forbidden, x is adjacent to y, z, by the same statement. This implies that $D_2 \subset G$. If $|T_2| \geq 2$, then let v be a vertex of $T_2 \setminus \{w\}$ and, without loss of generality, we may suppose that $v \in T_{x_1x_3}$ by Fact 1. Since $K_{1,3}$ is forbidden and $\omega(G) = 3$, v is adjacent to x, z and it is non-adjacent to w, y. This implies that x, y, z, v, w, x_1 induce G_{11}, a contradiction. Thus, $|T_2| = 1$, and so $G = D_2 \subset D_7$.

It remains to reject the possibility that $yz \notin E(G)$. Assuming the contrary, we get that x is adjacent to at most one of y, z; otherwise, x, y, z, x_1 induce $K_{1,3}$. In the same way we conclude that $xw \notin E(G)$, and then we may suppose that $xz \notin E(G)$, but then x, w, z, x_1, x_2, x_3 induce G_{10}, a contradiction. ◇

Claim 2. *If $|T_2| = 3$, then $G \in \{D_5, D_{10}\}$.*

Proof. Since $K_{1,3}$ is forbidden and $T_1 \neq \emptyset$, H_{14} is a subgraph of G, where $V(H_{14}) = \{u, w, y, z, x_1, x_2, x_3\}$ as in Fig. 3 and $u \in T_1$. We first suppose that $uy \notin E(G)$. Since G_{11} is forbidden, y is adjacent to z, w, which implies $D_5 \subset G$. If $G \neq D_5$, then there exists $v \in T_1 \setminus \{u\}$ and we may suppose that v is adjacent to x_1. Since $K_{1,3}$ is forbidden, v is adjacent to both z, y which implies that y, z, x_1, v induce K_4, a contradiction. Thus, $G = D_5$.

We now suppose that $uy \in E(G)$. Since $\omega(G) = 3$, we have $wz \notin E(G)$ and we may suppose that $yz \in E(G)$ by the symmetry of z and w; otherwise, u, w, y, z induce $K_{1,3}$. Then either $D_5 \subset G$ or $D_{10} \subset G$. If some of these graphs is a proper induced subgraph of G, then there exists $v \in T_1 \setminus \{u\}$. As before, v is adjacent to x_2, y, w, and so $D_5 \subset G$. If v is non-adjacent to u, then u, v, x_1, y induce $K_{1,3}$ (see H_{14} of Fig. 3), and thus v is adjacent to u. This implies that z is not adjacent to v (otherwise, u, v, y, z induce K_4), providing that y, z, x_1, x_2, v, w induce G_{11}. This confirms that $T_1 = \{u\}$, and hence $G = D_5$ or $G = D_{10}$. ◇

Claim 3. *If $|T_2| = 2$ and $|T_1| \leq 2$, then G is an induced subgraph of some of $D_5, D_7, D_9, D_{10}, D_{14}$.*

Proof. We first suppose that $|T_1| = 1$ and set $T_1 = \{x\}$, $T_2 = \{y, z\}$, where y and z are adjacent to some vertex w of x_1, x_2, x_3. If $xw \in E(G)$, then $G = W_3 \subset D_{10}$. For otherwise, we get that G_{11} is a subgraph of G, as $K_{1,3}$ is forbidden. Since G_{11} is also forbidden, we have $G \in \{H_8, H_{15}, H_{16}\}$. It is easily checked that $H_8, H_{15} \subset D_5$ and $H_{16} \subset D_{14}$.

We next suppose that $|T_1| = 2$. It follows that either H_{17} or H_{18} is a subgraph of G, where $T_1 = \{u, w\}$ (see Fig. 3). In the former case we must have $yz \notin E(G)$, and then $uz \in E(G)$ (otherwise,

u, y, z, x_1, x_2, x_3 induce G_{11}) and $uw \in E(G)$ (otherwise, u, z, w, x_3 induce $K_{1,3}$), and thus $G = D_5$. In the latter case, there must be $uw \in E(G)$. Indeed, if $uw \notin E(G)$, then $yw \notin E(G)$ (as $K_{1,3}$ is forbidden), which yields $G_{10} \subset G$. If further $yz \in E(G)$, then either $G = D_2 \subset D_7$ or $G = D_5$, as $\omega(G) = 3$. For $yz \notin E(G)$, since G_{11} is forbidden, we have $yw \in E(G)$ and $uz \in E(G)$, giving $G = D_9$. ◇

Claim 4. *If $|T_2| = 1$ and $|T_1| \leq 2$, then G is an induced subgraph of some of $D_3, D_5, D_7, D_{12}, D_{14}$.*

Proof. If $|T_1| = |T_2| = 1$, then $G \subset D_5$ or $G \in \{H_7, W_1\} \subset D_{12}$, as $K_{1,3}$ is forbidden. If $|T_2| = 1$, $|T_1| = 2$, either D_3 or G_{10} is a subgraph of G, where $T_1 = \{x, y\}$ as in Figs. 2 and 4. In the former case, we have either $G = D_3$ (for $xy \notin E(G)$) or $G = H_8 \subset D_5$ (for $xy \in E(G)$). In the latter case, we have $G = H_9 \subset D_7$ or $G = H_{16} \subset D_{14}$, as $K_{1,3}$ and G_{10} are forbidden. ◇

Amalgamating the obtained results, we arrive at the assertion given in the formulation of the statement. ■

On the basis of Lemmas 3.2 and 3.4 we obtain the following remark.

Remark 3.5. If G is a connected $K_{1,3}$-free graph with $\omega(G) \leq 3$, then $\lambda_2(G) \leq 1$ if and only if G is an induced subgraph a graph belonging to $\{C_5, D_h, D_{12}, D_{14}, D_{15} \mid 3 \leq h \leq 10\} \cup \mathcal{D}$.

We now turn our attention to the case $\omega(G) = 4$.

Lemma 3.6. *If $G \in \mathcal{G}$ and $\omega(G) = 4$, then G is an induced subgraph of some of graphs of $\{D_4, D_7, D_8, D_h \mid 11 \leq h \leq 15\} \cup \mathcal{D}$.*

Proof. Let i, j, k, s be different positive integers. Since G_{12} is forbidden and $\omega(G) = 4$, by Lemma 3.3(1) and (5), we get the following fact.

Fact 2. *We have $|T_{x_i}| \leq 1$ and $|T_{x_ix_j}| \leq 2$, where $|T_{x_ix_j}| = 2$ implies that $T_{x_ix_j}$ induce an edge. Moreover, every vertex of $T_{x_ix_j}$ is adjacent to every vertex of $T_{x_ix_k}$.*

We proceed with the following one.

Fact 3. *If $|T_{x_ix_j}| = 2$, then $|T_{x_ix_k}| = 0$, every vertex of $T_{x_ix_j}$ is adjacent to every vertex of $T_{x_sx_k}$ and every vertex of T_{x_k} is adjacent to exactly one vertex of $T_{x_ix_j}$.*

Proof. If $|T_{x_ix_k}| \geq 1$, then H_{19} is an induced subgraph of G by Fact 2, and so $G_3 \subset G$, a contradiction.

We now suppose that $T_{x_sx_k} \cup T_{x_k} \neq \emptyset$ and that some vertex of $T_{x_ix_j}$ is not adjacent to a vertex, say u, of $T_{x_sx_k} \cup T_{x_k}$. If $u \in T_{x_sx_k}$, since G_1 is forbidden and the vertices of $T_{x_ix_j}$ are adjacent, by Fact 2, u is adjacent to at least one vertex of $T_{x_ix_j}$. Combining this with the fact that G_3 is forbidden, we deduce that u is adjacent to both vertices of $T_{x_ix_j}$. If $u \in T_{x_k}$, since G_4 is forbidden, u is adjacent to at least one vertex of $T_{x_ix_j}$. As before, since G_3 is forbidden, it follows that u is adjacent to exactly one vertex of $T_{x_ix_j}$. ◇

Fact 4. *If $|T_2| \geq 3$, then $|T_1| = 0$.*

Proof. Assume that $T_{x_1} \neq \emptyset$, then $T_{x_1x_j} = \emptyset$ by Lemma 3.3(5), and so $|T_2| \leq 3$ by Fact 3. This implies that $|T_2| = 3$. Further, by Fact 3, we get $|T_{x_2x_3}| = |T_{x_3x_4}| = |T_{x_2x_4}| = 1$ and we may suppose that $T_{x_1} = \{x\}$. Then $T_1 = \{x\}$ and the vertices of T_2 induce a triangle K_3' by Fact 2 and Lemma 3.3(5). Thus, H_{20} is a subgraph of G. Since G_9 is forbidden, x is adjacent to at least one vertex of K_3'. If x is adjacent to exactly one vertex of K_3', then $G_{10} \subset G$. Otherwise, x is adjacent to either two or three vertices of K_3', which implies $G_{13} \subset G$. ◇

Fact 5. *If $T_{x_i} \neq \emptyset$ and $T_{x_jx_s} \neq \emptyset$, then $T_{x_jx_k} = \emptyset$ for $k \notin \{i, j, s\}$.*

Proof. If $T_{x_jx_k} \neq \emptyset$ then, by Lemma 3.3(5), the vertices of $T_{x_jx_s} \cup T_{x_jx_k}$ are adjacent. Since G_{10} and G_{13} are forbidden, a vertex x of T_{x_i} is adjacent to exactly one vertex of $T_{x_jx_s} \cup T_{x_jx_k}$ but then $K_{1,3} \subset G$, and we are done. $\diamond$

Claim 5. *If $T_0 = \emptyset$, $T_1 \neq \emptyset$ and $T_2 \neq \emptyset$, then G is an induced subgraph of D_{11}, D_{12} or some graph of $\mathcal{D}$.*

Proof. Suppose that $T_{x_1} \neq \emptyset$. By Lemma 3.3(5) and Fact 4, $T_{x_1x_j} = \emptyset$ and $|T_2| \leq 2$. By Fact 2, we have $|T_{x_1}| = 1$, say $T_{x_1} = \{x\}$.

Case 1: $|T_2| = 2$. By Lemma 3.3(5) and Fact 3, we have either $|T_{x_ix_j}| = 2$ or $|T_{x_ix_j}| = |T_{x_ix_k}| = 1$ for $1 \notin \{i, j, k\}$. From Fact 5, we have $|T_{x_ix_j}| = 2$, and we may suppose that $|T_{x_2x_3}| = 2$. Then the vertices of $T_{x_2x_3}$ are adjacent, by Fact 2. If $|T_1| = 1$ (which means that $T_1 = \{x\}$), then from Fact 3, x is adjacent to exactly one vertex of $T_{x_2x_3}$, and thus $G = H_{21} \subset D_{11}$. Let further $|T_1| = 2$, by Fact 2 and Lemma 3.3(5). Then, by Fact 2 and Lemma 3.3(5), we may take $T_{x_4} = \{y\}$. By Fact 3, y is adjacent to exactly one vertex of $T_{x_2x_3}$. If x and y are adjacent to the same vertex of $T_{x_2x_3}$, then $xy \in E(G)$, as $K_{1,3}$ is forbidden. In this case, $G_{12} \subset G$. Thus, x and y are adjacent to different vertices of $T_{x_2x_3}$, and thus $xy \notin E(G)$, as $K_{1,3}$ is forbidden. This implies $G = D_{11}$.

Case 2: $|T_2| = 1$. By Lemma 3.3(5), we may suppose that $|T_{x_2x_3}| = 1$, say $T_{x_2x_3} = \{u\}$. If $T_1 = \{x\}$, then either $G \subset H_{22} \subset \mathcal{D}$ (for $ux \notin E(G)$) or $G \subset H_{23} \subset D_{12}$ (for $ux \in E(G)$). For $T_1 \neq \{x\}$, by Fact 2 and Lemma 3.3(5), we have $|T_1| = 2$, and then we may suppose that $T_{x_4} = \{y\}$.

If $xy \in E(G)$, then u is adjacent to exactly one of x, y, as G_3 and G_9 are forbidden, but then $K_{1,3} \subset G$. Thus, $xy \notin E(G)$. Since $K_{1,3}$ is forbidden, u is adjacent to at most one of x, y, which implies either $G = H_{22} \subset \mathcal{D}$ or $G = H_{23} \subset D_{12}$. $\diamond$

Claim 6. *If $T_0 = \emptyset$, $T_1 = \emptyset$ and $T_2 \neq \emptyset$, then G is an induced subgraph of D_7, D_{13}, D_{14} or D_{15}.*

Proof. We first suppose that $|T_{x_ix_j}| = 2$ for some edge x_ix_j of K_4 and without loss of generality that this edge is x_1x_2. The vertices of $T_{x_1x_2}$ are adjacent, by Fact 2, and then since T_0, T_1 are empty, from Fact 3, we conclude that $|T_{x_ix_3}| = |T_{x_ix_4}| = 0$ for $i \in \{1, 2\}$, and thus $G \subset D_{15}$ irrespective of $|T_{x_3x_4}|$.

We now suppose that $|T_{x_ix_j}| \leq 1$ holds for each edge x_ix_j of K_4. Then $1 \leq |T_2| \leq 6$, and in what follows we consider all the possibilities.

If $|T_2| = 1$, then it is easily checked that $G \subset D_7$.

If $|T_2| = 2$, then the neighbours of T_2 in K_4 induce either $2K_2$ or P_3. In the former case, H_{24} is a subgraph of G, and thus $G \subset D_{13}$ independently on whether $xy \in E(G)$ or $xy \notin E(G)$, where $T_2 = \{x, y\}$ as in Fig. 3. In the latter case, we get $G \subset D_7$, by Lemma 3.3(5).

If $|T_2| = 3$, then the neighbours of T_2 in K_4 induce either P_4 or K_3. As before, we get $G \subset D_{13}$ (in the former case, since H_{25} is a subgraph of G) and $G = H_{26} \subset D_7$ (in the latter).

If $|T_2| = 4$, then the neighbours of T_2 in K_4 induce either C_4 or U, where U is obtained by deleting the pendant vertex from H_2. In the former case, H_{27} is a subgraph of G, by Fact 2. Then either $G = H_{27} \subset D_7$ or $G \in \{D_{13}, D_{14}\}$. In the latter case, H_{28} is a subgraph of G, by Fact 2. Since G_{13} is forbidden, we have $xy \notin E(G)$ (see Fig. 3), and thus $G = H_{28} \subset D_7$.

If $|T_2| = 5$, then the neighbours of T_2 in K_4 induce $K_4 - e$, and thus G contains H_{29} as a subgraph, by Fact 2. If either $ux \in E(G)$ or $yv \in E(G)$ (see Fig. 3), then $G_{13} \subset G$. Thus, $G = H_{29} \subset D_7$.

If $|T_2| = 6$, then D_7 is a subgraph of G, by Fact 2. As before, we easily get $G = D_7$. $\diamond$

Claim 7. *If $T_2 = \emptyset$, then G is an induced subgraph of D_4, D_{12} or some graph of $\mathcal{D}$.*

Proof. We may suppose that $T_1 \neq \emptyset$, since for otherwise $G = K_4 \subset \mathcal{D}$. If $T_0 \neq \emptyset$, then G contains G_{14} as an induced subgraph. Hence, $T_0 = \emptyset$. Together with the assumption of this claim and Fact 2, this implies $|T_1| \leq 4$.

If $|T_1| = 1$, then G is obtained by deleting the pendant vertex of G_{14}, and thus $G \subset D_{12}$. If $|T_1| = 2$, then H_{30} is a subgraph of G, by Fact 2. In this case, either $G = D_4$ (if the vertices of T_1 are adjacent) or $G = H_{30} \subset \mathcal{D}$ (otherwise).

If $|T_1| = 3$ or $|T_1| = 4$, in the same way we conclude that H_{31} is a subgraph of G, and then we easily deduce that the vertices of T_1 induce an empty graph (as G_6, G_7, G_8 are forbidden), which yields $G \subset H_{32} \subset \mathcal{D}$. ◇

Claim 8. *If $T_0 \neq \emptyset$, $T_1 = \emptyset$ and $T_2 \neq \emptyset$, then G is an induced subgraph of D_8.*

Proof. We first eliminate the possibility that $|T_0| \geq 2$. Namely, since every vertex of T_2 is adjacent to at most one vertex of T_0 then, by Lemma 3.3(2) and Fact 2, one of H_{33}, H_{34} or H_{35} is a subgraph of G. Since every vertex of T_2 is adjacent to at most one vertex of T_0, $G_4 \subset G$ if H_{33} is a subgraph of G, and $K_{1,3} \subset G$ if H_{34} is a subgraph of G. If H_{35} is a subgraph of G, then H_{36} is an induced subgraph of G, as G_9 is forbidden, but then $K_{1,3} \subset G$.

Thus, $|T_0| = 1$. We first suppose that $|T_{x_ix_j}| = 2$ for some edge x_ix_j of K_4, say $T_{x_1x_2} = \{x, y\}$ and $T_0 = \{u\}$. Then, $xy \in E(G)$ and $|T_{x_1x_3}| = |T_{x_1x_4}| = |T_{x_2x_3}| = |T_{x_2x_4}| = 0$ by Facts 2, 3. Since G_1 and G_4 are forbidden, u is non-adjacent to x, y. This implies that $T_{x_3x_4} \neq \emptyset$ and u is adjacent to some vertex of $T_{x_3x_4}$, as $T_0 \neq \emptyset$. If $|T_{x_3x_4}| = 2$, then either $G_1 \subset G$ or $G_4 \subset G$. Hence, $|T_{x_3x_4}| = 1$, and so H_{37} is a subgraph of G, by Fact 3. Concerning once again $ux, uy \notin E(G)$, we get $K_{1,3} \subset G = H_{37}$, a contradiction.

We now suppose that $|T_{x_ix_j}| \leq 1$ for all edges of K_4. If G contains H_{38} as a subgraph, then either $K_{1,3}$ or G_{11} is an induced subgraph of G. For otherwise, on the basis of Lemma 3.3(5), we get $|T_2| \leq 2$. If $|T_2| = 1$, then $G = W_6 \subset D_8$. If $|T_2| = 2$, then H_{39} is a subgraph of G (since H_{38} is not). If $xy \in E(G)$, where $x, y \in V(H_{39})$ as in Fig. 3, then $K_{1,3} \subset G$ or $G_3 \subset G$. If $xy \notin E(G)$, since G_9 is forbidden, observing once again H_{39}, we get $xz \in E(G)$, and thus $G = D_8$. ◇

Claim 9. *There is no graph of $\mathcal{G}$ for which T_0, T_1 and T_2 are all non-empty.*

Proof. Assume that T_0, T_1 and T_2 are non-empty for some $G \in \mathcal{G}$. Since G_{14} is forbidden, there are no edges between T_0 and T_1. Combining this with Lemma 3.3(5), we get that G contains H_{40} as a subgraph. In this case G_6 or $K_{1,3}$ is an induced subgraph of G, a contradiction. ◇

Amalgamating the obtained results, we arrive at the desired assertion. ■

We now proceed with $\omega(G) \geq 5$.

Lemma 3.7. *If $G \in \mathcal{G}$ and $\omega(G) \geq 5$, then G is an induced subgraph of some of graphs of $\{D_{12}, D_{16}\} \cup \mathcal{D}$.*

Proof. Let K_q be a fixed maximal clique of G, and let i, j, k be different positive integers. Since $K_5 - e$ is forbidden, every vertex outside K_q is adjacent to at most two vertices of K_q. Since $K_{1,3}$, G_{12} are forbidden, we have the following fact.

Fact 6. *$|T_{x_ix_j}| \leq 1$ holds for each edge x_ix_j of K_q and every vertex of K_q is adjacent to at most one vertex of T_1.*

Fact 7. *If $|T_{x_ix_j}| = 1$, then $|T_{x_ix_k}| = 0$ holds for each edge x_ix_k.*

Proof. If $|T_{x_ix_j}| = |T_{x_ix_k}| = 1$ (by Fact 6, this is the only possibility that contradicts our statement) then, since $K_{1,3}$ is forbidden, the vertices of $T_{x_ix_j}$ and $T_{x_ix_k}$ are adjacent, which implies $G_5 \subset G$, a contradiction. ◇

Fact 8. *Every vertex of K_q is adjacent to at most one vertex out of K_q.*

Proof. Otherwise, a vertex of K_q with at least two neighbours outside K_q would be adjacent to a vertex of T_1 and a vertex of T_2 (by Figs. 6, 7), but this contradicts Lemma 3.3(5). ◇

Fact 9. $T_0 = \emptyset$.

Proof. A vertex of T_0 would be adjacent to a vertex of T_1 or a vertex of T_2, but in any case we would have $G_{14} \subset G$. ◇

Fact 10. *Let $u_1, u_2 \in T = V(G) \setminus V(K_q)$ and suppose that u_i is adjacent to exactly p_i vertices of K_q, for $1 \leq i \leq 2$. If $q \geq 3 + p_1 + p_2$, then u_1 is non-adjacent to u_2.*

Proof. If $u_1u_2 \in E(G)$, by Fact 8, u_1 and u_2 do not have a common neighbour in K_q. Combining this with $q \geq 3 + p_1 + p_2$, we get $G_{14} \subset G$. ◇

To complete the proof, we assume that there is no graph of $\mathcal{D}$ such that G is its induced subgraph. Since every vertex of K_q is adjacent to at most one vertex out of K_q and every vertex out of K_q is adjacent to at most two vertices of K_q, we may suppose the existence of vertices $u_1, u_2 \in T$ such that $u_1u_2 \in E(G)$ (otherwise, $G \subset D \in \mathcal{D}$). Suppose that u_i is adjacent to exactly p_i vertices of K_q, for $1 \leq i \leq 2$. Then we may assume that $1 \leq p_1 \leq p_2 \leq 2$, and so $5 \leq q \leq 6$, by Fact 10.

Case 1: $q = 6$. Then $p_1 = p_2 = 2$, by Fact 10. If $n = 8$, then $G = D_{16}$, by Fact 8, as G is not an induced subgraph of some D of $\mathcal{D}$.

Assume further that $n \geq 9$, and let u be a vertex of $V(G) \setminus (V(K_6) \cup \{u_1, u_2\})$. By Fact 9, we have $u \notin T_0$. If $u \in T_1$, then u is non-adjacent to u_1, u_2, by Fact 10. This implies $G_6 \subset G$, by Fact 8. If $u \in T_2$ then, since $K_{1,3}$ and G_9 are forbidden, u is adjacent to u_1, u_2, and then u, u_1, u_2 induce a triangle whence $G_3 \subset G$.

Case 2: $q = 5$. Then either $p_1 = p_2 = 2$ or $p_1 = 1$ and $p_2 = 2$, by Fact 10. If $n = 7$, then $G \subset D_{16}$, as $u_1u_2 \in E(G)$.

Assume further that $n \geq 8$, and let u be a vertex of $V(G) \setminus \big(V(K_5) \cup \{u_1, u_2\}\big)$. As before we have $u \notin T_0$.

We first suppose that $p_1 = p_2 = 2$. By Fact 8, we have $u \in T_1$ and $n = 8$. If u is non-adjacent to u_1, u_2, then $G = D_{12}$, as $u_1u_2 \in E(G)$. Otherwise, u is adjacent to both u_1, u_2, as $K_{1,3}$ is forbidden, but this yields $G_3 \subset G$.

We now suppose that $p_1 = 1$ and $p_2 = 2$. If $u \in T_1$, then u is adjacent to at least one of u_1, u_2, by Fact 8, as G_6 is forbidden and $u_1u_2 \in E(G)$. Combining this with the fact that $K_{1,3}$ is forbidden, we get that u is adjacent to both u_1, u_2. This implies $G_8 \subset G$. If $u \in T_2$, since G_9 is forbidden, u is adjacent to at least one of u_1, u_2, as follows by Fact 8 since $u_1u_2 \in E(G)$. As before, we get that u is adjacent to both u_1, u_2, which implies $G_3 \subset G$, and we are done. ■

We are ready to prove our main result.

Proof of Theorem 2.1. For every graph of $\mathcal{S} = \{C_5, D_3, D_4, \ldots, D_{16}\} \cup \mathcal{D}$ we have $\lambda_2 \leq 1$. Namely, for $C_5, D_3, D_4, \ldots, D_{16}$ this is checked by inspection. Moreover, we know from [8, Theorem 1] that every graph of $\mathcal{D}$ has exactly one eigenvalue greater than 1. Therefore, if G is an induced subgraph of a graph of $\mathcal{S}$, then its second largest eigenvalue does not exceed 1.

Conversely, if $\lambda_2(G) \leq 1$, then from Lemmas 3.2, 3.4, 3.6 and 3.7, we can conclude that G is an induced subgraph of some graph of $\mathcal{S}$, and the proof is completed. ■

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The Maximum Number of Spanning Trees of a Graph with Given Matching Number

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Abstract
The number of spanning trees of a graph G is the total number of distinct spanning subgraphs of G that are trees. Feng et al. determined the maximum number of spanning trees in the class of connected graphs with n vertices and matching number β for $2 \leq \beta \leq n/3$ and $\beta = \lfloor n/2 \rfloor$. They also pointed out that it is still an open problem to the case of $n/3 < \beta \leq \lfloor n/2 \rfloor - 1$. In this paper, we solve this problem completely.

Keywords Graph · Spanning tree · Matching number

Mathematics Subject Classification 05C50 · 15A18

1 Introduction

Throughout this paper, we consider simple graph $G = (V, E)$ with vertex set $V(G)$ ($|V(G)| = n$) and edge set $E(G)$. The Laplacian matrix of graph G is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees and $A(G)$ is the adjacency matrix of G. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ be the eigenvalues of $L(G)$. The number of spanning trees of G, denoted by $\kappa(G)$, is the total number of distinct spanning subgraphs of G that are trees. It is well known that

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$$\kappa(G) = \frac{1}{n}\prod_{i=1}^{n-1}\mu_i.$$

We consider the problem of determining the extremal graphs with the maximum number of spanning trees from some special classes of graphs. The application of this problem is (i) in the area of experimental design [2] and (ii) in the network theory [15]. For calculating $\kappa(G)$ of a graph G, we do not have any clear formula in the literature except for some special cases. However, in the design of reliable probabilistic networks, the value (or the bound) on the number of spanning trees is very important (see, [22]).

As usual, we denote by K_n and $K_{1,n-1}$, the complete graph and the star of order n, respectively. We now recall some definitions in graph theory. Two distinct edges in a graph G are independent if they do not have a common end vertex. A **matching** in G is a set of pairwise independent edges. A **maximum matching** in G is a matching of maximum cardinality. The **matching number** of the graph G, denoted by $\beta(G)$, is the number of edges in a maximum matching. Obviously, $\beta(G) = 0$ if and only if G is an empty graph. For a connected graph G with $n \geq 2$ vertices, $\beta(G) = 1$ if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$. Thus, we consider graphs with matching number at least 2. The vertex disjoint union of the graphs G and H is denoted by $G \cup H$. The joint of two graphs G and H is $G \vee H = \overline{\overline{G} \cup \overline{H}}$, where $\overline{G}$ is the complement of graph G.

Problem 1.1 *Given a set $\mathcal{G}$ of graphs, find an upper bound for the number of spanning trees in this set and characterize the graphs at which the maximal number of spanning trees is attained.*

This problem attracts much attention in the literature. Li et al. [16] completely resolved this problem for given connectivity or chromatic number of graphs. For bicyclic and tricyclic graphs, this problem has been resolved in [21,22]. In [1], the authors obtained several sharp upper bounds for $\kappa(G)$ based on the so-called normalized Laplacian eigenvalues (for details on this subject, see [3,4]). Ma and Yao [18] studied the number of spanning trees of a class of self-similar fractal models and obtained an approximate numerical value of its spanning tree entropy. For some other excellent results on this topic including lower and upper bounds, please refer to [5,6,8–15,17,19,20].

Let $\mathcal{G}_{n,\beta}$ be the set of graphs on n vertices with matching number β, and denote by $\overline{G}$ the complement graph of G. Feng et al. presented the following result in the proof of Theorem 1.1 [7].

Proposition 1.2 [7] *Let $G \in \mathcal{G}_{n,\beta}$ and $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. Then*

$$\kappa(G) \leq \max\left\{ n^k (k+1)^{n-2\beta+k} (2\beta-k)^{2\beta-2k-2} : \ 0 \leq k \leq \beta-1 \right\},$$

where equality holds if and only if $G \cong K_{k+1} \vee \left(K_{2\beta-2k-1} \cup \overline{K_{n+k-2\beta}}\right)$.

Hereafter, let

$$f(x) = n^x\,(x+1)^{n-2\beta+x}(2\beta-x)^{2\beta-2x-2}, \quad \text{and}$$
$$\varphi(x) = \ln\, f(x) = x\ln\, n + (n-2\beta+x)\ln\,(x+1) + (2\beta-2x-2)\ln\,(2\beta-x).$$

Then,

$$\varphi'(x) = \ln\, n + \ln\,(x+1) - 2\ln\,(2\beta-x) + \frac{n-2\beta-1}{x+1} + \frac{x+2}{2\beta-x}$$

and

$$\begin{aligned}\varphi'(0) &= n-2\beta-1+\frac{1}{\beta}+\ln\left(\frac{n}{4\beta^2}\right),\ \ \varphi'(\beta-1)\\ &= \frac{n-\beta-1}{\beta}+\ln\left(\frac{n\beta}{(\beta+1)^2}\right) > 0. \end{aligned} \tag{1.1}$$

In [7], Feng et al. obtained a sharp upper bound on the number of spanning trees of graph G with given matching number β and the statement is as follows:

Theorem 1.3 [7] *Let $G \in \mathcal{G}_{n,\beta}$ and $2 \le \beta \le \lfloor \frac{n}{2} \rfloor$. The following statements hold:*

(1) For $\beta = \lfloor \frac{n}{2} \rfloor$, $\kappa(G) \le n^{n-2}$ with equality if and only if $G \cong K_n$;
(2) For $2 \le \beta \le \frac{n}{3}$, $\kappa(G) \le n^{\beta-1}\beta^{n-\beta-1}$ with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.

For the case of $n = 2\beta+2$ and $\beta \ge 9$, Feng et al. pointed out that (See Remark 1 of [7]), in the class of $\mathcal{G}_{n,\beta}$, $K_1 \vee \left(K_{2\beta-1} \bigcup \overline{K_{n-2\beta}}\right)$ is the maximal graph of $\kappa(G)$. They also raised the problem to solve the case of $\frac{n}{3} < \beta < \lfloor \frac{n}{2} \rfloor - 1$. In this paper, we give a solution to this problem completely (as they have solved the situation of $\beta = \lfloor \frac{n}{2} \rfloor$ and $n = 2\beta+2$, we only consider the case of $n \ge 2\beta+3$ in the following).
For $n \ge 2.3\,\beta$ and $\beta \ge 9$, in this paper, we give an upper bound on the number of spanning trees of graph G in terms of n and β, and the statement is as follows.

Theorem 1.4 *Let $G \in \mathcal{G}_{n,\beta}$ with $n \ge 2.3\,\beta$ and $\beta \ge 9$. Then*

$$\kappa(G) \le n^{\beta-1}\beta^{n-\beta-1},$$

with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.

For $2\beta+3 \le n < 2.3\beta$, in this paper, we present an upper bound on the number of spanning trees of graph G in terms of n and β, and the statement is as follows.

Theorem 1.5 *Let $G \in \mathcal{G}_{n,\beta}$ with $2\beta+3 \le n < 2.3\beta$.*

(1) If $n-2\beta-1+\frac{1}{\beta}+\ln\left(\frac{n}{4\beta^2}\right) < 0$, then

$$\kappa(G) \le \max\left\{(2\beta)^{2\beta-2},\ n^{\beta-1}\,\beta^{n-\beta-1}\right\}.$$

(2) If $n-2\beta-1+\frac{1}{\beta}+\ln\left(\frac{n}{4\beta^2}\right)>0$, *then* $\varphi'(x)$ *contains exactly two roots in the interval* $(0,\beta-1)$. *Let* α *be the smallest root of* $\varphi'(x)$ *in the interval* $(0,\beta-1)$. *Then,*

$$\kappa(G)\leq\max\Big\{f(\beta-1),\ f(\lceil\alpha\rceil),\ f(\lfloor\alpha\rfloor)\Big\}.$$

As K_n is a special case, by comparing the results of Theorem 1.3 (2) and Theorems 1.4–1.5, it is natural to ask the following problem:

Problem 1.6 *Let* $G\in\mathcal{G}_{n,\beta}$ *with* $2\beta+3\leq n<2.3\beta$. *Whether* $\kappa(G)\leq n^{\beta-1}\beta^{n-\beta-1}$ *is true or not, that is, whether* $n^{\beta-1}\beta^{n-\beta-1}$ *also uniquely maximizes* $\kappa(G)$ *in Theorem 1.5?*

However, the answer to Problem 1.6 is negative, as we have the following example.

Example 1.7 *Let* $G\in\mathcal{G}_{n,\beta}$, *where* $2\beta+3\leq n<2.3\beta$.

(i) Let $\beta=10000$ and $n=20004$. Then, $\varphi'(0)<4+\ln\left(\frac{5001}{10000^2}\right)<-5.9$, and thus, the condition of Theorem 1.5 (1) is satisfied. Using **MATLAB**, we have

$$\begin{aligned}&2(\beta-1)\ln 2\beta-(\beta-1)\ln n-(n-\beta-1)\ln\beta\\&\quad=2\times9999\times\ln(2\times10000)-9999\times\ln 20004-10003\times\ln 10000>6891,\end{aligned}$$

and thus,

$$2(\beta-1)\ln 2\beta>(\beta-1)\ln n+(n-\beta-1)\ln\beta,$$

which implies that $(2\beta)^{2\beta-2}>n^{\beta-1}\beta^{n-\beta-1}$.
(ii) Let $\beta=10000$ and $n=21000$. Then, using **Matlab** it follows that

$$\begin{aligned}&\varphi'(0)>999+\ln\left(\frac{5250}{10000^2}\right)>989,\ \varphi'(226)>0.005,\ \varphi'(227)<-0.009,\\&\varphi'(5598)<-3.6\times10^{-4}\ \text{ and }\ \varphi'(5599)>1.79\times10^{-5},\end{aligned}$$

and thus, Theorem 1.5 (2) implies that the smallest root of $\varphi'(x)$ is in $(226,227)$. Using **Matlab**, one can easily see that

$$f(226)=\max\Big\{f(226),\ f(227),\ f(9999)\Big\}.$$

2 Proofs of Theorems 1.4 and 1.5

This section is dedicated to the proofs of Theorems 1.4 and 1.5 . We firstly give the proof to Theorem 1.4.

Proof of Theorem 1.4 Let $g(x) = 2.3\beta^{2.3} - (2\beta - x)^2(x+1)^{0.3}$, where $0 \le x \le \beta - 1$. Then,

$$g'(x) = 0.1(x+1)^{-0.7}(23x + 20 - 6\beta)(2\beta - x). \tag{2.1}$$

Since $2\beta - x > 0$ always holds for $0 \le x \le \beta - 1$ and $\beta \ge 9$, by (2.1) we have

$$\begin{aligned} g(x) &\ge g\left(\frac{6\beta - 20}{23}\right) \\ &= 2.3\beta^{2.3} - \frac{400}{12167} \times 3^{0.3} \times 23^{0.7}(2\beta + 1)^{2.3} \\ &= \frac{1}{121670}\beta^{2.3}\left(279841 - 4000 \times 3^{0.3} \times 23^{0.7}\left(2 + \frac{1}{\beta}\right)^{2.3}\right) \\ &\ge \frac{1}{121670}\beta^{2.3}\left(279841 - 4000 \times 3^{0.3} \times 23^{0.7}\left(2 + \frac{1}{9}\right)^{2.3}\right) > 0. \end{aligned} \tag{2.2}$$

When $n \ge 2.3\,\beta$ and $0 \le k \le \beta - 2$, by (2.2), we obtain

$$\begin{aligned} &\left(\frac{n(k+1)}{(2\beta - k)^2}\right)^{\beta - k - 1}\left(\frac{\beta}{k+1}\right)^{n - \beta - 1} \\ &= \left(\frac{n\beta^{1.3}(k+1)}{(2\beta - k)^2(k+1)^{1.3}}\right)^{\beta - k - 1}\left(\frac{\beta}{k+1}\right)^{n - 2.3\beta + 1.3k + 0.3} \\ &\ge \left(\frac{n\beta^{1.3}}{(2\beta - k)^2(k+1)^{0.3}}\right)^{\beta - k - 1} \\ &\ge \left(\frac{2.3\beta^{2.3}}{(2\beta - k)^2(k+1)^{0.3}}\right)^{\beta - k - 1} > 1. \end{aligned}$$

Thus, for $0 \le k \le \beta - 2$ and $\beta \ge 9$,

$$n^k(k+1)^{n - 2\beta + k}(2\beta - k)^{2\beta - 2k - 2} < n^{\beta - 1}\beta^{n - \beta - 1},$$

and hence, the result follows from Proposition 1.2. □

To present the proof of Theorem 1.5, we need more lemmas as follows:

Lemma 2.1 *If $2\beta + 3 \le n < 2.3\beta$, then there exists some real number p with $0 < p < \beta - 1$ such that $\varphi'(x)$ is a strictly decreasing function for $0 \le x \le p$, and $\varphi'(x)$ is a strictly increasing function for $p \le x \le \beta - 1$.*

Proof For $0 \le x \le \beta - 1$, we define $\psi(x)$ as follows:

$$\begin{aligned}\psi(x) &= (x+1)^2 (2\beta - x)^2 \varphi''(x) \\ &= -x^3 + (4\beta - n)x^2 + 2\,(2n\beta \\ &\quad -2\beta^2 + 2\beta + 1\Big)\, x + 8\beta^3 + 8\beta^2 + 6\beta + 2 - 4n\beta^2.\end{aligned}$$

Claim 1 $\psi(x)$ **is a strictly increasing function on** $[0,\ \beta - 1]$.

Proof of Claim 1 Note that $\psi''(x) = 2\,(4\beta - n - 3x)$. Then $\psi''(x) < 0$ for $x > \frac{1}{3}\,(4\beta - n)$ and $\psi''(x) > 0$ for $x < \frac{1}{3}\,(4\beta - n)$, that is, $\psi'(x)$ is a strictly increasing function on $0 \le x \le \frac{1}{3}\,(4\beta - n)$ and a strictly decreasing function on $\frac{1}{3}\,(4\beta - n) \le x \le \beta - 1$. Thus,

$$\psi'(x) \ge \min\Big\{\psi'(0),\ \psi'(\beta - 1)\Big\}.$$

Recall that $0 \le x \le \beta - 1$ and $n \ge 2\beta$. Thus, $\psi'(\beta - 1) = \beta^2 + 2(\beta + 1)(n + 1) - 3 > 0$ and $\psi'(0) = 4n\beta - 4\beta^2 + 4\beta + 2 \ge 4\beta^2 + 4\beta + 2 > 0$. Therefore, $\psi'(x) > 0$, and hence, $\psi(x)$ is a strictly increasing function on $[0,\ \beta - 1]$. This completes the proof of **Claim** 1.

Since $0 \le x \le \beta - 1$ and by **Claim** 1, we have $\psi(0) \le \psi(x) \le \psi(\beta - 1)$. Again since $\beta \ge 11$ by $2\beta + 3 \le n < 2.3\beta$, we obtain

$$\begin{aligned}\psi(0) &= -4\beta^2\, n + 8\beta^3 + 8\beta^2 + 6\beta + 2 \\ &\le -4\beta^2(2\beta + 3) + 8\beta^3 + 8\beta^2 + 6\beta + 2 = -2(2\beta^2 - 3\beta - 1) < 0,\end{aligned}$$

and

$$\begin{aligned}\psi(\beta - 1) &= (\beta + 1)(4\beta - n(\beta + 1) + 7\,\beta^2 + 1) \\ &> (\beta + 1)\Big(4\,\beta - 2.3\,\beta\,(\beta + 1) + 7\,\beta^2 + 1\Big) \\ &= (\beta + 1)(1.7\,\beta + 4.7\,\beta^2 + 1) > 0.\end{aligned}$$

Combining with **Claim** 1 and $\psi(0) < 0 < \psi(\beta - 1)$, we can conclude that there is some real number p with $0 < p < \beta - 1$ such that $\psi(p) = 0$. Once again, **Claim** 1 implies that $\psi(x) < 0$ for $0 \le x < p$, $\psi(x) > 0$ for $p < x \le \beta - 1$ and $\psi(p) = 0$. Recall that $\psi(x) = (x + 1)^2(2\beta - x)^2\varphi''(x)$ and $0 \le x \le \beta - 1$. Thus, $\varphi''(x) < 0$ for $0 \le x < p$, $\varphi''(x) > 0$ for $p < x \le \beta - 1$ and $\varphi''(p) = 0$. This completes the proof of this result. □

Lemma 2.2 *If* $n - 2\beta - 1 + \frac{1}{\beta} + \ln\left(\frac{n}{4\beta^2}\right) > 0$ *and* $2\beta + 3 \le n < 2.3\beta$, *then* $\varphi'(0.2\beta) < 0$ *and* $\varphi'(x)$ *contains exactly two roots in the interval* $(0,\ \beta - 1)$.

Proof By (1.1), we have $\varphi'(0) > 0$ and $\varphi'(\beta - 1) > 0$. Combining this with Lemma 2.1, to complete the proof, it suffices to show that $\varphi'(0.2\beta) < 0$.

Since $2\beta + 3 \le n < 2.3\beta$, we have

$$\begin{aligned}\varphi'(0.2\beta) &= \ln(0.2\beta+1) - 2\ln(1.8\beta) + \ln n + \frac{n-2\beta-1}{0.2\beta+1} + \frac{0.2\beta+2}{1.8\beta} \\ &< \ln(0.2\beta+1) - 2\ln(1.8\beta) + \ln(2.3\beta) + \frac{0.3\beta-1}{0.2\beta+1} + \frac{0.2\beta+2}{1.8\beta} \\ &= \ln\left(\frac{2.3\beta\,(0.2\beta+1)}{(1.8\beta)^2}\right) + \frac{29\beta^2-60\beta+100}{18\beta(\beta+5)}. \end{aligned} \tag{2.3}$$

Denote by

$$h(t) = \ln\left(\frac{2.3t\,(0.2t+1)}{(1.8t)^2}\right) + \frac{29t^2-60t+100}{18t(t+5)}.$$

Then, $h'(t) = \dfrac{5(23t^2-130t-100)}{18t^2(t+5)^2}$, which implies that $h'(t) > 0$ for $t > \dfrac{65+15\sqrt{29}}{23}$ and $h'(t) < 0$ for $11 \le t < \dfrac{65+15\sqrt{29}}{23}$. Furthermore, since $h(11) < -0.64$ and $h(+\infty) = \ln\left(\frac{23}{162}\right) + \frac{29}{18} < -0.34$, we can conclude that $h(t) < 0$ for $t \ge 11$. Combining this with $\beta \ge 11$ by $2\beta+3 \le n < 2.3\beta$, we have $\varphi'(0.2\beta) < 0$ by (2.3), as desired. □

We are now ready to prove Theorem 1.5.

Proof of Theorem 1.5 **(1)** $n - 2\beta - 1 + \frac{1}{\beta} + \ln\left(\frac{n}{4\beta^2}\right) < 0$. Then $\varphi'(0) < 0$ and $\varphi'(\beta-1) > 0$, by (1.1). Combining this with $\varphi'(x)$ being a strictly decreasing function on $[0, p]$ and a strictly increasing function on $[p, \beta-1]$ by Lemma 2.1, we can conclude the existence of some real number q with $0 < q < \beta - 1$ such that $\varphi'(x) < 0$ holds for $0 \le x < q$, $\varphi'(x) > 0$ holds for $q < x \le \beta - 1$ and $\varphi'(q) = 0$. Thus, $\varphi(x)$ is a strictly decreasing function on $[0, q]$ and a strictly increasing function on $[q, \beta-1]$. Since $\varphi(x) = \ln f(x)$ with Proposition 1.2, we obtain

$$\begin{aligned}\kappa(G) &\le \max\left\{n^k(k+1)^{n-2\beta+k}(2\beta-k)^{2\beta-2k-2} : 0 \le k \le \beta-1\right\} \\ &= \max\left\{(2\beta)^{2\beta-2},\ n^{\beta-1}\,\beta^{n-\beta-1}\right\}.\end{aligned}$$

(2) $n - 2\beta - 1 + \frac{1}{\beta} + \ln\left(\frac{n}{4\beta^2}\right) > 0$. By Lemma 2.2, $\varphi'(0.2\beta) < 0$ and $\varphi'(x)$ contains exactly two roots in the interval $(0, \beta-1)$. Let α be the smallest root of $\varphi'(x)$ in the interval $(0, \beta-1)$. Then $\varphi'(x) > 0$ holds for $0 < x < \alpha$, as $\varphi'(0) > 0$.

Recall that $\varphi'(x)$ is strictly decreasing on $[0, p]$ and strictly increasing on $[p, \beta-1]$ by Lemma 2.1. Combining this with $\varphi'(x) > 0 = \varphi'(\alpha)$ holds for $0 \le x < \alpha$, $\varphi'(\beta-1) > 0$ and $\varphi'(0.2\beta) < 0$ by Lemma 2.2, we can conclude that $\alpha < p < \beta-1$.

In this case, $\varphi'(p) < \varphi'(\alpha) = 0$. Since $\varphi'(x)$ is strictly increasing on $[p, \beta-1]$ by Lemma 2.1 and since $\varphi'(\beta-1) > 0$, there exists $\gamma \in (p, \beta-1)$ such that $\varphi'(\gamma) = 0$.

Once again, Lemma 2.2 implies that $\varphi'(x) < 0$ for $x \in (\alpha, \gamma)$ and $\varphi'(x) > 0$ for $x \in (0, \alpha) \bigcup (\gamma, \beta - 1)$. Thus, $\varphi(x)$ is strictly increasing for $x \in [0, \alpha]$, $\varphi(x)$ is strictly decreasing for $x \in [\alpha, \gamma]$ and $\varphi(x)$ is strictly increasing for $x \in [\gamma, \beta - 1]$. This completes the proof of (2). □

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Note

Some notes on the extremal k-generalized quasi-unicyclic graphs with respect to Zagreb indices

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ABSTRACT

In this note, we point out some problems in the proofs and the main results of Javaid, Jamil and Tomescu (2019), and we also give the correct versions of them.

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1. Introduction

In this paper, we only consider simple undirected graphs. For a graph G and a vertex u of G, denote by $N_G(u)$ and $d_G(u)$ the neighbor set and the degree of vertex u, respectively. If there is no risk of confusion, we always simplify $N_G(u)$ and $d_G(u)$ as $N(u)$ and $d(u)$, respectively. Especially, a vertex with degree one will also be referred as a *pendant vertex*. Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$ and the degree of vertex v_i equals d_i for $i = 1, 2, \ldots, n$, then $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G. In the following discussions we always enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$.

Among all (vertex) degree-based graph invariants, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ [6] are two famous topological indices. They are defined as

$$M_1(G) = \sum_{v \in V(G)} d^2(v), \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

For graph G and a subset X of $V(G)$, $G - X$ is the graph obtained from G by removing the vertices of X and all edges incident to any of them. In particular, when X consists of only one vertex v, $G - \{v\}$ is always abbreviated to $G - v$. As usual, K_n, C_n and P_n denote the complete graph, cycle and path with n vertices. If G is a connected graph with n vertices and $n + c - 1$ edges, then G is called a c-*cyclic* graph. When $c = 0, 1, 2, 3$, G is called a tree, unicyclic graph, bicyclic graph and tricyclic graph, respectively. The *quasi-tree* is a graph G in which there exists a vertex $v \in V(G)$ such that $G - v$ is a tree. Similarly, if graph G has the property that $G - v$ induces a unicyclic graph for a suitable vertex v, then G is called a *quasi-unicyclic graph*. In [8], Xu et al. generalized the concept of quasi-tree to *k-generalized quasi-tree* as:

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Definition 1.1 (*[8]*). For any integer $k \geq 1$, the connected graph G is called a k-generalized quasi-tree, if there exists a subset $V_k \subseteq V(G)$ with cardinality k such that $G - V_k$ is a tree, but $G - V_{k-1}$ is not a tree for any $(k-1)$-subset of $V(G)$.

A *k-apex tree* [7,9] is defined as a connected graph G with a k-subset $V_k \subseteq V(G)$ such that $G - V_k$ is a tree but $G - X$ is not a tree for any subset $X \subseteq V(G)$ with $|X| < k$. It is not difficult to check that k-generalized quasi-trees and k-apex trees are two equivalent concepts.

In [8], the authors pointed out that any tree with at least three vertices is a quasi-tree since the deletion of any pendant vertex will produce another new tree. Thus, they called any tree a trivial quasi-tree, and other quasi-trees as non-trivial quasi-trees. With the similar reason, any unicyclic graph with at least one pendant vertex is also a quasi-unicyclic graph. Motivated by Definition 1.1, Javaid et al. [3] generalized the concept of quasi-unicyclic graph to *k-generalized quasi-unicyclic graph* as:

Definition 1.2 (*[3]*). For any integer $k \geq 1$, the connected graph G is called a k-generalized quasi-unicyclic graph, if there exists a subset $V_k \subseteq V(G)$ with cardinality k such that $G - V_k$ is a unicyclic graph but for every subset V_{k-1} of cardinality $k-1$ of $V(G)$, the graph $G - V_{k-1}$ is not unicyclic.

A 1-generalized quasi-unicyclic graph is just a quasi-unicyclic graph, but not vice versa, as $V_{k-1} = \emptyset$ in Definition 1.2 when $k = 1$. In what follows, we call the vertex set V_k in Definitions 1.1 and 1.2 as a *k-quasi vertex set*, and we use the symbol $\mathcal{U}_n^k$ to denote the class of k-generalized quasi-unicyclic graphs with n vertices.

In [3], the authors deduced the maximum and minimum values of first and second Zagreb indices in the class of k-generalized quasi-unicyclic graphs with n vertices. To prove these results, they relied on the following key lemma, namely, Lemma 1.1. However, the proof of Lemma 1.1 in [3] is not true. To be clear, we first list Lemma 1.1 together with its proof appearing in [3]:

Lemma 1.1. *If $k \geq 1$, $G \in \mathcal{U}_n^k$ and z is a vertex in a k-quasi vertex set, then for $j \in \{1, 2\}$,*
(i) $d(z) = n - 1$ if $M_j(G)$ is maximal; and (ii) $d(z) = 2$ if $M_j(G)$ is minimal.

Proof. (*i*) Let $G \in \mathcal{U}_n^k$ such that $M_j(G)$ is as large as possible. On contrary, suppose $d(z) < n - 1$, where z is a vertex of a k-quasi vertex set V_k of G. Then there exists a vertex $v \in V(G)$ such that zv is not an edge. As $G + zv \in \mathcal{U}_n^k$, we get $M_j(G + zv) > M_j(G)$, a contradiction. Hence, $d(z) = n - 1$.

(*ii*) *Let $G \in \mathcal{U}_n^k$, and suppose that $M_j(G)$ is as small as possible. If $d(z) = 1$, then z cannot be a k-quasi vertex. Suppose that $d(z) > 2$. Then there exist more than two vertices in G which are adjacent with z. Therefore, for an edge $zv \in E(G)$, we have $M_j(G - zv) < M_j(G)$ and $G - zv \in \mathcal{U}_n^k$, which is again a contradiction. It follows that $d(z) = 2$.* ■

Hereafter, let H_1, H_2, H_3, H_4, H_5, and $F_{n,k}$ be the graphs as shown in Fig. 1.1.

There are the following three problems in the proof of Lemma 1.1:

(1) The statement '$G + zv \in \mathcal{U}_n^k$' is not true in the proof of Lemma 1.1 (*i*). By Definition 1.2, H_1 is a 2-generalized quasi-unicyclic graph, since $S_1 = \{v_2, v_5\}$ is a 2-quasi vertex set of H_1, and $H_1 - u$ is not unicyclic for any vertex u. Here, we have $d_{H_1}(v_5) = 2 < 5 = n - 1$. However, $H_2 = H_1 + v_1v_5$ is not a 2-generalized quasi-unicyclic graph, as $H_2 - v_6$ is a unicyclic graph. Actually, H_2 is a quasi-unicyclic graph.

(2) The statement '*If $d(z) = 1$, then z cannot be a k-quasi vertex*' is not true in the proof of Lemma 1.1 (*ii*). By Definition 1.2, H_3 is a 2-generalized quasi-unicyclic graph, since $S_2 = \{v_6, v_7\}$ is a 2-quasi vertex set of H_3 and $H_3 - v$ is not unicyclic for any vertex v. However, $d_{H_3}(v_7) = 1$.

(3) The statement '$G - zv \in \mathcal{U}_n^k$' is not true in the proof of Lemma 1.1 (*ii*). By Definition 1.2, H_4 is a 2-generalized quasi-unicyclic graph, as $S_3 = \{v_1, v_4\}$ is a 2-quasi vertex set of H_4 with $d_{H_4}(v_4) = 3 > 2$ and $H_4 - w$ is not unicyclic for any vertex w. Denote by $G_1 = H_4 - e$, where e is an edge with v_4 as one of its end vertex. When $e \in \{v_3v_4, v_4v_8\}$, G_1 is not a 2-generalized quasi-unicyclic graph, as $G_1 - v_5$ is a unicyclic graph. When $e = v_4v_5$, G_1 is not a 2-generalized quasi-unicyclic graph, as $G_1 - v_2$ is a unicyclic graph.

Let $G_1 \vee G_2$ denote the *join graph* of two vertex disjoint graphs G_1 and G_2, that is, $G_1 \vee G_2$ is the graph having vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$. By employing Lemma 1.1, the authors proved the following main results of [3]:

Theorem 1.1 (*[3]*). *If $k \geq 1$, $n \geq k + 3$ and $G \in \mathcal{U}_n^k$, then for $j \in \{1, 2\}$, we have*

$$M_j(G) \leq M_j\left(K_{k+1} \vee \left(K_2 \cup (n-k-3)K_1\right)\right),$$

with equality if and only if $G = K_{k+1} \vee \left(K_2 \cup (n-k-3)K_1\right)$.

Theorem 1.2 (*[3]*). *If $G \in \mathcal{U}_n^1$ and $n \geq 7$, then $M_2(G) \geq 4n + 16$, where the equality holds if and only if G has two vertices of degree three and $n - 2$ vertices of degree two, where the two vertices of degree three are not adjacent.*

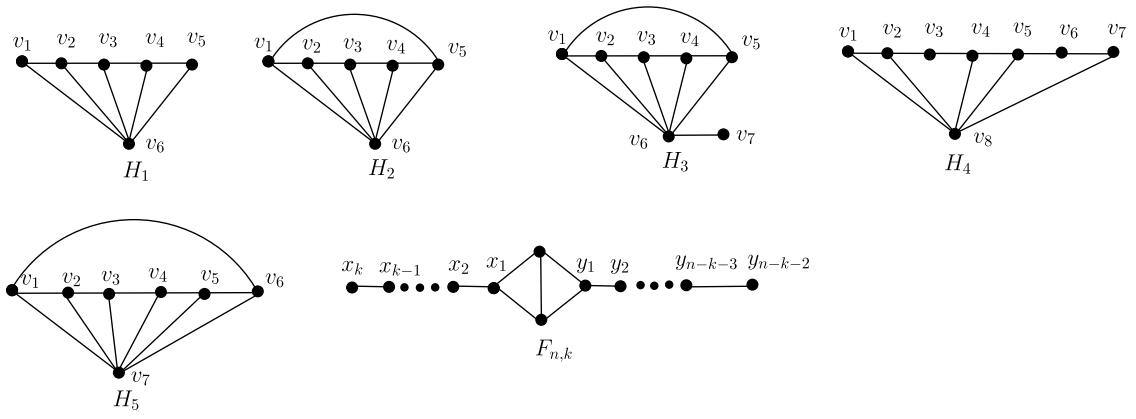


Fig. 1.1. The graphs H_1, H_2, H_3, H_4, H_5, and $F_{n,k}$.

Theorem 1.3 ([3]). *If $k \geq 1$, $n \geq 3(k+1)$ and $G \in \mathcal{U}_n^k$, then $M_1(G) \geq 4n + 10k$, with equality if and only if G has $2k$ vertices of degree three and $n - 2k$ vertices of degree two.*

If $k = 1$, then Theorem 1.3 is right, as we will show in Lemma 3.2 (i) (see Section 3). However, when $k \geq 2$, Theorem 1.3 is not true. For instance, when $k \geq 2$ and $n \geq 2k + 2$, let $S_4 = \{x_1, x_2, \ldots, x_k\}$ (see Fig. 1.1). Since $F_{n,k} - S_4$ is a unicyclic graph, and $F_{n,k} - V_{k-1}$ is not unicyclic for any subset V_{k-1} of cardinality $k-1$ of $V(F_{n,k})$, we have $F_{n,k} \in \mathcal{U}_n^k$ by Definition 1.2. On the other hand, $M_1(F_{n,k}) = 4n + 14 < 4n + 10k$, as $k \geq 2$.

In what follows, we shall give another proof to Theorems 1.1 and 1.2 respectively, which is much simpler than the proof of [3] and not depend on Lemma 1.1. Furthermore, we shall prove the following correct result in place of Theorem 1.3:

Theorem 1.4. *If $k \geq 2$, $n \geq 2k + 2$ and $G \in \mathcal{U}_n^k$, then $M_1(G) \geq 4n + 14$, with equality if and only if $G = F_{n,k}$.*

Theorem 1.4 also implies that Lemma 1.1 (ii) is not true, since $\{x_1, x_2, \ldots, x_k\}$ is a k-quasi vertex set of $F_{n,k}$ and $d_{F_{n,k}}(x_k) = 1$. Except for these problems referred as above to the paper [3], we shall remark another aspect. Actually, Definition 1.2 allows for a graph to be k-generalized quasi-unicyclic graph for several values of k. For instance, H_5 is a (1-generalized) quasi-unicyclic graph, as $H_5 - v_7$ is a unicyclic graph; it is also a 3-generalized quasi-unicyclic graph, as $S_5 = \{v_1, v_2, v_4\}$ is a 3-quasi vertex set of H_5 and any deletion of two vertices from H_5 is not unicyclic. Thus, similar to the concept of k-apex trees, we put forward the following concept:

Definition 1.3. For any integer $k \geq 1$, the connected graph G is called a k-apex unicyclic graph, if there exists a subset $V_k \subseteq V(G)$ with cardinality k such that $G - V_k$ is a unicyclic graph but for every subset W of $V(G)$ with $0 \leq |W| \leq k - 1$, the graph $G - W$ is not unicyclic. Furthermore, a 1-apex unicyclic graph is called an apex-unicyclic graph.

One can easily check that Definition 1.3 is well-defined, as if G is a k-apex unicyclic graph, then k is unique. Moreover, any unicyclic graph is not a k-apex unicyclic graph introduced in Definition 1.3, since W may be empty in Definition 1.3.

Hereafter, we denote by $\mathbb{U}_n^k$ the class of k-apex unicyclic graphs with n vertices. By Definitions 1.2 and 1.3, we easily check that any k-apex unicyclic graph is also a k-generalized quasi-unicyclic graph, and hence $\mathbb{U}_n^k \subseteq \mathcal{U}_n^k$. Besides, we also have

Proposition 1.1. *If $k \geq 1$, $n \geq k + 3$ and U is a unicyclic graph with $n - k$ vertices, then $K_k \vee U$ is a k-apex unicyclic graph with n vertices.*

By Proposition 1.1, $K_{k+1} \vee \big(K_2 \cup (n - k - 3)K_1\big) \in \mathbb{U}_n^k$ for $n \geq k + 3$. Except for this, one can easily check that any extremal graph of Theorems 1.2 and 1.4 is also a k-apex unicyclic graph with n vertices. Thus, Theorems 1.1–1.2 and 1.4 are also the corresponding extremal results for k-apex unicyclic graphs with n vertices.

2. Proofs of Theorem 1.1 and Proposition 1.1

We first give the proof to Proposition 1.1.

Proof of Proposition 1.1. Denote by $G_1 = K_k \vee U$. By contradiction, we assume that $G_1 \notin \mathbb{U}_n^k$. According to Definition 1.3 and U is a unicyclic graph, there exists $W \subset V(G_1)$ such that $F = G_1 - W$ is a unicyclic graph, where $0 \leq |W| = s \leq k-1$. For convenience, we suppose that $|W \cap V(K_k)| = s_1$ and $S_2 = W \cap V(U)$. Then, $s = s_1 + |S_2|$ and $F = K_{k-s_1} \vee \big(U - S_2\big)$.

Since $K_{k-s_1} \subseteq F$ and F is a unicyclic graph, we have $k - 3 \leq s_1 \leq k - 1$.

If $s_1 = k-3$, then $0 \le |S_2| \le 2$, as $0 \le s \le k-1$. In this case, K_{k-s_1} is a triangle and $U - S_2$ has at least one vertex since $|U| = n-k \ge 3$. Thus, $K_4 \subseteq F$, a contradiction.

If $s_1 = k-2$, then $0 \le |S_2| \le 1$ and so $U - S_2$ has at least one edge since U is a unicyclic graph. Combining this with $K_{k-s_1} = K_2$, we can conclude that $K_4 \subseteq F$, a contradiction.

If $s_1 = k-1$, then $|S_2| = 0$ and so $K_1 \vee U = F$, contrary with the fact that both U and F are unicyclic graphs. ■

In what follows, we shall provide the proof to Theorem 1.1 and we need the following lemmas:

Lemma 2.1 ([4,10,11]). *If G is a unicyclic graph with $n \ge 3$ vertices, then for $j \in \{1,2\}$, we have*

$$M_j(G) \le M_j\left(K_1 \vee \left(K_2 \cup (n-3)K_1\right)\right),$$

where the equality holds if and only if $G = K_1 \vee \left(K_2 \cup (n-3)K_1\right)$.

Lemma 2.2. *If $k \ge 1$, $G \in \mathcal{U}_n^k$ and z is a vertex in a k-quasi vertex set of G, then for $j \in \{1,2\}$, we have $d(z) = n-1$ if $M_j(G)$ is maximal.*

Proof. Let G be a graph of $\mathcal{U}_n^k$ such that $M_j(G)$ is as large as possible. By contradiction, we assume that $d(z) < n-1$ for some vertex z of a k-quasi vertex set V_k of G. From Definition 1.2, $U = G - V_k$ is a unicyclic graph. Let $G_1 = K_k \vee U$. Since $d(z) < n-1$ and $z \in V_k$, we have $G \subset G_1$ and so $M_j(G) < M_j(G_1)$. On the other hand, in view of $\mathbb{U}_n^k \subseteq \mathcal{U}_n^k$ and Proposition 1.1, we deduce that $G_1 \in \mathcal{U}_n^k$, a contradiction. ■

Proof of Theorem 1.1. Let G be a graph of $\mathcal{U}_n^k$ such that $M_j(G)$ is as large as possible. By Lemma 2.2, $G = K_k \vee U$, where U is a unicyclic graph with $n-k$ vertices.

Case 1. $j = 1$. Since $G = K_k \vee U$ and $|E(U)| = |V(U)| = n-k$, it follows that

$$\begin{aligned} M_1(G) &= k(n-1)^2 + \sum_{u \in V(U)} \left(d_U(u) + k\right)^2 = k(n-1)^2 + k^2(n-k) + 4k|E(U)| + M_1(U) \\ &= k(n-1)^2 + k^2(n-k) + 4k(n-k) + M_1(U) = k(n-1)^2 + k(n-k)(k+4) + M_1(U). \end{aligned}$$

By Lemma 2.1, $M_1(U) \le M_1\left(K_1 \vee \left(K_2 \cup (n-k-3)K_1\right)\right)$, where equality holds if and only if $U = K_1 \vee \left(K_2 \cup (n-k-3)K_1\right)$.

Case 2. $j = 2$. Recall that $G = K_k \vee U$ and $\sum_{uv \in E(U)} \left(d_U(u) + d_U(v)\right) = M_1(U)$. Thus,

$$\begin{aligned} M_2(G) &= \binom{k}{2}(n-1)^2 + k(n-1)\sum_{u \in V(U)} \left(d_U(u)+k\right) + \sum_{uv \in E(U)} \left(d_U(u)+k\right)\left(d_U(v)+k\right) \\ &= \binom{k}{2}(n-1)^2 + k(n-1)\left(2|E(U)| + k(n-k)\right) + \sum_{uv \in E(U)} \left(d_U(u)+k\right)\left(d_U(v)+k\right) \\ &= \binom{k}{2}(n-1)^2 + k(n-1)(n-k)(k+2) + \sum_{uv \in E(U)} \left(d_U(u)d_U(v) + k\left(d_U(v)+d_U(v)\right) + k^2\right) \\ &= \binom{k}{2}(n-1)^2 + k(n-1)(n-k)(k+2) + M_2(U) + kM_1(U) + k^2(n-k). \end{aligned}$$

By Lemma 2.1, $M_j(U) \le M_j\left(K_1 \vee \left(K_2 \cup (n-k-3)K_1\right)\right)$, where equality holds if and only if $U = K_1 \vee \left(K_2 \cup (n-k-3)K_1\right)$. This completes the proof of Theorem 1.1. ■

3. Proofs of Theorems 1.2 and 1.4

This section is dedicated to the proofs of Theorems 1.2 and 1.4. Actually, one can easily check that Theorem 1.2 follows from Lemma 3.2 (*ii*):

Lemma 3.1 ([1,2]). *If G is a bicyclic graph with $n \ge 7$ vertices, then for $j \in \{1,2\}$, we have $M_j(G) \ge 4n + 10 + 6(j-1)$. (i) When $j = 1$, then the equality holds if and only if G has two vertices of degree three and $n-2$ vertices of degree two, (ii) When $j = 2$, then the equality holds if and only if G has two vertices of degree three and $n-2$ vertices of degree two, where the two vertices of degree three are not adjacent.*

Lemma 3.2. *If $G \in \mathcal{U}_n^1$ and $n \ge 7$, then for $j \in \{1,2\}$, we have $M_j(G) \ge 4n + 10 + 6(j-1)$.*

(i) When $j = 1$, then the equality is reached if and only if G has two vertices of degree three and $n-2$ vertices of degree two, (ii) When $j = 2$, then the equality is reached if and only if G has two vertices of degree three and $n-2$ vertices of degree two, where the two vertices of degree three are not adjacent.

Proof. Since $G \in \mathcal{U}_n^1$, there exists one vertex v_0 such that $U = G - v_0$ is a unicyclic graph with $n-1$ vertices. We first prove the following claim:

Claim 1. $d_G(v_0) = 2$.

Proof of Claim 1: By Definition 1.2 with $k = 1$, G is not a unicyclic graph and so $d_G(v_0) \geq 2$. By contradiction, we assume that $d_G(v_0) \geq 3$ and we suppose that $v_0u \in E(G)$. Denote by $G_1 = G - v_0u$. Since $U = G_1 - v_0$ and $|E(G_1)| = |E(U)| + d_G(v_0) - 1 \geq n+1$, we have $G_1 \in \mathcal{U}_n^1$ and $M_j(G) > M_j(G_1)$, a contradiction. This completes the proof of Claim 1.

By Claim 1, $|E(G)| = |E(U)| + d_G(v_0) = n+1$ and so G is a bicyclic graph. Thus, the result follows from Lemma 3.1. ■

To prove Theorem 1.4, we need to introduce more concepts and lemmas. Let $b^{(s)}$ define s copies of integer b. Let $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ be two non-increasing sequences of real numbers. The ordering $\pi \trianglelefteq \pi'$ is called *majorization* [4,5], where $(x) \trianglelefteq (y)$ if and only if

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i, \quad \text{and} \quad \sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i \quad \text{for all } j = 1, 2, \ldots, n.$$

By $(x) \triangleleft (y)$, we means that $(x) \trianglelefteq (y)$ and $(x) \neq (y)$.

Lemma 3.3 ([4]). *Let G and G' be two connected graphs with degree sequences π and π', respectively. If $\pi \triangleleft \pi'$, then $M_1(G) < M_1(G')$.*

Lemma 3.4. *Let G be a c-cyclic graph with n vertices and degree sequence π, where $c \geq 1$. If $n \geq 2(p+c)$, $\pi \neq \pi_1$, and G has at least p pendant vertices, then $\pi_1 \triangleleft \pi$, where $p \geq 0$ and $\pi_1 = \left(3^{(p+2(c-1))}, 2^{(n-2p-2c+2)}, 1^{(p)}\right)$.*

Proof. Suppose that $\pi_1 = (d_1', d_2', \ldots, d_n')$ and $\pi = (d_1, d_2, \ldots, d_n)$. Suppose that G contains n_1 vertices of degree at least three, n_2 vertices of degree two and n_3 pendant vertices. If $d_1 = 2$, then $G = C_n$, as $c \geq 1$. This implies that $\pi = \pi_1$, a contradiction. Thus, $d_1 \geq 3$. Combining this with G containing at least p pendant vertices, we have $n_3 \geq p \geq 0$ and $n_1 \geq 1$.

We assume that $\sum_{i=1}^{j} d_i < \sum_{i=1}^{j} d_i'$ for some j.

Since $n_3 \geq p$, we have $\sum_{i=1}^{s} d_i = 2(n+c-1) - (n-s) = \sum_{i=1}^{s} d_i'$ for each s with $n-p+1 \leq s \leq n$, and $\sum_{i=1}^{s} d_i = 2(n+c-1) - (n-s) \geq 2(n+c-1) - p - 2(n-s-p) \geq \sum_{i=1}^{s} d_i'$ for each s with $n_1 + n_2 + 1 \leq s \leq n-p$.

Thus, $n_1 + 1 \leq j \leq n_1 + n_2$, and we may suppose that $j = n_1 + t$, where $1 \leq t \leq n_2$.

If $1 \leq j \leq p + 2(c-1)$, then $\sum_{i=1}^{j} d_i < 3j = \sum_{i=1}^{j} d_i'$ and so $d_n = d_{n-1} = \cdots = d_{n-p+1} = 1 \leq d_{n-p} \leq d_{n-p-1} \leq \cdots \leq d_{j+1} \leq 2$. This implies that $\sum_{i=1}^{n} d_i < 3j + 2(n-j-p) + p = 2n + j - p \leq 2(n+c-1)$, contrary with G being a c-cyclic graph. Thus, $j \geq p + 2(c-1) + 1$. Combining with $j = n_1 + t \geq p + 2(c-1) + 1$, $n = n_1 + n_2 + n_3$ and $1 \leq t \leq n_2$, we have

$$\sum_{i=1}^{j} d_i = 2(n+c-1) - n_3 - 2(n_2 - t) \geq 2(n+c-1) - p - 2(n_2 + n_3 - t - p) = \sum_{i=1}^{j} d_i',$$

a contradiction. From the above argument, we have $\pi_1 \trianglelefteq \pi$.

If $d_1 = 3$ and $n_3 = p$, then $2n - 2p + n_1 = 3n_1 + 2n_2 = 2(n+c-1) - p$, which implies that $n_1 = 2(c-1) + p$ and so $\pi_1 = \pi$, a contradiction. Thus, either $d_1 \geq 4$ or $n_3 > p$, and hence $\pi_1 \triangleleft \pi$. ■

For any connected graph H with at least one cycle, we define the *basic graph* of H, denoted by $\mathcal{B}(H)$, as the graph obtained from H by recursively deleting pendant vertices such that the resulting graph contains no pendant vertices. From the definition of basic graph, $\mathcal{B}(H)$ is unique and H is obtained from $\mathcal{B}(H)$ by attaching some trees to the vertices of $\mathcal{B}(H)$. In the coming discussion, we use the notation T_v to denote a rooted tree with root v, and we agree that T_v includes the root v.

In what follows, we may suppose that G_0 is a graph of $\mathcal{U}_n^k$ such that $M_1(G_0)$ is minimum, where $k \geq 2$ and $n \geq 2k+2$.

Lemma 3.5. *G_0 is a bicyclic graph.*

Proof. We suppose that G_0 is a c-cyclic graph with degree sequence π. We first suppose that $c = 3$. By Lemma 3.4, we have $\pi_2 \trianglelefteq \pi$, where $\pi_2 = \left(3^{(4)}, 2^{(n-4)}\right)$. By Lemma 3.3, $M_1(G_0) \geq 9 \times 4 + 4(n-4) = 4n + 20 > 4n + 14 = M_1(F_{n,k})$, contrary with the choice of G_0. Now, we consider the case of $c \geq 4$. Since there exists an edge e in some cycle of G_0 such that $G_0 - e$ is a $(c-1)$-cyclic graph and $M_1(G_0) > M_1(G_0 - e)$, we also have $M_1(G_0) > M_1(F_{n,k})$, a contradiction. Combining with $G_0 \in \mathcal{U}_n^k$, we have $1 \leq c \leq 2$.

We assume that G_0 is a unicyclic graph with unique cycle C_g. Then, G_0 is obtained from C_g by attaching some rooted trees to these vertices of C_g, and $U = G_0 - V_k$ is also a unicyclic graph with the unique cycle C_g. This implies that V_k comes from these rooted trees and so there exists W with $|W| = k-1$ (as $k \geq 2$) such that $G - W$ is also a unicyclic graph, contrary with $G_0 \in \mathcal{U}_n^k$. This completes the proof of this result. ■

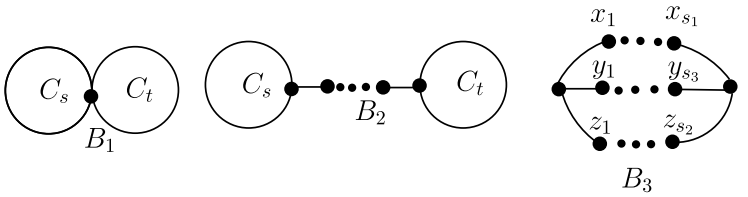


Fig. 3.1. The bicyclic graphs B_1, B_2 and B_3.

Proof of Theorem 1.4. By Lemma 3.5, G_0 is a bicyclic graph with degree sequence π and p pendant vertices. Denote by $\pi_3 = \left(3^{(4)}, 2^{(n-6)}, 1^{(2)}\right)$ and $\pi_4 = \left(3^{(5)}, 2^{(n-8)}, 1^{(3)}\right)$. Let B_1, B_2 and B_3 be the bicyclic graphs as shown in Fig. 3.1.

If $p \geq 3$, then $\pi_3 \lhd \pi_4 \trianglelefteq \pi$ by Lemma 3.4, which implies that $M_1\left(F_{n,k}\right) < M_1(G_0)$ by Lemma 3.3, a contradiction. Otherwise, $p \leq 2$. Since G_0 is a bicyclic graph, we have $\mathcal{B}(G_0) \in \{B_1, B_2, B_3\}$, where $s \geq t \geq 3$, and $s_1 \geq s_2 \geq s_3 \geq 0$ with $\min\{s_1, s_2\} \geq 1$.

Claim 1. $p = 2$.

Proof of Claim 1: By contradiction, we assume that $0 \leq p \leq 1$. We may suppose that $p = 1$, as the case of $p = 0$ can be proved similarly. In this case, G contains exactly one rooted tree T_{v_0}, where $G[V(T_{v_0})]$ is a path.

If $\mathcal{B}(G_0) \in \{B_1, B_2\}$, since $s \geq t \geq 3$ and $p = 1$, we can choose $u_1 \in C_s$ or $u_1 \in C_t$ such that $d_{G_0}(u_1) = 2$. If $\mathcal{B}(G_0) = B_3$, since $s_1 \geq 1$ and $p = 1$, we can choose $u_1 \in P_{s_1}$ such that $d_{G_0}(u_1) = 2$, where $P_{s_1} = x_1x_2 \cdots x_{s_1}$. In both cases, $U_1 = G_0 - u_1$ is a unicyclic graph. Now, we can easily obtain W_1 with $|W_1| = k - 1$ so that $G_0 - W_1$ is also a unicyclic graph, contrary to $G_0 \in \mathcal{U}_n^k$. This completes the proof of Claim 1.

Claim 2. $\mathcal{B}(G_0) = K_4 - e$ and $\pi = \pi_3$.

Proof of Claim 2: Since $p = 2$ by Claim 1 and in view of Lemmas 3.3–3.4, we have $\pi = \pi_3$. This implies that $\mathcal{B}(G_0) \in \{B_2, B_3\}$.

If $\mathcal{B}(G_0) = B_2$, then since $s \geq t \geq 3$ and $p = 2$, we can choose $u_2 \in C_s$ or C_t such that $d_{G_0}(u_2) = 2$, and hence $U_2 = G_0 - u_2$ is a unicyclic graph. Now, we can easily obtain W_2 with $|W_2| = k - 1$ so that $G_0 - W_2$ is also a unicyclic graph, contrary to $G_0 \in \mathcal{U}_n^k$.

Otherwise, $\mathcal{B}(G_0) = B_3$. If $\mathcal{B}(G_0) \neq K_4 - e$, then since $p = 2$, we can choose $u_3 \in B_3$ such that $d_{G_0}(u_3) = 2$ (Here, if possible, it is better for us to choose $u_3 \in P_{s_1}$). Similarly as the former arguments, we can prove that $G_0 \notin \mathcal{U}_n^k$, a contradiction. Thus, Claim 2 holds.

By Claim 2, we have $\pi = \pi_3$ and $\mathcal{B}(G_0) = K_4 - e$. Combining this with $G_0 \in \mathcal{U}_n^k$, it follows that $G_0 = F_{n,k}$. Conversely, if $G_0 = F_{n,k}$, then $G_0 \in \mathcal{U}_n^k$ and $M_1(G_0) = 4n + 14$, as $n \geq 2k + 2$. This completes the proof of this result. ■

CRediT authorship contribution statement

Muhuo Liu: Conceptualization, Formal analysis, Writing - original draft. **Kun Cheng:** Writing review & editing. **Ioan Tomescu:** Formal analysis, Writing review & editing.

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Spectral characterization of the complete graph removing a path

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ABSTRACT

A graph G is said to be $A-DS$ if every graph having the same adjacency spectrum is isomorphic to G. Let $K_n \setminus P_k$ be the graph obtained from the complete graph K_n with n vertices by removing all edges of a path P_k with k vertices. It was shown by Doob and Haemers that $K_n \setminus P_n$ is $A-DS$. In 2014, Cámara and Haemers conjectured that $K_n \setminus P_k$ is $A-DS$ for every $2 \leq k \leq n$, and they succeeded in proving it for $2 \leq k \leq 6$. Recently, Mao, Cioabă and Wang verified the conjecture for $7 \leq k \leq 9$. In this paper, we show that the conjecture is true for all $k \geq 20$.

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1. Introduction

Throughout this paper, G is a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $v \in V(G)$, the degree of v is denoted by $d_G(v)$, or $d(v)$ for short if no confusion occurs. Hereafter, we assume that $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$, where $d_i(G) = d_G(v_i)$ for $1 \leq i \leq n$. We call $\big(d_1(G), d_2(G), \ldots, d_n(G)\big)$ the *degree sequence* of G, and we use $\Delta(G)$ and $\delta(G)$ to denote the maximum and the minimum degree of G, respectively. A t-vertex is a vertex with degree t, and an r-*regular graph* is a graph G with $\Delta(G) = \delta(G) = r$. In particular, a 1-vertex is called a *pendant vertex*. When t is a non-negative integer, we denote by tG the union of t vertex-disjoint copies of graph G. A connected graph with n vertices and $n + c - 1$ edges is called a c-*cyclic graph*. When $c = 0$, 1, 2 and 3, a c-cyclic graph is called a tree, unicyclic graph, bicyclic graph and tricyclic graph, respectively. As usual, let K_n, C_n, P_n and $K_{1,n-1}$ be the complete graph, cycle, path and star with n vertices, respectively.

The adjacency matrix $A(G)$ of G is an $n \times n$ matrix with each entry $a_{i,j} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Since $A(G)$ is real and symmetric, its eigenvalues are real and can be ordered in a non-increasing order $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$. Denote by $S_A(G)$ the multiset of these eigenvalues, namely, $S_A(G) = \big\{\rho_1(G), \rho_2(G), \ldots, \rho_n(G)\big\}$. Two graphs G and H are said to be A-*cospectral* if they have equal adjacency spectrum. If G and H are isomorphic, then they are necessarily A-cospectral. A graph G is said to be $A-DS$ if $S_A(H) = S_A(G)$ implies that $H \cong G$ for any graph H.

In 2002, Doob and Haemers [4] showed that $K_n \setminus P_n$ is $A-DS$. In 2014, Cámara and Haemers [2] showed that $K_n \setminus P_k$ is $A-DS$ for $2 \leq k \leq 6$ and proposed the following conjecture.

Conjecture 1.1 (*Cámara and Haemers [2]*). *For any $2 \leq k \leq n$, $K_n \setminus P_k$ is $A-DS$.*

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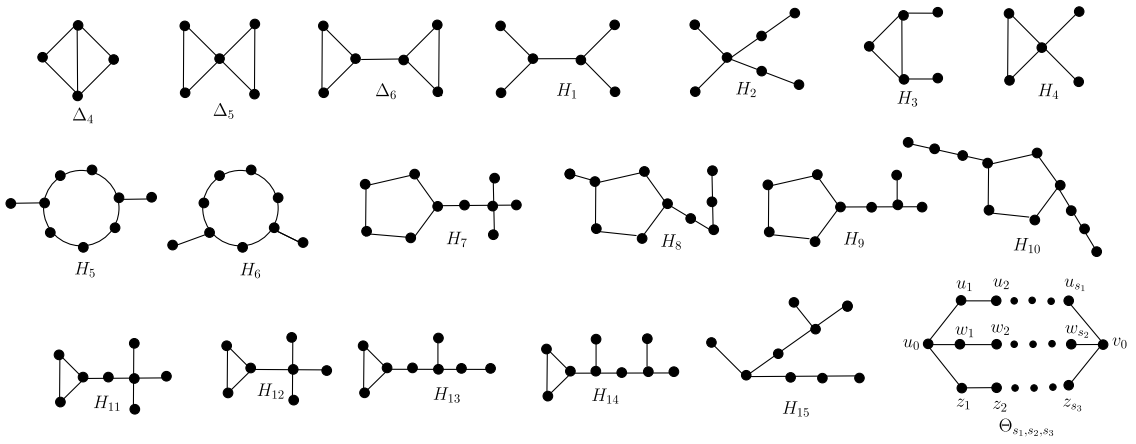


Fig. 1. The graphs Δ_4, Δ_5, Δ_6, H_1, H_2, …, H_{15} and Θ_{s_1,s_2,s_3}.

Recently, Mao, Cioabă and Wang [8] proved that Conjecture 1.1 is true for $7 \le k \le 9$. In this paper, we will prove Conjecture 1.1 holds for $k \ge 20$, as below.

Theorem 1.1. *If $k \ge 20$, then $K_n \setminus P_k$ is $A - DS$.*

We denote by $\overline{G}$ the complement graph of G. Suppose that Γ is A-cospectral with $K_n \setminus P_k$, and we will show that $\overline{\Gamma} = P_k \cup (n-k)K_1$ in the following steps.

1. We first show that $\overline{\Gamma}$ must have a specific structure, namely, $\overline{\Gamma} = \Gamma_1 \cup F \cup \left(n - |V(F)| - |V(\Gamma_1)|\right) K_1$, where Γ_1 is a c-cyclic graph and F is a forest with $\Delta(F) \le 3$ (Section 4).
2. We then show that $c \in \{0, 1\}$ (Section 5).
3. We show that $c = 1$ is impossible, and thus Γ_1 is a tree (Section 6).
4. We complete the proof by showing that $\Gamma_1 = P_k$ and F is empty (Section 7).
5. Finally, we give some concluding remarks in Section 8.

In Section 2, we describe some families of graphs that we will use as forbidden induced subgraphs of $\overline{\Gamma}$ in subsequent sections. In Section 3, we recall spectral and combinatorial properties for general graphs.

2. Forbidden induced subgraphs of $\overline{\Gamma}$

Hereafter, we let Δ_4, Δ_5, Δ_6, H_1, H_2, …, H_{15} and Θ_{s_1,s_2,s_3} be the graphs as shown in Fig. 1.

Definition 2.1. (*i*) Let W_q the tree on q vertices obtained from the path $P_{q-2} = u_1u_2\cdots u_{q-2}$ and two isolated vertices u_{q-1} and u_q by adding two edges u_2u_{q-1} and $u_{q-3}u_q$, where $q \ge 6$.

(*ii*) Let $Z_{s_1,s_2,\ldots,s_t}$ be the tree with maximum degree t (≥ 1) obtained by attaching t paths P_{s_1}, P_{s_2}, …, P_{s_t} to a single vertex.

(*iii*) Denote by $U_{g;s,t}$ the unicyclic graph obtained from a cycle C_g by attaching one path P_s to the vertex u of C_g, and then attaching another path P_t to the vertex v of C_g, where $uv \in E(C_g)$.

(*iv*) Let $U^g_{s_1,s_2,\ldots,s_t}$ be the unicyclic graph obtained from a cycle C_g by attaching t paths P_{s_1}, P_{s_2}, …, P_{s_t} to one common vertex of C_g.

From Definition 2.1, we have $H_1 = W_6$, $H_2 = Z_{2,2,1,1}$, $H_3 = U_{3;1,1}$, and $H_4 = U^3_{1,1}$.

Definition 2.2. (*i*) For any connected graph G with at least one cycle, we define the **base** of G, denoted by $\mathcal{R}(G)$, as the graph obtained from H by recursively deleting pendant vertices, to the resultant graph until no pendant vertices remain.

(*ii*) If $d_G(v) \ge 3$ and v contains at least one neighbor not in $\mathcal{R}(G)$, then v is called a **special-vertex** of G. Let $q(G)$ be **the number of special-vertices** of G.

By Definition 2.2, it is easy to see that if G is a c-cyclic graph with $c \ge 1$, then $\mathcal{R}(G)$ is the unique c-cyclic subgraph of G such that $\mathcal{R}(G)$ contains no pendant vertices, and $\mathcal{R}(G) = G$ if G contains no pendant vertices. Moreover, every vertex of degree at least three in a tree is a special-vertex, and for graphs Δ_6 and H_3, we have $\mathcal{R}(\Delta_6) = \Delta_6$, $\mathcal{R}(H_3) = C_3$, $q(\Delta_6) = 0$ and $q(H_3) = 2$.

3. Spectral and combinatorial properties of graphs

Let $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ be the eigenvalues of a symmetric matrix M of order n.

Lemma 3.1 (*Courant–Weyl Inequalities, see Theorem 2.8.1 of [1]*). *Let A and B be two Hermitian matrices of order n. For $1 \leq i, j \leq n$, we have*
(i) If $i+j-1 \leq n$, then $\lambda_{i+j-1}(A+B) \leq \lambda_i(A) + \lambda_j(B)$;
(ii) If $i+j-1 \geq n$, then $\lambda_{i+j-n}(A+B) \geq \lambda_i(A) + \lambda_j(B)$.

By taking $i = n$ and $j = 1$ or $i = j = 1$ in Lemma 3.1(i), the following corollary follows.

Corollary 3.2. *For any graph with n vertices, $\rho_1(G) + \rho_n(\overline{G}) \geq -1$ and $\rho_1(G) + \rho_1(\overline{G}) \geq n-1$.*

Let G be a graph with n vertices. Denote by $\theta_1(G;\alpha) \geq \theta_2(G;\alpha) \geq \cdots \geq \theta_n(G;\alpha)$ the eigenvalues of $A(G) + \alpha D(G)$.

Corollary 3.3. *Let G be a graph with n vertices. If $i \in \{2, 3, \ldots, n\}$ and $\alpha \geq 0$, then*

$$\alpha(n-1) - 1 - \theta_{n+1-i}(\overline{G};\alpha) \leq \theta_i(G;\alpha) \leq \alpha(n-1) - 1 - \theta_{n+2-i}(\overline{G};\alpha).$$

Proof. By setting $j = n+2-i$ in Lemma 3.1(ii), we have $\theta_i(G;\alpha) + \theta_{n+2-i}(\overline{G};\alpha) \leq \theta_2(K_n;\alpha) = \alpha(n-1)-1$. Let $j = n+1-i$ in Lemma 3.1(i). It follows that $\theta_i(G;\alpha) + \theta_{n+1-i}(\overline{G};\alpha) \geq \theta_n(K_n;\alpha) = \alpha(n-1) - 1$, and so the result follows. ■

Denote by $m_G(\alpha)$ the multiplicity of α as an eigenvalue of $A(G)$.

Lemma 3.4. *Let G be a graph with n vertices. Then, for any real number β, we have*

$$m_G(\beta) - 1 \leq m_{\overline{G}}(-1-\beta) \leq m_G(\beta) + 1.$$

Proof. We consider the following two cases:
Case 1. $m_G(\beta) \geq 2$. We may suppose that $\beta \notin \{\rho_n(G), \rho_1(G)\}$, as the case $\beta \in \{\rho_n(G), \rho_1(G)\}$ can be proved similarly. In this case, we suppose that there exists t with $1 \leq t \leq n-s-1$ such that

$$\rho_{t+s+1}(G) < \rho_{t+s}(G) = \rho_{t+s-1}(G) = \cdots = \rho_{t+2}(G) = \rho_{t+1}(G) = \beta < \rho_t(G).$$

By Lemma 3.1, we have

$$\rho_{n-t}(\overline{G}) + \beta = \rho_{n-t}(\overline{G}) + \rho_{t+1}(G) \geq \lambda_n(A(K_n)) = -1,$$
$$\rho_{n-t+2}(\overline{G}) + \beta < \rho_{n-t+2}(\overline{G}) + \rho_t(G) \leq \lambda_2(A(K_n)) = -1,$$
$$\rho_{n-t-s+2}(\overline{G}) + \beta = \rho_{n-t-s+2}(\overline{G}) + \rho_{s+t}(G) \leq \lambda_2(A(K_n)) = -1, \quad \text{and}$$
$$\rho_{n-t-s}(\overline{G}) + \beta > \rho_{n-t-s}(\overline{G}) + \rho_{s+t+1}(G) \geq \lambda_n(A(K_n)) = -1.$$

Thus, $\rho_{n-t-s}(\overline{G}) > \rho_{n-t-s+2}(\overline{G}) = \rho_{n-t-s+3}(\overline{G}) = \cdots = \rho_{n-t}(\overline{G}) = -1-\beta > \rho_{n-t+2}(\overline{G})$,
which implies the desired result.
Case 2. $m_G(\beta) \in \{0, 1\}$. Suppose to the contrary that $m_{\overline{G}}(-1-\beta) \geq m_G(\beta) + 2$. By Case 1 and in view of $\overline{(\overline{G})} = G$, $m_G(\beta) \geq m_{\overline{G}}(-1-\beta) - 1 \geq m_G(\beta) + 1$, a contradiction. ■

Lemma 3.5 (*Cauchy Interlacing, see Corollary 2.2 of [5]*). *Let B be an $n \times n$ real symmetric matrix and let B_k be a principal submatrix of B. Then for $i = 1, 2, \ldots, k$, we have*

$$\theta_{n-k+i}(B) \leq \theta_i(B_k) \leq \theta_i(B).$$

Lemma 3.6 (*Smith [9]*). *Let G be a connected graph with n vertices. Then, $\rho_1(G) < 2$ if and only if $G \in \{P_n, Z_{n-3,1,1}, Z_{2,2,1}, Z_{3,2,1}, Z_{4,2,1}\}$.*

Let $q^{(s)}$ denote the s-tuple $(q, q, \ldots, q)$. Since the sum of squares of the degrees (also famous as the first Zagreb index) is monotone with respect to the majorization ordering and the degree sequence $(3^{(2c-2)}, 2^{(n+2-2c)})$ is minimum (if exists) in the majorization ordering of degree sequences of all c-cyclic graph with n vertices (see Lemma 3.4 of [7]), we can deduce the following result by induction on c, which firstly appeared in the proof of Lemma 9 of [4].

Lemma 3.7 (*Doob and Haemers [4]*). *Let G be a c-cyclic graph with n vertices. If $c \geq 1$, then*

$$\sum_{i=1}^{n} d_i^2(G) \geq 4n + 10(c-1),$$

with equality holds if and only if the degree sequence of G is $(3^{(2c-2)}, 2^{(n+2-2c)})$.

A component (tree) of G with at least two vertices is called a *non-trivial component* (*tree*). Recall that $q(G)$ is the number of special-vertices of G (see Definition 2.2(ii)).

Lemma 3.8. *Let G be a forest with no isolated vertex. If G has n vertices and s non-trivial trees, then*

$$\sum_{i=1}^{n} d_i^2(G) \geq 4n - 6s + 2q(G), \tag{3.1}$$

with equality holds if and only if each special-vertex of G is a 3-vertex.

Proof. It suffices to show the case of $s = 1$, and we will prove it by induction on n. When $2 \leq n \leq 4$, it is easy to check that the result holds. Now, we suppose that the result holds for all trees with $n-1$ vertices, and we will prove it is also true for the case $|V(G)| = n$, where $n \geq 5$.

Let v be a pendant vertex of G and let $G_1 = G - v$. Suppose that $N_G(v) = \{u\}$. From the inductive hypothesis and $d_{G_1}(u) + 1 = d_G(u)$, we have

$$\begin{aligned}\sum_{i=1}^{n} d_i^2(G) &= \sum_{w \in V(G_1)} \big(d_{G_1}(w)\big)^2 + 1 + \big(d_G(u)\big)^2 - \big(d_{G_1}(u)\big)^2,\\ &\geq 4(n-1) - 6 + 2q\big(G_1\big) + 1 + \big(d_G(u)\big)^2 - \big(d_{G_1}(u)\big)^2\\ &= 4n - 8 + 2q\big(G_1\big) + 2d_{G_1}(u). \end{aligned}\tag{3.2}$$

If $d_G(u) = 2$, then $d_{G_1}(u) = 1$ and $q\big(G_1\big) = q\big(G\big)$. In this case, by (3.2), we have $\sum_{i=1}^{n} d_i^2(G) \geq 4n - 6 + 2q\big(G\big)$, where the equality requires that each special-vertex of G is a 3-vertex by the inductive hypothesis.

Otherwise, $d_G(u) \geq 3$, hence $d_{G_1}(u) \geq 2$ and $q(G) \leq q(G_1) + 1$. By (3.2), we have $\sum_{i=1}^{n} d_i^2(G) \geq 4n - 6 + 2q\big(G\big)$, where the equality requires that $d_{G_1}(u) = 2$ and hence $d_G(u) = 3$. Combining this with the inductive hypothesis, each special-vertex of G is a 3-vertex.

Conversely, if each special-vertex of G is a 3-vertex, it is not hard to see that equality holds in (3.1) (one only needs to consider the cases: $d_G(u) = 2$, $d_G(u) = 3$ and $d_G(u) \geq 4$). ■

The following corollary is a slight improvement of Lemma 3.7.

Corollary 3.9. *Let G be a c-cyclic graph with n vertices. If $c \geq 1$, then*

$$\sum_{i=1}^{n} d_i^2(G) \geq 4n + 10(c-1) + 2q(G), \tag{3.3}$$

where the equality holds if and only if each special-vertex of G is a 3-vertex and $\mathcal{R}(G)$ contains exactly $2(c-1)$ vertices of degree three.

Proof. We argue by induction on $q(G)$. When $q(G) = 0$, then $G \cong \mathcal{R}(G)$ and hence the result holds from Lemma 3.7. Now, we suppose that the result holds for all c-cyclic graphs with at most t special-vertices, and we will prove that the statement is true for the case $q(G) = t + 1$.

Let v be a rooted vertex of $\mathcal{R}(G)$ and T_v be the corresponding rooted tree of G, where T_v includes the root v. Let G_1 be the graph obtained from G by deleting all the vertex of $V(T_v)\backslash\{v\}$. Then, G_1 contains at most t special-vertices.

Note that $q(G_1) + q\big(T_v\big) \geq q(G) - 1$, $|V\big(G_1\big)| + |V\big(T_v\big)| = n + 1$ and $d_{G_1}(v) \geq 2$, as $v \in V\big(\mathcal{R}(G)\big)$. Thus, by the inductive hypothesis and Lemma 3.8 it follows that

$$\begin{aligned}\sum_{i=1}^{n} d_i^2(G) &= \sum_{u \in V(G_1)} \big(d_{G_1}(u)\big)^2 + \sum_{w \in V(T_v)} \big(d_{T_v}(w)\big)^2 + \big(d_{G_1}(v) + d_{T_v}(v)\big)^2 - \big(d_{G_1}(v)\big)^2 - \big(d_{T_v}(v)\big)^2,\\ &\geq 4n + 10c - 12 + 2q(G_1) + 2q\big(T_v\big) + 2d_{T_v}(v)d_{G_1}(v), \qquad (3.4)\\ &\geq 4n + 10(c-1) + 2q(G). \qquad (3.5)\end{aligned}$$

If equality holds in (3.3), then both equalities of (3.4) and (3.5) must hold. In this case, equality in (3.5) requires that $d_{T_v}(v) = 1$ and $d_{G_1}(v) = 2$. Thus, $d_G(v) = 3$. By the inductive hypothesis and Lemma 3.8, equality in (3.4) implies that each special-vertex of G_1 is a 3-vertex and $\mathcal{R}(G_1)$ contains exactly $2(c-1)$ vertices of degree three. This implies that $\mathcal{R}(G)$ contains exactly $2(c-1)$ vertices of degree three and each special-vertex of G is a 3-vertex.

Conversely, if each special-vertex of G is a 3-vertex and $\mathcal{R}(G)$ contains exactly $2(c-1)$ vertices of degree three, then (3.4) and (3.5) hold by the inductive hypothesis. ■

4. The structure of $\overline{\Gamma}$

Suppose that Γ is A-cospectral with $K_n \setminus P_k$. Recall that we will show that $\overline{\Gamma} = P_k \cup (n-k)K_1$. In this section, we show the first step, that is, $\overline{\Gamma} = \Gamma_1 \cup F \cup \big(n - |V(F)| - |V(\Gamma_1)|\big)K_1$, where Γ_1 is a c-cyclic graph and F is a forest with $\Delta(F) \le 3$. This will be presented in Remark 4.4. We also prove some useful lemmas in this section.

For any vertex subset $S \subseteq V(G)$, we denote by $G[S]$ the subgraph of G induced by S. If $\overline{\Gamma}$ does not contain a graph H as an *induced subgraph*, then H is *forbidden* in $\overline{\Gamma}$.

Lemma 4.1. *The following inequalities are true for any $n \ge k \ge 5$:*

$$(i)\ 2\cos\left(\frac{3\pi}{k+1}\right) \le \rho_2(\overline{\Gamma}) \le 2\cos\left(\frac{\pi}{k+1}\right) < 2,$$

$$(ii)\ -3 < -2\cos\left(\frac{\pi}{k+1}\right) - 1 \le \rho_n(\Gamma) \le -2\cos\left(\frac{2\pi}{k+1}\right) - 1 \le -2, \quad \textit{and}$$

$$(iii)\ 2\cos\left(\frac{2\pi}{k+1}\right) - 1 \le \rho_2(\Gamma) \le 2\cos\left(\frac{\pi}{k+1}\right) - 1 < 1 \le n-3 < n-1-\rho_1(P_k) \le \rho_1(\Gamma).$$

Proof. It is well-known that $S_A(P_k) = \left\{ 2\cos\left(\frac{j\pi}{k+1}\right), \text{where } j = 1, 2, \ldots, k \right\}$ (see [1], Page 18).

By Lemma 3.1, we have $2\cos\left(\frac{3\pi}{k+1}\right) = \rho_3(P_k) = \rho_3\big(P_k \cup (n-k)P_1\big) \le -1 - \rho_{n-1}\big(K_n \setminus P_k\big) = -1 - \rho_{n-1}(\Gamma) \le \rho_2(\overline{\Gamma}) \le -1 - \rho_n(\Gamma) = -1 - \rho_n\big(K_n \setminus P_k\big) \le -1 - \big(-1 - \rho_1\big(P_k \cup (n-k)P_1\big)\big) = \rho_1(P_k) = 2\cos\left(\frac{\pi}{k+1}\right) < 2$, and thus (i) holds.

Similarly, $-1 - 2\cos\left(\frac{\pi}{k+1}\right) = -1 - \rho_1(P_k) = -1 - \rho_1\big(P_k \cup (n-k)P_1\big) \le \rho_n\big(K_n \setminus P_k\big) = \rho_n(\Gamma) \le -1 - \rho_2\big(P_k \cup (n-k)P_1\big) = -1 - \rho_2(P_k) = -1 - 2\cos\left(\frac{2\pi}{k+1}\right)$, and so (ii) holds.

Once again, Lemma 3.1 implies that $-1 + 2\cos\left(\frac{2\pi}{k+1}\right) = -1 + \rho_2(P_k) = -1 - \rho_{n-1}\big(P_k \cup (n-k)P_1\big) \le \rho_2(\Gamma) = \rho_2(K_n \setminus P_k) \le -1 - \rho_n\big(P_k \cup (n-k)P_1\big) = -1 - \rho_k(P_k) = -1 + \rho_1(P_k) = -1 + 2\cos\left(\frac{\pi}{k+1}\right) < 1$. Combining this with $\rho_1\big(\Gamma\big) = \rho_1\big(K_n \setminus P_k\big) \ge n - 1 - \rho_1\big(P_k \cup (n-k)P_1\big) = n - 1 - \rho_1(P_k) > n - 3$ by Corollary 3.2, we deduce (iii). ■

The following properties have been proved in [8].

Lemma 4.2 (*Mao, Cioabă and Wang [8]*). *(i) Except for -1, every eigenvalue of graph $K_n \setminus P_k$ has multiplicity one. Furthermore, the multiplicity of -1 is $n-k$ if k is odd, and it is $n-k-1$ if k is even.*

(ii) No two non-trivial components of $\overline{\Gamma}$ are paths of the same nonzero length except for P_3, and $\overline{\Gamma}$ does not have the disjoint union of two cycles as an induced subgraph.

(iii) No component of $\overline{\Gamma}$ is a cycle except for C_3 and C_4.

By Lemmas 3.4 and 4.2, we obtain the following corollary.

Corollary 4.3. *(i) If k is odd, then $n-k-1 \le m_{\overline{\Gamma}}(0) \le n-k+1$.*

(ii) If k is even, then $n-k-2 \le m_{\overline{\Gamma}}(0) \le n-k$.

Remark 4.4. If $T \in \left\{Z_{p,1,1},\ Z_{2,2,1},\ Z_{3,2,1},\ Z_{4,2,1}\right\}$ for $p \ge 1$, then T is called a **first-type tree**. Let $\eta(\overline{\Gamma})$ be **the number of non-trivial components** of $\overline{\Gamma}$, and let $\varepsilon(F)$ be **the number of non-trivial paths** of a forest F. Since $\rho_2(\overline{\Gamma}) < 2$ by Lemma 4.1(i), it follows from Lemma 3.6 that $\overline{\Gamma}$ consists of a c-cyclic graph Γ_1 and a forest F consisting of $\varepsilon(F)$ non-trivial paths, $\eta(\overline{\Gamma}) - \varepsilon(F) - 1$ first-type trees, and $n - |V(\Gamma_1)| - |V(F)|$ isolated vertices. Recall that $q(F)$ is the number of special-vertices of F by Definition 2.2(ii). Then, $q(F) + \varepsilon(F) = \eta(\overline{\Gamma}) - 1$.

Since there are $n - |V(\Gamma_1)| - |V(F)|$ isolated vertices, by Corollary 4.3 we have

$$n-k-2 \le m_{\Gamma_1}(0) + m_F(0) + n - |V(\Gamma_1)| - |V(F)| = m_{\overline{\Gamma}}(0) \le n-k+1, \tag{4.1}$$

where the right (resp., left) equality holds implies that k is odd (resp., even).

Lemma 4.5. *Suppose that Γ_1 has a c-cyclic subgraph (not necessary induced) with t vertices and F contains an induced subgraph consisting with p vertices and s non-trivial trees. If $c \ge 2$, then $(c-1)p^2 < st^2$.*

Proof. Let G_1 be a c-cyclic subgraph of Γ_1 with t vertices, and let F_1 be an induced subgraph of F consisting with p vertices and s non-trivial trees. By contradiction, we assume that $(c-1)p^2 \ge st^2$. Define the vector $\mathbf{f}$, indexed by the vertices of $\overline{\Gamma}$, as follows:

$$f(u_i) = \begin{cases} 1 & \text{if } u_i \in G_1, \\ -\frac{t}{p} & \text{if } u_i \in F_1, \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to check that $\mathbf{f} \perp \mathbf{1}$, $\mathbf{f}^T\mathbf{f} = t + \frac{t^2}{p}$ and

$$\mathbf{f}^T A(\overline{\Gamma})\mathbf{f} \geq \sum_{u\in V(G_1)} d(u) + \frac{t^2}{p^2}\sum_{v\in V(F_1)} d(v) \geq 2(t+c-1) + 2\big(p-s\big)\frac{t^2}{p^2}.$$

As $(c-1)p^2 \geq st^2$, by using Rayleigh's inequality (see Theorem 4.2.2 of [6]) we obtain

$$\rho_n\big(\Gamma\big) \leq \frac{\mathbf{f}^T A\big(\Gamma\big)\mathbf{f}}{\mathbf{f}^T\mathbf{f}} = \frac{\mathbf{f}^T\big(J_n - A(\overline{\Gamma}) - I_n\big)\mathbf{f}}{t+\frac{t^2}{p}} \leq -\frac{2(t+c-1)+2\big(p-s\big)\frac{t^2}{p^2}}{t+\frac{t^2}{p}} - 1 \leq -3,$$

which is contrary to Lemma 4.1(ii). ■

By Lemma 4.5, we immediately have that following corollary.

Corollary 4.6. *Suppose that Δ_t is a subgraph (not necessarily induced) of $\overline{\Gamma}$. If F contains a non-trivial tree with p vertices as its induced subgraph, then $p < t$ for $t \in \{4, 5, 6\}$.*

Lemma 4.7. *Let H be an induced subgraph of $\overline{\Gamma}$.*

(i) H is not a cycle with even length.

(ii) If $|V(H)| = s \geq 2$, then $\rho_2(H) \leq 2\cos\left(\frac{\pi}{k+1}\right) < 2$ and

$$-3 < -2\cos\left(\frac{\pi}{k+1}\right) - 1 \leq \rho_s\big(K_s \setminus H\big) \leq \rho_2\big(K_s \setminus H\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) - 1 < 1.$$

Proof. Suppose to the contrary that H is a cycle with even length. It is well-known that $S_A(C_g) = \left\{ 2\cos\left(\frac{2j\pi}{g}\right), \text{where } j = 0, 1, \ldots, g-1 \right\}$ (see [1], Page 18). For $j \in \{1, 2, \ldots, g-1\}$, since C_g is 2-regular, the eigenvector of each eigenvalue of $2\cos\left(\frac{2j\pi}{g}\right)$ is orthogonal to all-one vector $\mathbf{1}$ of length g, so it is easy to see that $-1-2\cos\left(\frac{2j\pi}{g}\right)$ is also an eigenvalue of $S_A\big(K_g \setminus C_g\big)$. Since $K_g \setminus C_g$ is $(g-3)$-regular, we have $\rho_1\big(K_g \setminus C_g\big) = g-3 \geq 1$. By Lemma 3.5, it follows that $\rho_2\big(\Gamma\big) \geq \rho_2\big(K_g \setminus C_g\big) = 1$, which is contrary to Lemma 4.1(iii). Thus, (i) holds.

Now we prove (ii). By Lemmas 3.5 and 4.1 we have

$$-2\cos\left(\frac{\pi}{k+1}\right) - 1 \leq \rho_n\big(\Gamma\big) \leq \rho_s\big(K_s \setminus H\big) \leq \rho_2\big(K_s \setminus H\big) \leq \rho_2\big(\Gamma\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) - 1$$

and

$$\rho_2\big(H\big) \leq \rho_2\big(\overline{\Gamma}\big) \leq 2\cos\left(\frac{\pi}{k+1}\right) < 2,$$

as desired. ■

Corollary 4.8. *Neither any cycle nor Δ_6 is a component of $\overline{\Gamma}$.*

Proof. Suppose that $V(\overline{\Gamma}) = \{w_1, w_2, w_3, \ldots, w_n\}$. If C_g is a component of $\overline{\Gamma}$, then $g = 3$ by Lemmas 4.2(iii) and 4.7(i). We may suppose that $V(C_3) = \{w_1, w_2, w_3\}$. Now, $\big(1, -1, 0^{(n-2)}\big)$ and $\big(-\frac{1}{2}, -\frac{1}{2}, 1, 0^{(n-3)}\big)$ are two independent eigenvectors corresponding to the eigenvalue 0 of $A\big(\Gamma\big)$. Thus, $m_\Gamma(0) \geq 2$, contrary to Lemma 4.2(i).

Now, we assume that Δ_6 is a component of $\overline{\Gamma}$. Suppose that $w_1w_2 \in E\big(\Delta_6\big)$ and $w_3w_4 \in E\big(\Delta_6\big)$, where $\{w_1, w_2, w_3, w_4\}$ are four 2-vertices of Δ_6. In this case, $\big(1, -1, 0^{(n-2)}\big)$ and $\big(0, 0, 1, -1, 0^{(n-4)}\big)$ are two independent eigenvectors corresponding to the eigenvalue 0 of $A\big(\Gamma\big)$, which is also contrary to Lemma 4.2(i). ■

Corollary 4.9. *The following graphs are forbidden to $\overline{\Gamma}$:*

(i) $Z_{2,2,2}$, H_1, H_2, $Z_{1,3,4} \cup K_1 \cup P_3$, $H_5 \cup P_2 \cup P_3$, $H_6 \cup K_1 \cup P_3$, $U^5_{1,1} \cup 3P_2$, $H_7 \cup K_1$, $U^5_5 \cup P_3$, $H_8 \cup P_3$, $H_9 \cup P_3$, $W_8 \cup P_2 \cup P_3$, $H_{11} \cup P_3 \cup 2P_2$, $H_{12} \cup P_3$, H_{14}, $Z_{4,1,1,1} \cup P_3$, $Z_{3,1,1,1} \cup 2P_3 \cup K_1$, $Z_{2,1,1,1,1} \cup P_3$, $Z_{2,1,1,1} \cup K_{1,3} \cup P_3$, $Z_{2,1,1,1} \cup K_1 \cup P_3 \cup P_5$, $Z_{2,1,1,1} \cup 3P_3$, $K_{1,5} \cup 3P_3$, $Z_{4,4,1}$, $Z_{7,2,1} \cup K_1$, $Z_{6,2,1} \cup P_3$, $H_{15} \cup P_2 \cup P_3$.

(ii) $\Delta_5 \cup 2P_3$, $\Delta_6 \cup K_{1,3}$, $\Delta_6 \cup P_3 \cup P_4$, $\Delta_4 \cup P_2 \cup P_3$, $U^7_1 \cup K_1 \cup P_9$, $U^3_2 \cup 2P_3 \cup P_4$, $U^3_1 \cup P_2 \cup P_3 \cup K_{1,3}$, $U^3_6 \cup P_2 \cup 2P_3$, $H_3 \cup 2P_2 \cup P_4$, $\Theta_{3,0,1} \cup 2P_3 \cup P_2$, $U^5_1 \cup Z_{1,1,3}$, $U^5_1 \cup Z_{2,2,1}$, $U^5_1 \cup P_8$, $U^5_2 \cup P_7$, $U^5_1 \cup P_4 \cup P_7$, $U^5_1 \cup K_{1,3} \cup P_7$, $U^3_1 \cup P_6$, $H_4 \cup K_{1,3}$, $H_4 \cup P_2 \cup P_4$, $H_4 \cup P_2 \cup 2P_3$, $H_3 \cup P_5$, $H_3 \cup K_{1,3}$, $H_3 \cup P_3 \cup P_4$, $U_{3;4,1} \cup P_2 \cup 2P_3$, $U_{3;6,1} \cup P_2$, $U^3_7 \cup P_3$, $U^3_1 \cup Z_{2,1,1}$, $U^3_1 \cup K_{1,3} \cup P_2 \cup P_3$, $U^3_5 \cup P_2 \cup K_{1,3}$, $U^3_6 \cup P_2 \cup 2P_3$, $U^3_6 \cup P_2 \cup P_4$, $U^3_5 \cup P_5$, $U^3_5 \cup P_2 \cup P_3 \cup P_4$.

Proof. We may suppose that $|V(G)| = s$.

When $H \in \{ Z_{2,2,2}, H_1, H_2, Z_{1,3,4} \cup K_1 \cup P_3, H_5 \cup P_2 \cup P_3, H_6 \cup K_1 \cup P_3, U^5_{1,1} \cup 3P_2, H_7 \cup K_1, U^5_5 \cup P_3, H_8 \cup P_3, H_9 \cup P_3, W_8 \cup P_2 \cup P_3, H_{11} \cup P_3 \cup 2P_2, H_{12} \cup P_3, H_{14}, Z_{4,1,1,1} \cup P_3, Z_{3,1,1,1} \cup 2P_3 \cup K_1, Z_{2,1,1,1,1,1} \cup P_3, Z_{2,1,1,1} \cup K_{1,3} \cup P_3, Z_{2,1,1,1} \cup K_1 \cup P_3 \cup P_5, Z_{2,1,1,1} \cup 3P_3, K_{1,5} \cup 3P_3, Z_{4,4,1}, Z_{7,2,1} \cup K_1, Z_{6,2,1} \cup P_3, H_{15} \cup P_2 \cup P_3 \}$, it is easy to check that $\rho_2(K_s \setminus H) \geq 1$.

When $H \in \{ \Delta_5 \cup 2P_3, \Delta_6 \cup K_{1,3}, \Delta_6 \cup P_3 \cup P_4, \Delta_4 \cup P_2 \cup P_3, U^7_1 \cup K_1 \cup P_9, U^3_2 \cup 2P_3 \cup P_4, U^3_1 \cup P_2 \cup P_3 \cup K_{1,3}, U^3_6 \cup P_2 \cup 2P_3, H_3 \cup 2P_2 \cup P_4, \Theta_{3,0,1} \cup 2P_3 \cup P_2, C_5 \cup K_{1,4} \cup 3P_2, U^5_1 \cup Z_{1,1,3}, U^5_1 \cup Z_{2,2,1}, U^5_1 \cup P_8, U^5_2 \cup P_7, U^5_1 \cup P_4 \cup P_7, U^5_1 \cup K_{1,3} \cup P_7, U^3_1 \cup P_6, H_4 \cup K_{1,3}, H_4 \cup P_2 \cup P_4, H_4 \cup P_2 \cup 2P_3, H_3 \cup P_5, H_3 \cup K_{1,3}, H_3 \cup P_3 \cup P_4, U_{3;4,1} \cup P_2 \cup 2P_3, U_{3;6,1} \cup P_2, U^3_7 \cup P_3, U^3_1 \cup Z_{2,1,1}, U^3_1 \cup K_{1,3} \cup P_2 \cup P_3, U^3_5 \cup P_2 \cup K_{1,3}, U^3_6 \cup P_2 \cup 2P_3, U^3_6 \cup P_2 \cup P_4, U^3_5 \cup P_5, U^3_5 \cup P_2 \cup P_3 \cup P_4 \}$, it is easy to check that $\rho_s(K_s \setminus H) \leq -3$. Now, the result follows from Lemma 4.7(ii). ■

Let $\tau(G)$ be the number of triangles of G.

Lemma 4.10 (*Doob and Haemers [4]*). *If G is a graph with degree sequence $(d_1, d_2, \ldots, d_n)$ and e edges, then*

$$\tau(\overline{G}) + \tau(G) = \binom{n}{3} - (n-1)e + \frac{1}{2}\sum_{i=1}^{n} d_i^2.$$

Corollary 4.11. *If Γ_1 is a c-cyclic graph, then*

$$\sum_{i=1}^{|V(\Gamma_1)|} d_i(\Gamma_1)\big(d_i(\Gamma_1) - 2\big) = 2\big(\tau(\Gamma_1) + \varepsilon(F) - 1\big).$$

Furthermore, if $c \geq 1$, then $\tau(\Gamma_1) \geq 3c - 2 + q(\Gamma_1) - \varepsilon(F)$, with equality holds if and only if each special-vertex of Γ_1 is a 3-vertex and $\mathcal{R}(\Gamma_1)$ contains exactly $2(c-1)$ vertices of degrees three.

Proof. By Lemma 4.10, we have $\tau(K_n \backslash P_k) = \binom{n}{3} - (n-1)(k-1) + 2k - 3$ and hence

$$\tau(\Gamma) = \binom{n}{3} - (n-1)(k-1) + \frac{1}{2}\sum_{i=1}^{n} d_i^2(\overline{\Gamma}) - \tau(\overline{\Gamma}).$$

Since Γ is A-cospectral with $K_n \backslash P_k$, $\tau(K_n \backslash P_k) = \tau(\Gamma)$ [3] and hence $\sum_{i=1}^{n} d_i^2(\overline{\Gamma}) = 2\tau(\overline{\Gamma}) + 4k - 6$. Combining this with $\sum_{i=1}^{n} d_i(\overline{\Gamma}) = 2(k-1)$ and Remark 4.4, we have

$$\sum_{i=1}^{n} d_i(\overline{\Gamma})\big(d_i(\overline{\Gamma}) - 2\big) = 2\big(\tau(\overline{\Gamma}) - 1\big) = 2\big(\tau(\Gamma_1) - 1\big). \tag{4.2}$$

If T is a tree of F with $\Delta(T) \geq 3$, then $T \in \{Z_{p,1,1}, Z_{2,2,1}, Z_{3,2,1}, Z_{4,2,1}\}$ for some $p \geq 1$ by Remark 4.4, and this implies that

$$\sum_{i=1}^{n} d_i(\overline{\Gamma})\big(d_i(\overline{\Gamma}) - 2\big) = \sum_{i=1}^{|V(\Gamma_1)|} d_i(\Gamma_1)\big(d_i(\Gamma_1) - 2\big) - 2\varepsilon(F). \tag{4.3}$$

Since $\sum_{i=1}^{n} d_i^2(\Gamma_1) \geq 4|V(\Gamma_1)| + 10(c-1) + 2q(\Gamma_1)$ by Corollary 3.9 and in view of $\sum_{i=1}^{n} d_i(\Gamma_1) = 2\big(|V(\Gamma_1)| + c - 1\big)$, by combining (4.2) and (4.3), we have the desired result. ■

Recall that $\eta(\overline{\Gamma})$ is the number of non-trivial components of $\overline{\Gamma}$. The following result implies that Conjecture 1.1 is true if $\eta(\overline{\Gamma}) = 1$.

Lemma 4.12. *If $\eta(\overline{\Gamma}) = 1$, then $\overline{\Gamma} \cong P_k \cup (n-k)K_1$.*

Proof. Since $\eta(\overline{\Gamma}) = 1$ and $|E(\Gamma_1)| = k - 1$, we have $|V(\Gamma_1)| \leq k$ and $F = \emptyset$.
Case 1. $|V(\Gamma_1)| \leq k - 1$. In this case, $\overline{\Gamma}$ contains at least $n - k + 1$ isolated vertices. By (4.1), we conclude that $m_{\overline{\Gamma}}(0) = n - k + 1$ and $|V(\Gamma_1)| = k - 1$. Thus, Γ_1 is a unicyclic graph with $k-1$ vertices. By Corollary 4.11, it follows that $1 \geq \tau(\Gamma_1) \geq q(\Gamma_1) + 1$, and so $q(\Gamma_1) = 0 = \tau(\Gamma_1) - 1$. Thus $\Gamma_1 \cong C_3$, contrary to Corollary 4.8.
Case 2. $|V(\Gamma_1)| = k$. In this case, Γ_1 is a tree. By Lemma 3.8, it follows that $\sum_{i=1}^{k} d_i^2(\Gamma_1) \geq 4k - 6$, where equality holds if and only if $\Gamma_1 \cong P_k$. Now, since $\varepsilon(F) = \tau(\Gamma_1) = 0$, Corollary 4.11 implies that $\sum_{i=1}^{k} d_i^2(\Gamma_1) = 2\sum_{i=1}^{k} d_i(\Gamma_1) - 2 = 4k - 6$, and hence $\Gamma_1 \cong P_k$. ■

5. The graph Γ_1 is either a unicyclic graph or a tree

Since Conjecture 1.1 was settled for $2 \leq k \leq 9$ in [8,2], it is natural to assume that $k \geq 10$ in this section. Recall that in the previous section, we obtained that $\overline{\Gamma} = \Gamma_1 \cup F \cup \big(n - |V(F)| - |V(\Gamma_1)|\big)K_1$, where Γ_1 is a c-cyclic graph and F is

a forest with $\Delta(F) \leq 3$. In Theorem 5.5, we will show that for $k \geq 10$, Γ_1 is either a unicyclic graph or a tree, that is, $c \in \{0, 1\}$.

Lemma 5.1. *At most two non-trivial trees of $\overline{\Gamma}$ are isomorphic. Furthermore, if $\tau(\Gamma_1) \geq 2$, then no two non-trivial trees of F are isomorphic.*

Proof. If $\overline{\Gamma}$ contains at least three copy of a non-trivial tree T, then $m_{\overline{\Gamma}}(\alpha) \geq 3$ holds for some eigenvalue $\alpha \neq 0$ and hence $m_{\Gamma}(-1-\alpha) \geq 2$ by Lemma 3.4, contrary with Lemma 4.2(i).

If $\tau(\Gamma_1) \geq 2$, then since $\overline{\Gamma}$ does not contain a disjoint union of two cycles as an induced subgraph by Lemma 4.2(ii), $\overline{\Gamma}$ contains Δ_t as a subgraph, where $t \in \{4, 5, 6\}$. Suppose that F contains at least two copies of a tree T. By combining Lemmas 4.2(ii), 4.5, Corollary 4.6 and Remark 4.4, it follows that $T \in \{P_3,\ K_{1,3}\}$. In view of Lemma 4.5 and $|V(F)| \geq 6$, we have $t \in \{5,\ 6\}$. That is, Δ_4 is not a subgraph of $\overline{\Gamma}$.

If $t = 5$, then Δ_5 is an induced subgraph of $\overline{\Gamma}$, since Δ_4 is not a subgraph of $\overline{\Gamma}$. This implies that $\Delta_5 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(ii). Thus, $\overline{\Gamma}$ contains neither Δ_5 nor Δ_4 as a subgraph. Furthermore, since $\overline{\Gamma}$ contains no even cycle as an induced subgraph by Lemma 4.7(i), we conclude that $\overline{\Gamma}$ contains Δ_6 as an induced subgraph.

Since $\Delta_6 \cup K_{1,3}$ is forbidden by Corollary 4.9(ii) and notice that $T \in \{P_3,\ K_{1,3}\}$, we have $T = P_3$. Combining this with Lemma 4.5, it follows that $c = 2$. By Corollary 4.8, Δ_6 is not a component of $\overline{\Gamma}$, which implies that $q(\Gamma_1) \geq 1$. Since $c = 2$, by Corollary 4.11 we have $2 = \tau(\Gamma_1) \geq 4 + q(\Gamma_1) - \varepsilon(F) \geq 5 - \varepsilon(F)$, and so $\varepsilon(F) \geq 3$, where the equality requires that Γ_1 contains exactly one special vertex, which is a 3-vertex. On the other hand, $\Delta_6 \cup P_3 \cup P_4$ is forbidden by Corollary 4.9(ii). Now, we can conclude that $\varepsilon(F) = 3$ and $F = P_2 \cup 2P_3$.

As $\Delta_6 \cup P_2 \cup 2P_3$ is an induced subgraph of $\overline{\Gamma}$, by Lemma 4.7(ii) it follows that

$$-2\cos\left(\frac{\pi}{k+1}\right) - 1 \leq \rho_{14}\left(K_{14} \setminus \left(\Delta_6 \cup P_2 \cup 2P_3\right)\right) < -2.98$$

and so $k \geq 22$. In view of $c = 2$ and $F = P_2 \cup 2P_3$, we have $|V(\Gamma_1)| + 1 = |E(\Gamma_1)| = k - 1 - 5 \geq 16$, and so $|V(\Gamma_1)| \geq 15$. Recall that Γ_1 contains exactly one special 3-vertex and $|V(\Gamma_1)| \geq 15$. Thus, $U_7^3 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(ii). ■

Remark 5.2. By Lemma 4.2(ii), we can deduce that $P_2 \cup P_3$ is an induced subgraph of F when $\varepsilon(F) \geq 2$, and $P_2 \cup 2P_3$ is an induced subgraph of F if either $\eta(\overline{\Gamma}) \geq 4$ or $\varepsilon(F) \geq 3$. Lemma 5.1 implies that $P_2 \cup 2P_3 \cup P_4$ is an induced subgraph of F if $\varepsilon(F) \geq 4$. This observation will play an important role in the sequel.

Lemma 5.3. *If $\overline{\Gamma}$ contains a bicyclic graph as a subgraph, then $\eta(\overline{\Gamma}) \geq 4$ and $\tau\left(\overline{\Gamma}\right) = \tau\left(\Gamma_1\right) \leq 1$.*

Proof. First we claim that if $\eta(\overline{\Gamma}) \geq 4$, then $\tau\left(\Gamma_1\right) \leq 1$. By contradiction, we assume that $\eta(\overline{\Gamma}) \geq 4$ and $\tau\left(\Gamma_1\right) \geq 2$. This implies that Γ_1 contains Δ_t as a subgraph by Lemma 4.2(ii), where $t \in \{4, 5, 6\}$. In this case, since $\eta(\overline{\Gamma}) \geq 4$ and no two non-trivial trees of F are isomorphic by Lemma 5.1, we have $|V(F)| \geq 9$. Combining this with Lemma 4.5, we can conclude that $\overline{\Gamma}$ contains neither Δ_5 nor Δ_4 as a subgraph, and so Δ_6 is an induced subgraph of $\overline{\Gamma}$. Thus, either $\Delta_6 \cup P_3 \cup P_4$ or $\Delta_6 \cup K_{1,3}$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(ii). This proves the claim. Thus, it suffices to show that $\eta(\overline{\Gamma}) \geq 4$.

By Lemma 4.12, we may assume that $\eta(\overline{\Gamma}) \geq 2$. To show $\eta(\overline{\Gamma}) \geq 4$, suppose to the contrary that $2 \leq \eta(\overline{\Gamma}) \leq 3$. Then $\varepsilon(F) \leq 2$. Since $c \geq 2$, by Corollary 4.11, we have

$$\tau\left(\overline{\Gamma}\right) = \tau\left(\Gamma_1\right) \geq 3c - 2 + q(\Gamma_1) - \varepsilon(F) \geq 2. \tag{5.1}$$

Since $\tau(\overline{\Gamma}) \geq 2$ and $\overline{\Gamma}$ does not contain a disjoint union of two cycles as an induced subgraph by Lemma 4.2(ii), Γ_1 contains Δ_t as a subgraph, where $t \in \{4, 5, 6\}$.

Case 1. $t = 4$. If $\eta(\overline{\Gamma}) = 3$, then Lemma 4.2(ii) implies that F contains $P_2 \cup P_3$ as an induced subgraph, and so $c = 2$ by Lemma 4.5. This implies that $\Delta_4 \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(ii).

Thus $\eta(\overline{\Gamma}) = 2$. Then we have $F \in \{P_2,\ P_3\}$ by Lemma 4.5, and $\tau(\Gamma_1) \geq 3$ by (5.1), as $\varepsilon(F) = 1$. Thus $c \geq 3$. Combining this with $|V(\Gamma_1)| + c - 1 = |E(\Gamma_1)| = k - 1 - |E(F)|$, it follows that $|V(\Gamma_1)| = k - |E(F)| - c \leq k - 3 - |E(F)|$. Thus, $\overline{\Gamma}$ contains at least $n - |V(\Gamma_1)| - |V(F)| \geq n - (k - 3 - |E(F)|) - |V(F)| = n - k + 2$ isolated vertices, and so $m_{\overline{\Gamma}}(0) \geq n - k + 2$, contrary to (4.1).

Case 2. $t \in \{5,\ 6\}$. Since Δ_4 is not a subgraph of $\overline{\Gamma}$ by Case 1, we can conclude that $c \geq \tau\left(\Gamma_1\right)$. Combining this with (5.1), we have $2 + q(\Gamma_1) \leq 2(c-1) + q(\Gamma_1) \leq \varepsilon(F) \leq 2$. Thus,

$$q(\Gamma_1) = 0,\ \ \varepsilon(F) = 2,\ \text{ and } c = 2. \tag{5.2}$$

Since $q(\Gamma_1) = 0$ and $c = 2$ by (5.2), we conclude that $\Gamma_1 = \Delta_t$, and so $t = 6$ by Corollary 4.11. This implies that Δ_6 is a component of $\overline{\Gamma}$, contrary to Corollary 4.8. ■

Lemma 5.4. *If $c \geq 2$, then $\tau(\overline{\Gamma}) = 0$.*

Proof. By Lemma 5.3, $\eta(\overline{\Gamma}) \geq 4$ and $\tau\left(\overline{\Gamma}\right) = \tau\left(\Gamma_1\right) \leq 1$. To show that $\tau(\overline{\Gamma}) = 0$, we assume to the contrary that $\tau(\overline{\Gamma}) = 1$. In what follows, we suppose that C_3 is the unique triangle of $\overline{\Gamma}$. Since Γ_1 contains no even cycle as an induced subgraph and $\tau(\overline{\Gamma}) = 1$, we can conclude that U_2^3 is an induced subgraph of Γ_1. Throughout this proof, let B_1 be the bicyclic graph obtained from cycles C_g and C_3 by adding one edge u_1w_1, where $C_3 : u_1u_2u_3u_1$ and $C_g : w_1w_2 \cdots w_gw_1$.

Claim A. *$\varepsilon(F) = 3 = \eta(\overline{\Gamma}) - 1$ and $\Gamma_1 \in \left\{\Theta_{g-2,0,1},\ B_1\right\}$, where either $g = 5$ or $g = 7$.*

Proof of Claim A. If $\eta(\overline{\Gamma}) \geq 5$, then since F contains no two paths of length one by Lemma 4.2(ii) and since U_2^3 is an induced subgraph of Γ_1, by Lemma 5.1 and Remark 5.2, we conclude that either $U_2^3 \cup 2P_3 \cup P_4$ or $U_1^3 \cup P_2 \cup P_3 \cup K_{1,3}$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(ii). Thus, $\eta(\overline{\Gamma}) = 4$. If $c \geq 3$, then $\varepsilon(F) \geq 3(c-1) + q(\Gamma_1) \geq 6$ by Corollary 4.11, contrary to $\eta(\overline{\Gamma}) = 4$. This implies that $c = 2$. Combining this with $\varepsilon(F) \geq 3(c-1) + q(\Gamma_1) \geq 3$ by Corollary 4.11 and $\eta(\overline{\Gamma}) = 4$, it follows that $\varepsilon(F) = 3$, $q(\Gamma_1) = 0$, $\mathcal{R}(\Gamma_1) = \Gamma_1$ and Γ_1 contains exactly two 3-vertices. Furthermore, since $\overline{\Gamma}$ contains no induced even cycle by Lemma 4.7(i) and since $\overline{\Gamma}$ does not contain a disjoint union of two cycles as an induced subgraph by Lemma 4.2(ii), we have $\Gamma_1 \in \left\{\Theta_{g-2,0,1},\ B_1\right\}$, where $g \geq 5$ is odd.

If $g \geq 9$, then by Lemma 4.2(ii), we conclude that $\overline{\Gamma}$ contains $U_6^3 \cup P_2 \cup 2P_3$ as an induced subgraph of $\overline{\Gamma}$, contradicting Corollary 4.9(ii). Thus, either $g = 5$ or $g = 7$. This completes the proof of Claim A.

By Claim A, we have the following two cases.

Case 1. $\Gamma_1 = \Theta_{g-2,0,1}$. In this case, since $H_3 \cup 2P_2 \cup P_4$ are forbidden by Corollary 4.9(ii) and in view of $\varepsilon(F) = 3 = \eta(\overline{\Gamma}) - 1$ by Claim A, by Lemma 4.2(ii), it follows that $F = P_2 \cup 2P_3$.

Now, since $|E(\Gamma_1)| = k-6$ by $F = P_2 \cup 2P_3$ and in view of $\Gamma_1 = \Theta_{g-2,0,1}$, we have $|V(\Gamma_1)| = k-7$. Since $m_{\Theta_{5,0,1}}(0) = 1$ and $m_{P_2 \cup 2P_3}(0) = 2$, we have $\Gamma_1 = \Theta_{3,0,1}$ by (4.1). However, $\Theta_{3,0,1} \cup P_2 \cup 2P_3$ is forbidden by Corollary 4.9(ii), a contradiction.

Case 2. $\Gamma_1 = B_1$. Since $Z_{2,2,2}$ is forbidden by Corollary 4.9(i), we have $g = 5$. In this case, since $\rho_{17}\big(K_{17} \setminus (B_1 \cup P_2 \cup P_3 \cup P_4)\big) = -3$, by Lemmas 4.2(ii) and 4.7(ii), we have $F = P_2 \cup 2P_3$, as $\varepsilon(F) = 3 = \eta(\overline{\Gamma}) - 1$ by Claim A. Now, since $|E(\Gamma_1)| = k-6$ and $\Gamma_1 = B_1$, it follows that $k = 15$. By Lemma 4.7(ii),

$$0.979 < \rho_2\big(K_{16} \setminus (B_1 \cup P_2 \cup 2P_3)\big) \leq 2\cos\left(\frac{\pi}{16}\right) - 1 < 0.962,$$

a contradiction. ■

In the theorem below, we will show that Γ_1 must be a unicyclic graph or a tree.

Theorem 5.5. *If Γ_1 is a c-cyclic graph, then $c \in \{0, 1\}$.*

Proof. By contradiction, we assume that $c \geq 2$. Then, $\tau(\overline{\Gamma}) = 0$ by Lemma 5.4. Since Γ_1 is a c-cyclic graph with $c \geq 2$, we may suppose that C_{p_0} and C_{q_0} are two smallest cycles of Γ_1, that is, $p_0 + q_0 = \min\ \{\ p + q : \text{where } C_p \text{ and } C_q \text{ are two cycles of } \Gamma_1\ \}$. Subject to this, we may further suppose that $p_0 \geq q_0$ and $|V(C_{p_0}) \cap V(C_{q_0})|$ is as small as possible. By definition, both C_{p_0} and C_{q_0} are two induced subgraphs and C_{q_0} is the smallest cycle of $\overline{\Gamma}$. By Lemma 4.7(i), p_0 and q_0 are two odd integers such that $p_0 \geq q_0 \geq 5$, as $\tau(\overline{\Gamma}) = 0$. We suppose that $C_{p_0} : u_1u_2 \cdots u_{p_0}u_1$ and $C_{q_0} : w_1w_2 \cdots w_{q_0}w_1$.

Case 1. $|V(C_{p_0}) \cap V(C_{q_0})| = 0$. In this case, since $p_0 \geq q_0 \geq 5$ and since $\overline{\Gamma}$ does not contain a disjoint union of two cycles as an induced subgraph by Lemma 4.2(ii), H_1 is an induced subgraph of Γ_1, contrary to Corollary 4.9(i).

Case 2. $|V(C_{p_0}) \cap V(C_{q_0})| = 1$. In this case, we suppose that $w_1 = u_1$. If $p_0 \geq 7$, then H_2 is an induced subgraph of $\overline{\Gamma}$, which is contrary to Corollary 4.9(i). Thus, $p_0 = q_0 = 5$. By the choice of C_{p_0} and C_{q_0}, $\big(N(w_5) \cup N(w_2)\big) \cap V(C_{p_0}) = \{w_1\} = \big(N(u_5) \cup N(u_2)\big) \cap V(C_{q_0})$. Since H_2 is forbidden by Corollary 4.9(i), we may suppose that $w_4u_4 \in E(G)$ by symmetry. As $p_0 = q_0 = 5$, it is easy to see that $G\big[\{w_1, u_2, u_3, u_4, w_4, w_5\}\big]$ is an induced cycle with six vertices, contrary to Lemma 4.7(i).

Case 3. $|V(C_{p_0}) \cap V(C_{q_0})| \geq 2$. In this case, Θ_{s_1,s_2,s_3} is a subgraph of $\overline{\Gamma}$. By the choice of p_0 and q_0, and since H_1 and $Z_{2,2,2}$ are forbidden by Corollary 4.9(i), we may suppose that $s_1 + s_2 = p_0 - 2$, $s_2 + s_3 = q_0 - 2$ and $s_1 \geq s_3 \geq s_2 = 1$.

If $p_0 \geq q_0 \geq 7$, then $s_1 \geq s_3 \geq 4$ and so $Z_{2,2,2}$ is an induced subgraph of $\overline{\Gamma}$, contradicting Corollary 4.9(i). Otherwise, $q_0 = 5$. In this case, by the choice of p_0 and q_0, and since $q_0 = 5$, it is easy to see that $\Theta_{p_0-3,1,2}$ is an induced subgraph of $\overline{\Gamma}$, and hence C_{p_0+1} is an induced even cycle of $\overline{\Gamma}$, contrary to Lemma 4.7(i). Thus the theorem follows. ■

6. The graph Γ_1 is a tree for $k \geq 20$

By Theorem 5.5, we deduce that Γ_1 is a c-cyclic graph for $c \in \{0, 1\}$, that is, Γ_1 is a unicyclic graph or a tree. However, in this section, we will show that if $k \geq 20$, then $c = 0$, and thus Γ_1 is a tree. Actually, we prove it by contradiction and assume that Γ_1 is a unicyclic graph. We first show that the unique cycle in Γ_1 must be C_3 or C_5 in Lemma 6.5 and we further exclude C_5 in Lemma 6.6. Finally we show that C_3 shall also be excluded in Theorem 6.9, and thus Γ_1 is a tree.

We present some useful lemmas first. Denote by $m_1(G)$, $m_2(G)$, $m_3(G)$, and $m_4(G)$ the numbers of distinct (not necessarily induced) subgraphs in G isomorphic to P_3, $2K_2$, P_4 and C_4, respectively. In what follows, we define

$$\Phi(G) = \big(8n - 20\big)m_1(G) + 16m_2(G) - 8m_3(G).$$

Lemma 6.1 (*Cámara and Haemers [2]*). *If G is a graph with n vertices and e edges, then the number of 4-walks of $\overline{G}$ is equal to $(n-1)^4+(n-1)-(8n^2-32n+34)e+(8n-20)m_1(G)+16m_2(G)-8m_3(G)+8m_4(G)$.*

It is not hard to check that $m_1(P_k)=k-2$, $m_2(P_k)=\frac{1}{2}(k-2)(k-3)$, $m_3(P_k)=k-3$, and $m_4(P_k)=0$. Since Γ is A-cospectral with $K_n\setminus P_k$, they have the same number of 4-walks, and hence we have the following corollary by Lemmas 4.7(i) and 6.1.

Corollary 6.2. *If Γ_1 is either a tree or a unicyclic graph, then*

$$\Phi(\overline{\Gamma})=\Phi\big(P_k\cup(n-k)K_1\big)=(8n-20)(k-2)+8(k-3)^2.$$

Lemma 6.3. *Let $G=U_1^7\cup P_{q_1}\cup P_{q_2}$ and $t=q_1+q_2+7$. If $q_2\geq 2$ and $q_1\geq 3$, then $|E(G)|=|E(P_t)|$, $m_1(G)=m_1(P_t)$, $m_2(G)=m_2(P_t)$ and $m_3(G)\leq m_3(P_t)$, where the inequality is strict if $q_2\geq 3$.*

Proof. It is not hard to see that $|E(G)|=|E(P_t)|$, $m_1(G)=q_1+q_2+5=t-2=m_1(P_t)$ and

$$\begin{aligned}m_2(G)=&\frac{1}{2}(q_1-2)(q_1-3)+\frac{1}{2}(q_2-2)(q_2-3)+5+14+8(q_1+q_2-2)+(q_1-1)(q_2-1)\\=&\frac{1}{2}\big(q_1+q_2+5\big)\big(q_1+q_2+4\big)=\frac{1}{2}(t-2)(t-3)=m_2(P_t).\end{aligned}$$

If $q_2\geq 3$, then $m_3(G)=q_1-3+q_2-3+2+7=t-4<t-3=m_3(P_t)$.
If $q_1\geq 3>2=q_2$, then $m_3(G)=q_1-3+2+7=t-3=m_3(P_t)$. ■

Lemma 6.4. *Let $G=Z_{p_1,p_2,1}\cup P_s$ and $t=p_1+p_2+s+1$, where $p_1\geq p_2\geq 1$ and $s\geq 2$. Then, $|E(G)|=|E(P_t)|$, $m_1(G)=m_1(P_t)$, $m_2(G)=m_2(P_t)$, and $m_3(G)\leq m_3(P_t)$. Furthermore, if either $s\geq 3$ or $p_2=1$, then $m_3(G)<m_3(P_t)$.*

Proof. It is easy to see that $|E(G)|=|E(P_t)|$, $m_1(G)=m_1(P_t)=t-2$ and $m_2(G)=p_1+p_2-2+\frac{1}{2}\big(p_1+p_2-1\big)\big(p_1+p_2-2\big)+\frac{1}{2}(s-2)(s-3)+(s-1)\big(p_1+p_2+1\big)=\frac{1}{2}(t-2)(t-3)=m_2(P_t)$. If either $s\geq 3$ or $p_2=1$, then $m_3(G)\leq 2+p_1+p_2-2+s-3=t-4<t-3=m_3(P_t)$. Otherwise, $s=2$ and $p_2\geq 2$. In the later case, $m_3(G)=2+p_1+p_2-2+s-2=t-3=m_3(P_t)$. This completes the proof. ■

By Corollary 4.8, if Γ_1 is a unicyclic graph, then $\Delta(\Gamma_1)\geq 3$. In the rest of this section, we assume that $k\geq 20$.
Since F contains $|V(F)|+1-\eta(\overline{\Gamma})$ edges, by Corollary 4.11, we have

$$|V(\Gamma_1)|=|E(\Gamma_1)|=k-2+\eta(\overline{\Gamma})-|V(F)|,\ \text{and}\ 1\geq\tau(\Gamma_1)\geq q(\Gamma_1)-\varepsilon(F)+1,\tag{6.1}$$

where the second equality holds if and only if each special-vertex of Γ_1 is a 3-vertex.

Combining Lemma 4.1(i) and $k\geq 20$, it follows that

$$\rho_2(\overline{\Gamma})\geq 2\cos\left(\frac{3\pi}{k+1}\right)\geq 2\cos\left(\frac{\pi}{7}\right)>1.8.\tag{6.2}$$

Lemma 6.5. *If Γ_1 is a unicyclic graph with the unique cycle C_g, then $g\in\{3,5\}$.*

Proof. For short, we use Δ to denote $\Delta(\Gamma_1)$ in this proof. By Lemma 4.7(i), g must be odd. Suppose to the contrary that $g\geq 7$. Since $q(\Gamma_1)\geq 1$ by $\Delta\geq 3$ and in view of $\tau(\Gamma_1)=0$, it follows from (6.1) that $\varepsilon(F)\geq 2$, with equality holds if and only if Γ_1 contains exactly one special-vertex, which is a 3-vertex.

Since $Z_{1,3,4}\cup K_1\cup P_3$ is forbidden by Corollary 4.9(i) and $\varepsilon(F)\geq 2$, we have $g=7$ by Lemma 4.2(ii). Since $\{H_2,\ Z_{2,2,2}\}$ are forbidden by Corollary 4.9(i), we conclude that $\Delta=3$ and $\overline{\Gamma}$ does not contain U_2^7 as an induced subgraph. Furthermore, as $\{H_5\cup P_2\cup P_3,\ H_6\cup K_1\cup P_3,\ H_1\}$ are forbidden by Corollary 4.9(i) and $\Delta=3$, we have $\Gamma_1=U_1^7$ and so $\varepsilon(F)=2$ by (6.1).

Let P_{q_1} and P_{q_2} be the two non-trivial paths of F, and let $t=7+q_1+q_2$, where $q_1\geq q_2\geq 2$. Then $t\geq 11$. By Remark 4.4, denote by F_1 the forest consisting of all those first-type trees (if exist) of F. By Lemmas 6.3 and 6.4 we have $m_1(\overline{\Gamma})=m_1\big(U_1^7\cup P_{q_1}\cup P_{q_2}\big)+m_1(F_1)=m_1(P_t)+m_1(F_1)=m_1\big(P_t\cup F_1\big)=m_1(P_k)$, $m_2(\overline{\Gamma})=m_2\big(U_1^7\cup P_{q_1}\cup P_{q_2}\big)+m_2(F_1)+|E\big(U_1^7\cup P_{q_1}\cup P_{q_2}\big)|\cdot|E(F_1)|=m_2(P_t)+m_2(F_1)+|E(P_t)|\cdot|E(F_1)|=m_2\big(P_t\cup F_1\big)=m_2(P_k)$, and $m_3(\overline{\Gamma})=m_3\big(U_1^7\cup P_{q_1}\cup P_{q_2}\big)+m_3(F_1)\leq m_3\big(P_t\big)+m_3(F_1)=m_3\big(P_t\cup F_1\big)\leq m_3(P_k)$.

If either $q_2\geq 3$ or $F_1\neq\emptyset$, then $m_3(\overline{\Gamma})<m_3(P_k)$ by Lemmas 6.3 and 6.4. Combining this with $m_1(\overline{\Gamma})=m_1(P_k)$ and $m_2(\overline{\Gamma})=m_2(P_k)$, it follows that $\Phi(\overline{\Gamma})>\Phi\big(P_k\cup(n-k)K_1\big)$, contrary to Corollary 6.2. Therefore, $q_2=2$ and $F_1=\emptyset$. This implies that $F=P_{q_1}\cup P_2$.

Since $U_1^7\cup K_1\cup P_9$ is forbidden by Corollary 4.9(i) and $8=|E(U_1^7)|=|E(\Gamma_1)|=k-1-(q_1-1)-1=k-q_1-1$, we have $k=9+q_1\leq 17$, a contradiction. ■

Furthermore, we will show that $g = 5$ is impossible in the next lemma.

Lemma 6.6. *If Γ_1 is a unicyclic graph with the unique cycle C_g, then $g = 3$.*

Proof. By Lemma 6.5, suppose to the contrary that $g = 5$.

If $\Delta(\Gamma_1) \geq 4$, then $\varepsilon(F) \geq 3$ by (6.1). Since $\{U_{1,1}^5 \cup 3P_2,\ C_5 \cup K_{1,4} \cup 3P_2,\ H_1\}$ are forbidden by Corollary 4.9, Γ_1 contains $H_7 \cup K_1$ as an induced subgraph, contrary to Corollary 4.9(i). Thus, $\Delta(\Gamma_1) = 3$. In this case, Γ_1 contains U_1^5 as an induced subgraph. By (6.1) and $\Delta(\Gamma_1) = 3$, it follows that

$$\varepsilon(F) = q(\Gamma_1) + 1 \geq 2 \ \text{ and } \ \Delta(\Gamma_1) = 3.$$

If T is a tree with $\Delta(T) = 3$, then since $U_1^5 \cup Z_{1,1,3}$ and $U_1^5 \cup Z_{2,2,1}$ are forbidden by Corollary 4.9(ii), from Remark 4.4 we can conclude that $T \in \{K_{1,3}, Z_{2,1,1}\}$. Let P_s be the longest path of F, and let U_d^5 be an induced subgraph of Γ_1 such that d is as large as possible. Since $\{U_1^5 \cup P_8,\ U_5^5 \cup P_3\}$ are forbidden by Corollary 4.9, we have $s \leq 7$ and $d \leq 4$, as $\varepsilon(F) \geq 2$.

We first prove the following claim.

Claim B. $\rho_2(\overline{\Gamma}) = \rho_2(\Gamma_1)$

Proof of Claim B. By contradiction, we assume that $\rho_2(\overline{\Gamma}) = \rho_1(F)$, as $\rho_1(\Gamma_1) \geq \rho_1(C_5) = 2 > \rho_1(F)$ by Remark 4.4.

Case 1. $Z_{2,1,1}$ is a non-trivial tree of F. Since $s \leq 7$, $\rho_2(\overline{\Gamma}) = \rho_1(F) = \rho_1(Z_{2,1,1}) = 2\cos\left(\frac{\pi}{8}\right) \geq \rho_1(P_s)$. By (6.2), it follows that $\cos\left(\frac{\pi}{8}\right) \geq \cos\left(\frac{3\pi}{k+1}\right)$ and so $k \leq 23$. In this case, since $U_1^5 \cup Z_{2,1,1} \cup P_3 \cup P_2$ is an induced subgraph of $\overline{\Gamma}$ by Lemma 4.2(ii) and $\varepsilon(F) \geq 2$, from Lemma 4.7(ii) it follows that

$$-1 - 2\cos\left(\frac{\pi}{k+1}\right) \leq \rho_{16}\left(K_{16} \setminus \left(U_1^5 \cup Z_{2,1,1} \cup P_3 \cup P_2\right)\right) \leq -2.98,$$

and hence $22 \leq k \leq 23$. If either $U_1^5 \cup Z_{2,1,1} \cup 2P_3$ or $U_1^5 \cup Z_{2,1,1} \cup P_4 \cup P_2$ is an induced subgraph of $\overline{\Gamma}$, then by Lemma 4.7(ii) we have $-1 - 2\cos\left(\frac{\pi}{k+1}\right) \leq \max\left\{\rho_{17}\left(K_{17} \setminus \left(U_1^5 \cup Z_{2,1,1} \cup 2P_3\right)\right),\ \rho_{17}\left(K_{17} \setminus \left(U_1^5 \cup Z_{2,1,1} \cup P_2 \cup P_4\right)\right)\right\} \leq -2.9854$, and so $k \geq 25$, a contradiction. Thus $q(\Gamma_1) + 1 = \varepsilon(F) = 2 = \eta(\overline{\Gamma}) - 2$ and $s \leq 3$ by Lemma 4.2(ii). Combining this with $d \leq 4$ and $s \leq 3$, it follows that $k - 1 = |E(F)| + |E(\Gamma_1)| \leq 4 + 4 + 9$, contrary to $k \geq 22$.

Case 2. $Z_{2,1,1}$ is not a non-trivial tree of F. Since $k \geq 20$, we have $\rho_1(K_{1,3}) = 2\cos\left(\frac{\pi}{6}\right) = \rho_1(P_5) < \rho_2(\overline{\Gamma})$ by (6.2). This implies that $6 \leq s \leq 7$. Once again, (6.2) implies that $\cos\left(\frac{\pi}{s+1}\right) \geq \cos\left(\frac{3\pi}{k+1}\right)$, and hence $k \leq 3s + 2$.

If $s = 7$, then $k \leq 23$. In this case, since $U_1^5 \cup P_2 \cup P_7$ is an induced subgraph of $\overline{\Gamma}$, by Lemma 4.7(ii) it follows that $-1 - 2\cos\left(\frac{\pi}{k+1}\right) \leq \rho_{15}\left(K_{15} \setminus \left(U_1^5 \cup P_7 \cup P_2\right)\right) \leq -2.992$, and so $k \geq 35$, a contradiction. Thus, $s = 6$ and so $k = 20$, as we assume that $k \geq 20$.

If anyone of $\{U_1^5 \cup P_6 \cup 2P_3,\ U_1^5 \cup P_6 \cup P_4,\ U_1^5 \cup P_6 \cup K_{1,3},\ U_2^5 \cup P_6 \cup P_3\}$ is an induced subgraph of $\overline{\Gamma}$, then by Lemma 4.7(ii) we have $-1 - 2\cos\left(\frac{\pi}{k+1}\right) \leq \max\left\{\rho_{18}\left(K_{18} \setminus \left(U_1^5 \cup P_6 \cup 2P_3\right)\right),\ \rho_{16}\left(K_{16} \setminus \left(U_1^5 \cup P_4 \cup P_6\right)\right),\ \rho_{16}\left(K_{16} \setminus \left(U_1^5 \cup K_{1,3} \cup P_6\right)\right),\ \rho_{18}\left(K_{18} \setminus \left(U_2^5 \cup P_6 \cup P_3\right)\right)\right\} \leq -2.9797$, and so $k \geq 22$, a contradiction. Thus, $\{U_1^5 \cup P_6 \cup 2P_3,\ U_1^5 \cup P_6 \cup P_4,\ U_1^5 \cup P_6 \cup K_{1,3},\ U_2^5 \cup P_6 \cup P_3\}$ are forbidden. Combining this with $\varepsilon(F) \geq 2$ and Lemma 4.2(ii), we have

$$3 \leq \eta(\overline{\Gamma}) = \varepsilon(F) + 1 \leq 4.$$

When $\eta(\overline{\Gamma}) = \varepsilon(F) + 1 = 4$, since $\{U_1^5 \cup P_6 \cup 2P_3,\ U_1^5 \cup P_6 \cup P_4\}$ are forbidden, we have $F = P_6 \cup P_3 \cup P_2$ by Lemma 4.2(ii) and $q(\Gamma_1) = \varepsilon(F) - 1 = 2$. Combining this with the fact that $U_2^5 \cup P_6 \cup P_3$ is forbidden and $\Delta(\Gamma_1) = 3$, it follows that $|E(\Gamma_1)| = 7$, and so $k - 1 = |E(F)| + |E(\Gamma_1)| = 15$, a contradiction.

When $\eta(\overline{\Gamma}) = \varepsilon(F) + 1 = 3$, then $q(\Gamma_1) = 1$. Since $U_1^5 \cup P_6 \cup P_4$ is forbidden, we have $F \in \{P_6 \cup P_3,\ P_6 \cup P_2\}$. Combining this with $d \leq 4$, it follows that $k - 1 = |E(F)| + |E(\Gamma_1)| \leq 5 + 2 + 9 \leq 16$, a contradiction. This completes the proof of Claim B.

If $d = 4$, then since $\varepsilon(F) \geq 2$ and $\{W_8 \cup P_2 \cup P_3, H_1, H_8 \cup P_3,\ H_9 \cup P_3\}$ are forbidden by Corollary 4.9(i), we can conclude that $\Gamma_1 = U_4^5$, and so $\rho_2(\overline{\Gamma}) = \rho_2(U_4^5) < 1.619$ by Claim B, contrary to (6.2).

Thus, we can assume that $1 \leq d \leq 3$. Since $\varepsilon(F) \geq 2$ and $\{H_1,\ H_9 \cup P_3\}$ are forbidden by Corollary 4.9(i), we conclude that Γ_1 is a subgraph of H_{10}, and hence $\rho_2(\overline{\Gamma}) = \rho_2(\Gamma_1) \leq \rho_2(H_{10}) < 1.683$ by Claim B, contrary to (6.2). ■

By Lemma 6.6 and Corollary 4.8, in what follows, we may suppose that C_3 is the unique cycle of $\overline{\Gamma}$ with $V(C_3) = \{w_1, w_2, w_3\}$, where $d_{\Gamma_1}(w_1) \geq d_{\Gamma_1}(w_2) \geq d_{\Gamma_1}(w_3) \geq 2$ and $d_{\Gamma_1}(w_1) \geq 3$.

Lemma 6.7. *If $d_{\overline{\Gamma}}(w_1) \geq 3$, then $\eta(\overline{\Gamma}) \geq 3$.*

Proof. Assume to the contrary that $\eta(\overline{\Gamma}) = 2$. Then $|V(\Gamma_1)| = |E(\Gamma_1)| = k - |V(F)|$. Since $q(\Gamma_1) \geq 1$ by $d_{\overline{\Gamma}}(w_1) \geq 3$, it follows from (6.1) that $q(\Gamma_1) = 1 = \varepsilon(F)$. Thus, the equality holds in (6.1), and so $\Gamma_1 \cong U_d^3$ and F is a path, say P_s, where $s \geq 2$. Thus, $d + 3 = |E(\Gamma_1)| = k - |V(F)| = k - s$ and so $s + d = k - 3 \geq 17$. On the other hand, $U_1^3 \cup P_6$ is forbidden by Corollary 4.9(ii), and so $d \leq 7$ and $s \leq 5$, a contradiction. ■

Lemma 6.8. *If $d_{\overline{\Gamma}}(w_1) \geq 3$, then $d_{\overline{\Gamma}}(w_1) = 3$ and $d_{\overline{\Gamma}}(w_2) = 2$.*

Proof. To show $d_{\overline{\Gamma}}(w_1) = 3$, we assume to the contrary that $d_{\overline{\Gamma}}(w_1) \geq 4$. Then, H_4 is an induced subgraph of $\overline{\Gamma}$. Since $\{H_4 \cup K_{1,3},\ H_4 \cup P_2 \cup P_4,\ H_4 \cup P_2 \cup 2P_3\}$ are forbidden by Corollary 4.9(ii) and since $\eta(\overline{\Gamma}) \geq 3$ by Lemma 6.7, it follows from Lemma 4.2(ii) that $F \in \{P_2 \cup P_3,\ 2P_3\}$. Thus, $\varepsilon(F) = 2$. Combining this with $d_{\overline{\Gamma}}(w_1) \geq 4$ and (6.1), we have $q(\Gamma_1) = 1$. In view of Corollary 4.11, it follows that $\big(d_{\overline{\Gamma}}(w_1) - 1\big)\big(d_{\overline{\Gamma}}(w_1) - 2\big) = 4$, contrary to $d_{\overline{\Gamma}}(w_1) \geq 4$. Thus, $d_{\overline{\Gamma}}(w_1) = 3$.

Now to show $d_{\overline{\Gamma}}(w_2) = 2$, we assume to the contrary that $d_{\overline{\Gamma}}(w_2) = 3$. In this case, H_3 is an induced subgraph of $\overline{\Gamma}$. Note that $\{H_3 \cup P_5,\ H_3 \cup K_{1,3}\}$ are forbidden by Corollary 4.9(ii). Thus, each non-trivial tree of $\overline{\Gamma}$ is a path with at most four vertices, and (6.1) implies that $\varepsilon(F) \geq q(\Gamma_1) \geq 2$, where the first equality holds if and only if each special-vertex of Γ_1 is a 3-vertex. Since $H_3 \cup P_3 \cup P_4$ is forbidden by Corollary 4.9(ii) and $\varepsilon(F) \geq q(\Gamma_1) \geq 2$, it follows from Lemma 4.2(ii) and 5.1 that $F \in \{P_2 \cup P_3,\ 2P_3,\ P_2 \cup 2P_3,\ P_2 \cup P_4\}$.

Case 1. $F = P_2 \cup 2P_3$. Since $\varepsilon(F) = 3$, we have $2 \leq q(\Gamma_1) \leq 3$ by (6.1), where the second equality implies that Γ_1 contains exactly three special-vertices, which are 3-vertices. In addition, $U_{3;4,1} \cup P_2 \cup 2P_3$ is forbidden by Corollary 4.9(ii) and $d_{\overline{\Gamma}}(w_1) = d_{\overline{\Gamma}}(w_2) = 3$, this implies that $k - 6 = |E(\Gamma_1)| = |V(\Gamma_1)| \leq 12$, a contradiction.

Case 2. $F \in \{P_2 \cup P_3,\ 2P_3,\ P_2 \cup P_4\}$. In this case, $\varepsilon(F) = q(\Gamma_1) = 2$ and hence equality holds in (6.1). Therefore, Γ_1 contains exactly two special-vertices, which are 3-vertices. Since $U_{3;6,1} \cup P_2$ is forbidden by Corollary 4.9(ii), we have $\Gamma_1 = U_{3;s,t}$, where $1 \leq s \leq t \leq 5$. This implies that $k - 5 \leq k - 1 - |E(F)| = |E(\Gamma_1)| = |V(\Gamma_1)| \leq 13$, a contradiction. ■

Now we are ready to show that Γ_1 is a tree.

Theorem 6.9. *If Γ_1 is a c-cyclic graph, then $c = 0$.*

Proof. By Theorem 5.5, $c \in \{0, 1\}$. Assume to the contrary that $c = 1$. By Lemma 6.6 and Corollary 4.8, we may suppose that C_3 is the unique cycle of $\overline{\Gamma}$ with $V(C_3) = \{w_1, w_2, w_3\}$, where $d_{\Gamma_1}(w_1) \geq d_{\Gamma_1}(w_2) \geq d_{\Gamma_1}(w_3) \geq 2$ and $d_{\Gamma_1}(w_1) \geq 3$. Let P_s be the longest path of F and let U_d^3 be an induced subgraph of Γ_1 such that d is as large as possible. We have the following claim.

Claim C. *$\Delta(\Gamma_1) = 3$, $\eta(\overline{\Gamma}) - 1 = \varepsilon(F) = q(\Gamma_1) \geq 2$, $2 \leq s \leq 5$ and $5 \leq d \leq 6$*

Proof of Claim C. Since $\eta(\overline{\Gamma}) \geq 3$ by Lemma 6.7 and $\{U_7^3 \cup P_3,\ U_1^3 \cup P_6, U_1^3 \cup Z_{2,1,1}\}$ are forbidden by Corollary 4.9(ii), Lemma 4.2(ii) implies that $1 \leq d \leq 6$, $2 \leq s \leq 5$, and $T = K_{1,3}$ if $\Delta(T) = 3$. Since $\rho_1(K_{1,3}) = \rho_1(P_5) = 2\cos\left(\frac{\pi}{6}\right)$, we have $\rho_2(\overline{\Gamma}) = \rho_2(\Gamma_1) > 1.8$ by (6.2).

If $\Delta(\Gamma_1) \geq 4$, then since $d_{\overline{\Gamma}}(w_1) = 3 > d_{\overline{\Gamma}}(w_2) = d_{\overline{\Gamma}}(w_3) = 2$ by Lemma 6.8, from (6.1) it follows that $\varepsilon(F) \geq 3$. Let u_0 be the vertex of Γ_1 such that $d_{\overline{\Gamma}}(u_0) = \Delta(\Gamma_1)$ and the distance between u_0 and w_1 is as large as possible. Since $U_1^3 \cup K_{1,3} \cup P_2 \cup P_3$ is forbidden by Corollary 4.9(ii) and in view of $\varepsilon(F) \geq 3$, we can conclude that the distance between u_0 and w_1 is at most two, and so Γ_1 contains either $H_{11} \cup P_3 \cup 2P_2$ or $H_{12} \cup P_3$ as an induced subgraph by Lemma 4.2(ii), contrary to Corollary 4.9(i). Thus, $\Delta(\Gamma_1) = 3$, and so $\varepsilon(F) = q(\Gamma_1)$ by Corollary 4.11.

If $d \leq 4$, then since $d_{\overline{\Gamma}}(w_1) = 3 > d_{\overline{\Gamma}}(w_2) = d_{\overline{\Gamma}}(w_3) = 2$, $\Delta(\Gamma_1) = 3$ and $\{H_1, Z_{2,2,2}\}$ are forbidden by Corollary 4.9(i), Γ_1 is a subgraph of H_{13} or H_{14}. Combining with $\rho_2(H_{13}) < 1.76 < \rho_2(\Gamma_1) = \rho_2(\overline{\Gamma})$ by (6.2) and H_{14} being forbidden by Corollary 4.9(i), we can conclude that Γ_1 is a proper subgraph of H_{14}. Thus, $\rho_2(\overline{\Gamma}) = \rho_2(\Gamma_1) < 1.793$, contrary to (6.2). Thus, $5 \leq d \leq 6$. Combining this with $\varepsilon(F) = q(\Gamma_1) \geq 1$ and $U_5^3 \cup P_2 \cup K_{1,3}$ being forbidden by Corollary 4.9(ii), we have $\Delta(F) = 2$ by Remark 4.4, and so $\eta(\overline{\Gamma}) = \varepsilon(F) + 1$.

Now, to complete the proof, it suffices to show that $q(\Gamma_1) \geq 2$. By contradiction, we assume that $q(\Gamma_1) = 1$. Then Γ_1 is a subgraph of U_6^3, and so $\rho_2(\Gamma_1) \leq \rho_2(U_6^3) < 1.77$, contrary to $\rho_2(\Gamma_1) > 1.8$. This completes the proof of Claim C.

Case 1. $d = 6$. By Corollary 4.9(ii), $\{U_6^3 \cup P_2 \cup 2P_3,\ U_6^3 \cup P_2 \cup P_4\}$ are forbidden. Combining this with $\varepsilon(F) = q(\Gamma_1) \geq 2$ by Claim C, we conclude that $F \in \{2P_3,\ P_2 \cup P_3\}$ by Lemma 4.2(ii). Thus, $|V(\Gamma_1)| = |E(\Gamma_1)| = k - 1 - |E(F)| \geq k - 5 \geq 15$. Combining with $|V(\Gamma_1)| \geq 15$, $\Delta(\Gamma_1) = 3$ and $d_{\Gamma_1}(w_2) = 2$, it follows that $Z_{2,2,2}$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(i).

Case 2. $d = 5$. Since $\eta(\overline{\Gamma}) = \varepsilon(F) + 1 \geq 3$ by Claim C, and since $\{U_5^3 \cup P_5,\ U_5^3 \cup P_2 \cup P_3 \cup P_4\}$ are forbidden by Corollary 4.9(ii), it follows from Lemma 4.2(ii) and Claim 1 that $F \in \{P_2 \cup 2P_3, P_2 \cup P_3, P_2 \cup P_4, 2P_3, P_3 \cup P_4\}$. Combining this with $\Delta(\Gamma_1) = 3$ by Claim C, we have $|V(\Gamma_1)| = |E(\Gamma_1)| = k - 1 - |E(F)| \geq k - 6 \geq 14$. Combining with $|V(\Gamma_1)| \geq 14$, $\Delta(\Gamma_1) = 3$ and $d_{\Gamma_1}(w_2) = 2$, we conclude that $Z_{2,2,2}$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(i). ■

7. Completing the proof of Theorem 1.1

By Theorem 6.9, Γ_1 is a tree. In this section, we will complete the proof of Theorem 1.1 by showing that $\Gamma_1 = P_k$ and F is empty, and thus $\overline{\Gamma} = P_k \cup (n - k)K_1$.

Since $\tau(\Gamma_1) = 0$, Lemma 3.8 and Corollary 4.11 imply that

$$\sum_{i=1}^{|V(\Gamma_1)|} d_i(\Gamma_1)\big(d_i(\Gamma_1) - 2\big) = 2\big(\varepsilon(F) - 1\big) \geq 4|V(\Gamma_1)| - 6 + 2q(\Gamma_1) - 4\big(|V(\Gamma_1)| - 1\big) = 2\big(q(\Gamma_1) - 1\big),$$

and so

$$\varepsilon(F) \geq q(\Gamma_1), \tag{7.1}$$

with equality holds if and only if every special-vertex of Γ_1 is a 3-vertex.

Lemma 7.1. *Let $G = K_{1,4} \cup P_{s_1} \cup P_{s_2} \cup P_{s_3}$ and $t = s_1+s_2+s_3+2$. If $s_1 \geq s_2 \geq s_3 \geq 2$, then $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$, $m_2(G) = m_2(P_t)$, and $m_3(G) < m_3(P_t)$.*

Proof. It is not hard to see that $|E(G)| = |E(P_t)|$, $m_1(G) = s_1+s_2+s_3 = t-2 = m_1(P_t)$, $m_2(G) = 4\big(s_1+s_2+s_3-3\big) + \frac{1}{2}\big(s_1-2\big)\big(s_1-3\big) + \frac{1}{2}\big(s_2-2\big)\big(s_2-3\big) + \frac{1}{2}\big(s_3-2\big)\big(s_3-3\big) + \big(s_1-1\big)\big(s_2-1\big) + \big(s_1-1\big)\big(s_3-1\big) + \big(s_2-1\big)\big(s_3-1\big) = \frac{1}{2}\big(s_1+s_2+s_3\big)\big(s_1+s_2+s_3-1\big) = \frac{1}{2}(t-2)(t-3) = m_2(P_t)$, and $m_3(G) \leq s_1+s_2+s_3-6 = t-8 < t-3 = m_3(P_t)$. ■

Lemma 7.2. *Let $G = W_q \cup P_{s_1} \cup P_{s_2}$ and $t = s_1+s_2+q-2$, where $q \geq 7$. If $s_1 \geq s_2 \geq 2$ and $s_1 \geq 3$, then $|E(G)| = |E(P_t)|$, $m_1(G) = m_1(P_t)$, $m_2(G) = m_2(P_t)$, and $m_3(G) < m_3(P_t)$.*

Proof. It is not hard to see that $|E(G)| = |E(P_t)|$, $m_1(G) = q+s_1+s_2-4 = t-2 = m_1(P_t)$, $m_2(G) = 2q-9+\frac{1}{2}(q-4)(q-5)+(q-1)(s_1+s_2-2)+\frac{1}{2}(s_1-2)(s_1-3)+\frac{1}{2}(s_2-2)(s_2-3)+(s_1-1)(s_2-1) = \frac{1}{2}(q+s_1+s_2-4)(q+s_1+s_2-5) = \frac{1}{2}(t-2)(t-3) = m_2(P_t)$, and $m_3(G) \leq q-3+s_1+s_2-5 = t-6 < t-3 = m_3(P_t)$. ■

A path $P_s : u_1u_2\cdots u_s$ with $s \geq 2$ is called a *pendant path* of G if $d_G(u_s) = 1 < d_G(u_{s-1}) = d_G(u_{s-2}) = \cdots = d_G(u_2) = 2 < d_G(u_1)$, and u_1 is called the *initial vertex* of P_s.

Theorem 7.3. *If $k \geq 13$ and Γ_1 is a tree, then $\Gamma_1 = P_k$ and F is empty.*

Proof. Let P_s be the longest path of F. Let Γ_1 be the non-trivial tree of $\overline{\Gamma}$ such that $\Delta(\Gamma_1) = \Delta(\overline{\Gamma})$, and subject to this, $\rho_1(\Gamma_1)$ is as largest as possible. If $\Delta(\Gamma_1) = 2$, then by the choice of Γ_1, each non-trivial tree of F is a path. By Corollary 4.11, we have $\varepsilon(F) = 0$ and so the theorem holds. Thus, it suffices to consider the following two cases:

Case 1. $\Delta(\Gamma_1) \geq 4$. If $q(\Gamma_1) \geq 2$, then $\varepsilon(F) \geq 3$ by (7.1). Since $\big\{H_2,\ Z_{4,1,1,1} \cup P_3,\ Z_{3,1,1,1} \cup 2P_3 \cup K_1\big\}$ are forbidden by Corollary 4.9(i) and in view of Lemma 4.2(ii), we can conclude that H_1 is an induced subgraph of $\overline{\Gamma}$, contradicting Corollary 4.9(i).

Thus $q(\Gamma_1) = 1$. By Corollary 4.11 and $\tau(\Gamma_1) = 0$, we have

$$\varepsilon(F) = \frac{1}{2}\Delta(\Gamma_1)\big(\Delta(\Gamma_1)-3\big) + 1 \geq 3. \tag{7.2}$$

Since $\big\{H_2,\ Z_{3,1,1,1} \cup 2P_3 \cup K_1,\ Z_{2,1,1,1,1} \cup P_3\big\}$ are forbidden by Corollary 4.9(i) and $\Delta(\Gamma_1) \geq 4$, it follows from Lemma 4.2(ii) that either Γ_1 is a star or $\Gamma_1 = Z_{2,1,1,1}$.

If $\Gamma_1 = Z_{2,1,1,1}$, then since $\big\{Z_{2,1,1,1} \cup K_{1,3} \cup P_3, Z_{2,1,1,1} \cup K_1 \cup P_3 \cup P_5,\ Z_{2,1,1,1} \cup 3P_3\big\}$ are forbidden by Corollary 4.9(i) and in view of $\varepsilon(F) \geq 3$ by (7.2), we have $s \leq 4$ and $\varepsilon(F)+1 = \eta(\overline{\Gamma})$. Combining this with Lemma 4.2(ii) and (7.2), it follows that $\varepsilon(F) = 3$ and $F \in \big\{P_2 \cup P_3 \cup P_4,\ P_2 \cup 2P_3\big\}$. It is not hard to see that $5 = |E(\Gamma_1)| = k-1-|E(F)| \geq k-1-6$, a contradiction. Thus, $\Gamma_1 = K_{1,p-1}$, where $p \geq 5$.

If $p \geq 6$, then $\varepsilon(F) \geq 6$ by (7.2). By Lemma 4.2(ii), $K_{1,5} \cup 3P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(i). Thus, $p = 5$ and so $\varepsilon(F) = 3$ by (7.2).

By Remark 4.4, F consists of three non-trivial paths and $\eta(\overline{\Gamma}) - 4$ first-type trees. Let F_1 be the set of all those first-type trees, and let P_{q_1}, P_{q_2}, and P_{q_3} be the three non-trivial paths of F. By Lemmas 6.4 and 7.1, we have $m_1(\overline{\Gamma}) = m_1\big(K_{1,4} \cup P_{q_1} \cup P_{q_2} \cup P_{q_3}\big) + m_1(F_1) = m_1\big(P_{q_1+q_2+q_3+2}\big) + m_1(F_1) = m_1\big(P_{q_1+q_2+q_3+2} \cup F_1\big) = m_1(P_k)$, $m_2(\overline{\Gamma}) = m_2\big(K_{1,4} \cup P_{q_1} \cup P_{q_1} \cup P_{q_1}\big) + m_2(F_1) + |E\big(K_{1,4} \cup P_{q_1} \cup P_{q_1} \cup P_{q_1}\big)| \cdot |E(F_1)| = m_2\big(P_{q_1+q_2+q_3+2}\big) + m_2(F_1) + |E\big(P_{q_1+q_2+q_3+2}\big)| \cdot |E(F_1)| = m_2\big(P_{q_1+q_2+q_3+2} \cup F_1\big) = m_2(P_k)$, and $m_3(\overline{\Gamma}) = m_3\big(K_{1,4} \cup P_{q_1} \cup P_{q_1} \cup P_{q_1}\big) + m_3(F_1) < m_3\big(P_{q_1+q_2+q_3+2}\big) + m_3(F_1) \leq m_3(P_k)$. This implies that $\Phi(\overline{\Gamma}) > \Phi\big(P_k \cup (n-k)K_1\big)$, contrary to Corollary 6.2.

Case 2. $\Delta(\Gamma_1) = 3$.

Subcase 2.1. $q(\Gamma_1) = 1$. By Corollary 4.11, we have $\varepsilon(F) = q(\Gamma_1) = 1$. Combining this with $Z_{2,2,2}$ being forbidden by Corollary 4.9(i) and Remark 4.4, we can conclude that $\overline{\Gamma}$ contains exactly $\eta(\overline{\Gamma}) - 1$ non-trivial trees (each of which has exactly one 3-vertex) and one path P_s, where $s \geq 2$. We may suppose that $\Gamma_1 = Z_{p_1,p_2,1}$, where $p_1 \geq p_2 \geq 1$. By Lemma 6.4 and since $Z_{2,2,2}$ is forbidden by Corollary 4.9(i), we can obtain another forest G_1 with exactly $\eta(\overline{\Gamma}) - 2$ first-type trees and one path $P_{p_1+p_2+s+1}$ such that $\Phi(\overline{\Gamma}) \geq \Phi(G_1) \geq \Phi\big(P_k \cup (n-k)K_1\big)$, where the first inequality is strict if either $p_2 = 1$ or $s \geq 3$. Since $p_1+p_2+s+1 \geq 5$, by Corollary 6.2 and Lemma 6.4, it follows that $\Gamma_1 = Z_{p_1,p_2,1}$ and $F = P_2$, where $p_2 \geq 2$. Note that $\big\{Z_{4,4,1},\ Z_{7,2,1} \cup K_1\big\}$ are forbidden by Corollary 4.9(i). Thus, $2 \leq p_2 \leq 3$ and $2 \leq p_1 \leq 6$. In this case, $k-2 = |E(\Gamma_1)| = p_1+p_2+1 \leq 10$, a contradiction.

Subcase 2.2. $q(\Gamma_1) \geq 2$. In this case, $\varepsilon(F) = q(\Gamma_1) \geq 2$ by (7.1). Since $Z_{2,2,2,}$ is forbidden by Corollary 4.9(i), we may suppose that $Z_{p_3,p_4,1}$ is an induced subgraph of Γ_1 such that p_4 is as large as possible, and subject to this, p_3+p_4 is as large as possible, where $p_3 \geq p_4 \geq 1$. Furthermore, since $q(\Gamma_1) \geq 2$ and H_1 is forbidden by Corollary 4.9(i), we have $p_3 \geq 3$. Since $Z_{4,4,1}$ is forbidden by Corollary 4.9(i), we can conclude that $p_4 \leq 3$.

If $p_4 = 3$, then since $\{Z_{1,3,4} \cup K_1 \cup P_3, H_1\}$ are forbidden by Corollary 4.9(i) and $\varepsilon(F) = q(\Gamma_1) \geq 2$, we have $p_3 = 3$ and H_{15} is an induced subgraph of Γ_1. Combining this with $\varepsilon(F) \geq 2$ and Lemma 4.2(ii), $H_{15} \cup P_2 \cup P_3$ is an induced subgraph of $\overline{\Gamma}$, contrary to Corollary 4.9(i).

If $p_4 = 1$, then $\Gamma_1 = W_q$ and $\varepsilon(F) = q(\Gamma_1) = 2$ by the choice of p_4. As H_1 is forbidden by Corollary 4.9(i), $q \geq 7$. From Lemmas 6.4 and 7.2, we can deduce that $\Phi(\overline{\Gamma}) > \Phi\left(P_k \cup (n-k)K_1\right)$, contrary to Corollary 6.2.

Finally, we consider the case of $p_4 = 2$. Since $\{Z_{6,2,1} \cup P_3, H_1\}$ are forbidden by Corollary 4.9(i) and $\varepsilon(F) = q(\Gamma_1) \geq 2$, we have $3 \leq p_3 \leq 5$ and $\varepsilon(F) = q(\Gamma_1) = 2$ by the choice of p_4. Here, we rewrite p_3 as q, that is, $q = p_3$. Suppose that $P_{q+1} = uw_1w_2\cdots w_q$ is the longest pendant path of $Z_{q,2,1}$ with initial vertex u, where $d_{\Gamma_1}(u) = 3$. Let T_1 (resp., T_2) be the tree obtained from $Z_{p_3,2,1}$ and a vertex v by adding exactly one edge vw_{q-1} (resp., vw_{q-2}). By the choice of p_4 and $p_4 = 2$, $\Gamma_1 \in \{T_1, T_2\}$. Since $\varepsilon(F) = q(\Gamma_1) = 2$, we suppose that P_s and P_t are the two paths of F, where $s \geq t \geq 2$. By Lemma 4.2(ii), we have $s \geq 3$ and thus we can easily check that $|E(\Gamma_1 \cup P_s \cup P_t)| = |E(P_{q+s+t+3})|$, $m_1(\Gamma_1 \cup P_s \cup P_t) = q+s+t+1 = m_1(P_{q+s+t+3})$, $m_2(\Gamma_1 \cup P_s \cup P_t) = \frac{1}{2}(q+s+t+1)(q+s+t) = m_2(P_{q+s+t+3})$ and $m_3(\Gamma_1 \cup P_s \cup P_t) \leq q+s+t-1 < q+s+t = m_3(P_{q+s+t+3})$. Now, from Lemma 6.4, we can conclude that $\Phi(\overline{\Gamma}) > \Phi\left(P_k \cup (n-k)K_1\right)$, contrary to Corollary 6.2. ■

By Theorems 6.9 and 7.3, it follows that $\overline{\Gamma} = P_k \cup (n-k)K_1$ for $k \geq 20$, which completes the proof of Theorem 1.1.

8. Concluding remarks

In this paper, we show that $K_n \backslash P_k$ is $A - DS$ for $k \geq 20$, which almost solves Conjecture 1.1. It is continued work of [2,4,8], where Conjecture 1.1 was shown to hold for $2 \leq k \leq 9$ and $k = n$. Note that $K_n \backslash P_k$ is a dense graph. Thus, how to characterize dense graphs becomes an interesting problem to us. To this aim, under the hypothesis that G is cospectral with a dense graph, one should attempt to determine exact values or some useful properties for the eigenvalues of G, via which we can deduce the structure of G or its complement graph $\overline{G}$. This was well illustrated in [4,2,8]. However, these are not sufficient to attack Conjecture 1.1. In this paper, we pay more attention to the eigenvalues of $\overline{G}$. Toward this, the Courant–Weyl inequalities (Lemma 3.1) and Cauchy Interlacing theorem (Lemma 3.5) are two effective tools. By applying the Courant–Weyl inequalities, when Γ is A-cospectral with $K_n \backslash P_k$, we deduce that the second largest eigenvalue of $\overline{\Gamma}$ is less than 2 (Lemma 4.1(i)), through which we are able to determine the structure of $\overline{\Gamma}$ (Remark 4.4). We also employ the Cauchy Interlacing theorem to obtain many forbidden graphs, which play a crucial role in the proof of our main results.

By the current argument, we succeed in settling Conjecture 1.1 for $k \geq 20$. When k is small ($10 \leq k < 20$), in order to settle Conjecture 1.1 completely, we have to exclude many graphs, which makes the analysis much more complicated. We think it is interested to find a simpler method to solve the small case of k.

CRediT authorship contribution statement

Muhuo Liu: Conceptualization, Formal analysis, Writing - original draft. **Haiying Shan:** Writing - review & editing. **Xiaofeng Gu:** Formal analysis, Writing - review & editing.

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THE FAN GRAPH IS DETERMINED BY ITS SIGNLESS LAPLACIAN SPECTRUM

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Abstract. Given a graph G, if there is no nonisomorphic graph H such that G and H have the same signless Laplacian spectra, then we say that G is Q-DS. In this paper we show that every fan graph F_n is Q-DS, where $F_n = K_1 \vee P_{n-1}$ and $n \geqslant 3$.

Keywords: signless Laplacian spectrum; join graph; graph determined by its spectrum

MSC 2010: 05C50, 15A18

1. Introduction

Throughout this paper, G is an undirected simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let $N(u)$ and $d(u)$ be the neighbor set and the degree of vertex u, respectively. In the sequel, we enumerate the degrees in nonincreasing order, i.e., $d_1 \geqslant d_2 \geqslant \ldots \geqslant d_n$, where $d(v_i) = d_i$ for $i \in \{1, 2, \ldots, n\}$. Sometimes we write $d_i(G)$ and $d_G(u)$ in place of d_i and $d(u)$, respectively, in order to indicate the dependence on G. As usual, K_n, P_n and C_n denote the complete graph, path and cycle of order n, respectively, and $G_1 \vee G_2$ denotes the *join graph* of two vertex disjoint graphs G_1 and G_2. In other words, $G_1 \vee G_2$ is the graph having vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv\colon\ u \in V(G_1),\ v \in V(G_2)\}$.

Let $A(G)$ and $D(G)$, respectively, be the adjacency matrix and the diagonal matrix of G. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$, and the *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. Denote by $\Phi(G, x)$ the Q-characteristic polynomials of graph G.

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It is easy to see that $Q(G)$ is positive semidefinite [2] and hence its eigenvalues can be arranged as

$$\mu_1(G) \geqslant \mu_2(G) \geqslant \ldots \geqslant \mu_n(G) \geqslant 0.$$

If there is no confusion, sometimes we simply write $\mu_i(G)$ as μ_i. In the following, let $S_Q(G)$ denote the spectra, i.e., the eigenvalues of $Q(G)$.

Two graphs are said to be Q-cospectral or L-cospectral if they have the same signless Laplacian or Laplacian spectrum, respectively. A graph G is said to be Q-DS or L-DS if H Q-cospectral or L-cospectral to G implies that $H = G$, respectively.

Which graphs are determined by their spectra? This question was proposed by Dam and Haemers in [11], and has drawn much attention recently. The literature contains dozens of results on this topic. For details, we refer the readers to [5], [8], [10], [11], [12] and the references therein.

The fan graph is denoted by $F_n = K_1 \vee P_{n-1}$. In [10], it was proved that F_n is L-DS for any $n \geqslant 3$. In this note, we will show that:

Theorem 1.1. *For any $n \geqslant 3$, F_n is Q-DS.*

2. Some properties for the Q-cospectral graph with F_n

Consider two sequences of real numbers: $\alpha_1 \geqslant \alpha_2 \geqslant \ldots \geqslant \alpha_n$ and $\beta_1 \geqslant \beta_2 \geqslant \ldots \geqslant \beta_m$ with $m < n$. The latter sequence is said to *interlace* the former whenever $\alpha_i \geqslant \beta_i \geqslant \alpha_{n-m+i}$ for $i = 1, 2, \ldots, m$.

Lemma 2.1 ([7])**.** *Let A be a symmetric matrix. If B is a principal submatrix of A, then the eigenvalues of B interlace the eigenvalues of A.*

When M is a real symmetric matrix of order n, we use $\Theta_1(M) \geqslant \Theta_2(M) \geqslant \ldots \geqslant \Theta_n(M)$ to denote its eigenvalues.

Corollary 2.1. *Let G be a graph with n vertices. If the least degree vertex v_n and second minimum degree vertex v_{n-1} are not adjacent, then $\mu_{n-1} \leqslant d_{n-1}$.*

P r o o f. Since $v_n v_{n-1} \notin E(G)$, $Q(G)$ contains

$$B = \begin{pmatrix} d_n & 0 \\ 0 & d_{n-1} \end{pmatrix}$$

as a principal submatrix. By Lemma 2.1, $\mu_{n-1} \leqslant \Theta_1(B) = d_{n-1}$. □

Let uv be an edge of G. Let $m(v)$ denote the average of the degrees of the vertices being adjacent to v, i.e., $m(v) = \sum_{w \in N(v)} d(w)/d(v)$.

Lemma 2.2 ([3]). *If G is a connected graph with at least one edge, then*

$$\mu_1(G) \leqslant \max\{d(v) + m(v) \colon v \in V(G)\} \leqslant d_1(G) + d_2(G).$$

Lemma 2.3 ([4], [8]). *For any connected graph G with n vertices, $\mu_n < d_n$ and*

$$\mu_2 \geqslant \frac{1}{2}\big(d_1 + d_2 - \sqrt{(d_1 - d_2)^2 + 4}\big) \geqslant d_2 - 1.$$

Furthermore, if $d_3 = d_2 \leqslant d_1 - 2$, then $\mu_2 \geqslant d_2$.

Lemma 2.4 ([3]). *Let G be a graph with $U \subseteq V(G)$, where $U = \{u_1, u_2, \ldots, u_k\}$. If all vertices of U have the same set of neighbors, then G has at least $k - 1$ signless Laplacian eigenvalues equal to $d_G(u_1)$.*

Lemma 2.5 ([6]). *If G_i is an r_i-regular graph on n_i vertices for $i \in \{1, 2\}$, then*

$$\Phi(G_1 \vee G_2, x) = \frac{\Phi(G_1, x - n_2)\Phi(G_2, x - n_1)}{(x - 2r_1 - n_2)(x - 2r_2 - n_1)} f(x),$$

where $f(x) = x^2 - (2(r_1 + r_2) + (n_1 + n_2))x + 2(2r_1r_2 + r_1n_1 + r_2n_2)$.

Lemma 2.6 ([6]). *If G_i is an r_i-regular graph on n_i vertices for $i \in \{1, 2, 3\}$, then*

$$\Phi(G_1 \vee (G_2 \cup G_3), x) = \frac{\Phi(G_1, x - n_2 - n_3)\Phi(G_2, x - n_1)\Phi(G_3, x - n_1)}{(x - 2r_1 - n_2 - n_3)(x - 2r_2 - n_1)(x - 2r_3 - n_1)} f(x),$$

where $g(x) = x^3 - (2(r_1 + r_2 + r_3) + 2n_1 + n_2 + n_3)x^2 + \big((n_1 + n_2 + n_3)(n_1 + 2(r_2 + r_3)) + 4(r_1(n_1 + r_3) + r_2(r_1 + r_3))\big)x - \big(2n_1(n_1r_1 + n_2r_2 + n_3r_3 + 2r_1(r_2 + r_3)) + 4r_2r_3(2r_1 + n_2 + n_3)\big)$.

Let I_n be the identity matrix of order n.

Lemma 2.7. *If $S_Q(G) = S_Q(F_n)$ and $n \geqslant 5$, then $d_2(G) \leqslant 5$, $n - 4 \leqslant d_1(G) \leqslant n - 1$ and*

$$1 < \mu_{n-2}(G) \leqslant \mu_2(G) < 5 \leqslant n < \frac{1}{2}\big(n + 1 + \sqrt{n^2 - 2n + 9}\big) < \mu_1(G).$$

P r o o f. Note that $Q(F_n)$ contains $I_{n-1} + Q(P_{n-1})$ as its principal submatrix. By Lemma 2.1, we have $\mu_{n-2}(G) \geqslant 1 + \mu_{n-2}(P_{n-1}) > 1$ and $\mu_2(G) \leqslant \mu_1(I_{n-1} + Q(P_{n-1})) < 5$. Now, Lemma 2.3 implies that $d_2(G) - 1 \leqslant \mu_2(G) < 5$ and hence $d_2(G) \leqslant 5$.

Since each edge deletion from a connected graph G will strictly decrease the largest signless Laplacian eigenvalue (namely, $\mu_1(G)$), by Lemmas 2.5 and 2.6 we have

$$\mu_1(G) > \begin{cases} \mu_1\Big(K_1 \vee \Big(\dfrac{n-2}{2}K_2 \cup K_1\Big)\Big) & \text{when } n \text{ is even;} \\ \mu_1\Big(K_1 \vee \Big(\dfrac{n-1}{2}K_2\Big)\Big) & \text{when } n \text{ is odd.} \end{cases}$$

Note that

$$\begin{aligned} \mu_1\Big(K_1 \vee \Big(\frac{n-1}{2}K_2\Big)\Big) &= \frac{1}{2}\big(n+2+\sqrt{n^2-4n+12}\big) \\ &> \frac{1}{2}\big(n+1+\sqrt{n^2-2n+9}\big) = \mu_1\Big(K_1 \vee \Big(\frac{n-2}{2}K_2 \cup K_1\Big)\Big). \end{aligned}$$

Thus, we obtain the required inequality for $\mu_1(G)$.

Since $\mu_1(G) > n$ and $d_2(G) \leqslant 5$, we have $n-4 \leqslant d_1(G) \leqslant n-1$ by Lemma 2.2. □

Lemma 2.8 ([2])**.** *If G is a graph with n vertices and m edges, then*

$$\sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n} d_i = 2m, \quad \text{and} \quad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2.$$

If $S_Q(G) = S_Q(F_n)$, then $d_2 \leqslant 5$ and $d_1 \geqslant n-4$ by Lemma 2.7. Hereafter, we suppose that G has n_j vertices of degree j in $V(G) \setminus \{v_1\}$ for $j = 1, 2, \ldots, 5$. By Lemma 2.8 it follows that

$$\begin{cases} n_2 = \frac{1}{2}(n^2 - 9n + 12) - \frac{1}{2}d_1(d_1 - 7) - 3n_1 - n_5, \\ n_3 = -n^2 + 9n - 10 + d_1(d_1 - 6) + 3n_1 + 3n_5, \\ n_4 = \frac{1}{2}(n-1)(n-6) - \frac{1}{2}d_1(d_1 - 5) - n_1 - 3n_5. \end{cases} \tag{2.1}$$

Lemma 2.9. *If $S_Q(G) = S_Q(F_n)$, then G is connected with either $d_1(G) \geqslant n-2$ or $d_n(G) = 1$.*

P r o o f. From Lemma 2.7 it follows that $d_2(G) \leqslant 5$ and $n-4 \leqslant d_1(G) \leqslant n-1$. If $d_1(G) = n-4$ and $d_n(G) \geqslant 2$, then $d_2(G) = 5$ by Lemmas 2.2 and 2.7. So, $n \geqslant 9$. In this case, $n_1 = 0$. From (2.1) we have $n_3 + n_4 = 15 - 2n < 0$, a contradiction. Thus,

$$d_1(G) = n-4 \text{ implies that } d_n(G) = 1. \tag{2.2}$$

We first prove that G is connected. By contradiction, we assume that G is disconnected. Since F_n is nonbipartite, $\mu_n(G) = \mu_n(F_n) > 0$ (see [2], Proposition 2.1). Recall that $d_1(G) \geqslant n-4$. Thus, G contains a connected component with at least $n-3$ vertices. So, $G = G_1 \cup C_3$, where $d_1(G_1) = n-4$. Since $S_Q(G) = S_Q(F_n)$ and $S_Q(C_3) = \{4,1,1\}$,

$$d_{n-3}(G_1) > \mu_{n-3}(G_1) \geqslant \mu_{n-2}(G) > 1$$

by Lemmas 2.3 and 2.7. Now, we have $d_n(G) = 2$, contradicting (2.2).

We now show that either $d_1(G) \geqslant n-2$ or $d_n(G) = 1$. By contradiction, from (2.2) we assume that $d_n(G) \geqslant 2$ and $d_1(G) = n-3$. In this case, $n_1 = 0$ and $d_2(G) \geqslant 4$ by Lemmas 2.2 and 2.7. From (2.2) it follows that

$$n_3 + n_4 = 8 - n, \tag{2.3}$$

which implies that $n \in \{7,8\}$.

If $n = 8$, then $n_3 = n_4 = 0$ by (2.3). Recall that $n_1 = 0$. Thus, $0 = n_3 = -7 + 3n_5$ by (2.1), a contradiction. Otherwise, $n = 7$. Now, (2.3) implies that $n_3 + n_4 = 1$, and hence $n_4 = 5 - 3n_5 \in \{0,1\}$ by (2.1), a contradiction. □

Lemma 2.10. *If $d_1(G) \leqslant n-3$, then G and F_n are not Q-cospectral.*

P r o o f. By contradiction, we assume that $S_Q(G) = S_Q(F_n)$, and hence Lemmas 2.7 and 2.9 imply that G is connected with $d_2(G) \leqslant 5$ and $n-4 \leqslant d_1(G) \leqslant n-3$.

Case 1. $d_1(G) = n-4$. Suppose $\max\{d(v) + m(v)\colon v \in V(G)\}$ occurs at the vertex u_0. If $d(u_0) \leqslant 4$, by Lemmas 2.2 and 2.7 we have

$$\mu_1(G) \leqslant d(u_0) + m(u_0) \leqslant d(u_0) + d_1(G) = d(u_0) + n - 4 \leqslant n < \mu_1(F_n),$$

a contradiction.

If $5 \leqslant d(u_0) \leqslant n-4$, then

$$\begin{aligned} \mu_1(G) &\leqslant d(u_0) + m(u_0) \leqslant d(u_0) + \frac{2|E(G)| - d(u_0) - (n-1-d(u_0))d_n(G)}{d(u_0)} \\ &\leqslant d(u_0) + \frac{2(2n-3) - d(u_0) - (n-1-d(u_0))}{d(u_0)} = d(u_0) + \frac{3n-5}{d(u_0)}. \end{aligned} \tag{2.4}$$

When $n = 9$, by (2.4) we have $d(u_0) + m(u_0) \leqslant 9.4 < 9.6 < \mu_1(F_9)$, a contradiction.

When $n \geqslant 10$, it is easy to see that

$$d(u_0) + m(u_0) \leqslant \max\Big\{5 + \frac{3n-5}{5}, n-4 + \frac{3n-5}{n-4}\Big\} < \frac{1}{2}\big(n+1+\sqrt{n^2-2n+9}\big),$$

against Lemmas 2.2 and 2.7.

Case 2. $d_1(G) = n - 3$. We consider the following three subcases:

Subcase 2.1. $n = 7$. In this case, $d_1(G) = 4$ and hence $d_2(G) \leqslant 4$ and $n_5 = 0$ by Lemma 2.7. Now, (2.1) implies that $n_2 = 5 - 3n_1 \geqslant 0$ and $n_3 = 3n_1 - 4 \geqslant 0$, a contradiction.

Subcase 2.2. $n = 8$. In this case, by (2.1) it follows that $n_2 = 7 - 3n_1 - n_5$, $n_3 = 3n_1 + 3n_5 - 7$ and $n_4 = 7 - n_1 - 3n_5$. Thus, either $n_5 = n_2 = n_3 = 2$ and $n_1 = 1$, or $n_5 = 1$ and $n_4 = n_3 = n_1 = 2$. If $n_5 = 1$ and $n_4 = n_3 = n_1 = 2$, then Corollary 2.1 implies that $\mu_7(G) \leqslant 1 < 1.19 < \mu_7(F_8)$, a contradiction. Otherwise, $n_5 = n_2 = n_3 = 2$ and $n_1 = 1$.

We assume that there exist two vertices of degree five being not adjacent with each other, then by Lemma 2.1 we obtain $\mu_2(G) \geqslant 5 > \mu_2(F_8)$, a contradiction. Thus, every pair of vertices of degree five are adjacent. In this case, $Q(G)$ contains

$$B_1 = \begin{pmatrix} 5 & 1 & 1 \\ 1 & 5 & 1 \\ 1 & 1 & 5 \end{pmatrix}$$

as a principal submatrix. By Lemma 2.1, $\mu_3(G) \geqslant \Theta_3(B_1) = 4 > \mu_3(F_8)$, a contradiction.

Subcase 2.3. $n \geqslant 9$. We first suppose that $0 \leqslant n_5 \leqslant 1$. By (2.1) we have $n_2 + n_3 = 8 - n + 2n_5$. Thus, $n_5 = 1$ and $9 \leqslant n \leqslant 10$. No matter if $n = 9$ or $n = 10$, it will yield a contradiction by (2.1).

Next we suppose that $n_5 \geqslant 2$. When $n \geqslant 10$, by Lemma 2.3 we have $\mu_2(G) \geqslant 5$, against Lemma 2.7. When $n = 9$, by (2.1) we have $n_3 + n_4 = 2n_1 - 1$, and hence $n_1 \geqslant 1$. Now, Lemma 2.3 implies that $\mu_9(G) < 1 = \mu_9(F_9)$, a contradiction. □

Lemma 2.11. *If $d_1(G) = n - 2$ and $n \geqslant 7$, then G and F_n are not Q-cospectral.*

P r o o f. By contradiction, we assume that $S_Q(G) = S_Q(F_n)$. By Lemma 2.9, G is connected. If $n_1 \geqslant 4$, then v_1 is adjacent to at least three vertices of degree one, as $d(v_1) = d_1(G) = n - 2$. By Lemmas 2.3 and 2.4 we have $\mu_{n-2}(G) \leqslant 1$, which contradicts Lemma 2.7. Thus, $0 \leqslant n_1 \leqslant 3$.

When $n = 7$, since $\mu_7(F_7) = 1$, we have $n_1 = 0$ by Lemma 2.3. By (2.1), it follows that $n_5 = 1$, $n_2 = 3$, and $n_3 = 2$. There are exactly five connected graphs of order 7 with $n_2 = 3$, $n_3 = 2$ and $n_5 = 1$ and $d_1(G) = 5$ (see [1], pages 217–223). It can be easily checked that none of them is Q-cospectral with F_7, a contradiction.

When $n = 8$, if $n_5 \geqslant 1$, since $d_1 = 6$ and $d_2 = 5$, by Lemma 2.3 we have $\mu_2(G) > 4.38 > \mu_2(F_8)$, a contradiction. Otherwise, $n_5 = 0$. Now, (2.1) implies that

$n_3 = n_1 = 1$, $n_2 = 2$, and $n_4 = 3$. If the vertex of degree 6 is adjacent to at most two vertices of degree four, then by Lemma 2.2 we obtain

$$\begin{aligned}\mu(G) &\leqslant \max\Big\{6 + \frac{(4+2)\times 2 + 3 + 1}{6}, 4 + \frac{6 + 4\times 2 + 3}{4}, 3 + \frac{6 + 4\times 2}{3}, 2 + \frac{6+4}{2}\Big\} \\ &< 8.67 < \mu(F_8),\end{aligned}$$

a contradiction. Otherwise, the vertex of degree 6 is adjacent to three vertices of degree four, and hence $Q(G)$ contains B_1, B_2 or B_3 as a principle submatrix, where

$$B_1 = \begin{pmatrix} 6 & 1 & 1 & 1 \\ 1 & 4 & 0 & 0 \\ 1 & 0 & 4 & 0 \\ 1 & 0 & 0 & 4 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 6 & 1 & 1 & 1 \\ 1 & 4 & 1 & 0 \\ 1 & 1 & 4 & 0 \\ 1 & 0 & 0 & 4 \end{pmatrix},$$

$$B_3 = \begin{pmatrix} 6 & 1 & 1 & 1 \\ 1 & 4 & 1 & 1 \\ 1 & 1 & 4 & 0 \\ 1 & 1 & 0 & 4 \end{pmatrix}, \quad B_4 = \begin{pmatrix} 6 & 1 & 1 & 1 \\ 1 & 4 & 1 & 1 \\ 1 & 1 & 4 & 1 \\ 1 & 1 & 1 & 4 \end{pmatrix}.$$

Note that $\Theta_3(B_1) = \Theta_3(B_3) = \Theta_3(B_4) = 4 > \mu_3(F_8)$ and $\Theta_2(B_2) > 4.46 > \mu_2(F_8)$. By Lemma 2.1, we get a contradiction. So, we may suppose that $n \geqslant 9$ in the following.

If $n_5 \geqslant 2$, since $n \geqslant 9$, $d_1(G) \geqslant 7$. By Lemma 2.3 we have $\mu_2(G) \geqslant 5$, contradicting Lemma 2.7. Otherwise, we may suppose that $0 \leqslant n_5 \leqslant 1$ in what follows.

By (2.1), it follows that

$$(2.5)\quad n_2 = n - 3 - n_5 - 3n_1, \quad n_3 = 6 - n + 3n_5 + 3n_1, \quad n_4 = n - 4 - 3n_5 - n_1.$$

Since $0 \leqslant n_1 \leqslant 3$, $0 \leqslant n_5 \leqslant 1$ and $n_3 \geqslant 0$, we have $9 \leqslant n \leqslant 18$ by (2.5).

Case 1. n is odd. In this case, $n \in \{9, 11, 13, 15, 17\}$. Computer aided calculations show that $\mu_n(F_n) = 1$ and hence $n_1 = 0$ by Lemma 2.3. Now, (2.5) implies that $n = 9$ with $n_2 = 5$, $n_4 = 2$ and $n_5 = 1$. By Lemma 2.3, $\mu_2(G) > 4.58 > \mu_2(F_9)$, a contradiction.

Case 2. n is even. In this case, $n \in \{10, 12, 14, 16, 18\}$. Computer aided calculations show that $\mu_{n-1}(F_n) > 1$. Thus, by Corollary 2.1, we can conclude that $0 \leqslant n_1 \leqslant 1$. If $n_5 = 0$, then $n_3 = 6 - n + 3n_1 \geqslant 0$ by (2.5), against $0 \leqslant n_1 \leqslant 1$ and $n \geqslant 10$. Otherwise, $n_5 = 1$. Since $n_3 = 9 - n + 3n_1 \geqslant 0$ and $0 \leqslant n_1 \leqslant 1$, we have $n \in \{10, 12\}$. When $n \in \{10, 12\}$, since $d_1 \geqslant 8$ and $d_2 = 5$, by Lemma 2.3 we have $\mu_2(G) > 4.69 > \mu_2(F_n)$, a contradiction. □

Theorem 2.1. *If $S_Q(G) = S_Q(F_n)$ and $n \geqslant 7$, then G and F_n have the same degree sequence.*

P r o o f. Since $S_Q(G) = S_Q(F_n)$, by Lemmas 2.7, 2.9–2.11, G is connected with $d_2(G) \leqslant 5$ and $d_1(G) = n-1$. When $n = 7$, if $n_5 \geqslant 1$, since $d_1 = 6$ and $d_2 = 5$, by Lemma 2.3 we have $\mu_2(G) > 4.38 > \mu_2(F_7)$, a contradiction. Thus, $n_5 = 0$ and so G and F_7 have the same degree sequence by (2.1).

Now, we consider the case of $n \geqslant 8$. By Lemmas 2.3 and 2.7, we have $0 \leqslant n_5 \leqslant 1$. From (2.1) it follows that $n_4 + n_1 + 3n_5 = 0$, and hence G and F_n share the same degree sequence. □

Corollary 2.2. *If $S_Q(G) = S_Q(F_n)$ and $n \geqslant 7$, then either $G \cong K_1 \vee (C_b \cup P_{n-1-b})$ or $G \cong F_n$, where $3 \leqslant b \leqslant n-3$.*

P r o o f. From Theorem 2.1 and Lemma 2.9, if G is Q-cospectral with F_n, then G is connected and so $G \cong K_1 \vee (C_{k_1} \cup C_{k_2} \cup \ldots \cup C_{k_t} \cup P_a)$, where $k_1 + k_2 + \ldots + k_t = n - 1 - a$ and $a \geqslant 2$.

If $t \geqslant 2$, since $Q(G)$ contains $I_{n-1} + Q(C_{k_1} \cup C_{k_2} \cup \ldots \cup C_{k_t} \cup P_a)$ as its principal submatrix, by Lemma 2.1 we have $\mu_2(G) \geqslant 1 + \mu_2(C_{k_1} \cup C_{k_2} \cup \ldots \cup C_{k_t} \cup P_a) = 5$, which contradicts Lemma 2.7. Thus, $0 \leqslant t \leqslant 1$ and hence the result follows. □

3. The proof of Theorem 1.1

Let $\Theta(G)$ be the largest eigenvalue of $A(G) + \alpha D(G)$, where $\alpha \geqslant 0$. To complete the proof of Theorem 1.1, it suffices to show that $K_1 \vee (C_b \cup P_{n-1-b})$ and F_n are not Q-cospectral by Corollary 2.2 for $n \geqslant 7$ (since the case of $3 \leqslant n \leqslant 6$ can be checked easily). In what follows, we will prove the following more general result:

Theorem 3.1. *For any $\alpha \geqslant 0$ and $3 \leqslant b \leqslant n-3$, we have*

$$\Theta(K_1 \vee (C_b \cup P_{n-1-b})) > \Theta(F_n).$$

To prove Theorem 3.1, we need the following famous property of $\Theta(G)$.

Lemma 3.1 (See [9], page 18)**.** *Let G be a connected graph. If $\varphi = (\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n))^\top$ is a unit vector defined on $V(G)$, then*

$$\Theta(G) \geqslant \varphi^\top (A(G) + \alpha D(G))\varphi = 2 \sum_{uv \in E(G)} \varphi(u)\varphi(v) + \alpha \sum_{i=1}^{n} d(v_i)\varphi^2(v_i),$$

where the equality holds if and only if φ is an eigenvector corresponding to $\Theta(G)$.

When $\alpha \geqslant 0$ and G is connected, there is a unique positive unit eigenvector corresponding to $\Theta(G)$ (see [9], page 21), and we call such an eigenvector the *Perron vector* of G hereafter. In what follows, let $V(F_n) = \{w_1, w_2, \ldots, w_n\}$ with $d(w_n) = n-1$ and $w_j w_{j+1} \in E(F_n)$ for $1 \leqslant j \leqslant n-2$, and let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ be the Perron vector of F_n such that x_i corresponds to the vertex w_i, where $1 \leqslant i \leqslant n$. We call $w_p w_{p+1}$ a *special edge* if $p \leqslant \lfloor \frac{1}{2}(n-3) \rfloor$ and $x_p = x_{p+1}$, and we call w_p a *special vertex* if $p \leqslant \lfloor \frac{1}{2}(n-1) \rfloor$ and $x_p = x_{p-2}$.

Lemma 3.2. *If $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ is the Perron vector of F_n and $n \geqslant 3$, then $x_j = x_{n-j}$ holds for any $1 \leqslant j \leqslant \lfloor \frac{1}{2}(n-1) \rfloor$ and F_n contains neither a special edge nor a special vertex.*

P r o o f. In the proof of this result, we simplify $\Theta(F_n)$ as Θ. Let P be the permutation matrix that reverses the order of the vertices in the sequence $w_1, w_2, \ldots, w_{n-1}$, where the vertex w_n is fixed. Since $\mathbf{x}$ is an eigenvector for the eigenvalue Θ, so is $P\mathbf{x}$. Note that $\mathbf{x}$ is the unique positive unit vector corresponding to Θ and $P\mathbf{x}$ is also a positive unit vector corresponding to Θ. Thus, $P\mathbf{x} = \mathbf{x}$ and hence

$$x_j = x_{n-j} \text{ holds for any } 1 \leqslant j \leqslant \Big\lfloor \frac{n-1}{2} \Big\rfloor. \tag{3.1}$$

Now, from $(A(F_n) + \alpha D(F_n))\mathbf{x} = \Theta\mathbf{x}$ we have

$$\begin{cases} \Theta x_1 = 2\alpha x_1 + x_2 + x_n, \\ \Theta x_i = 3\alpha x_i + x_{i-1} + x_{i+1} + x_n \quad \text{for } i \in \Big\{2, 3, \ldots, \Big\lfloor \frac{n-1}{2} \Big\rfloor\Big\}. \end{cases} \tag{3.2}$$

From Lemma 3.1 we easily get $\Theta(G) \geqslant \alpha d(w_n) = \alpha(n-1)$ by setting $\varphi(w_n) = 1$ and $\varphi(w_j) = 0$ for $1 \leqslant j \leqslant n-1$. Now, by (3.2), it follows that $(\Theta + 1 - 2\alpha)(x_2 - x_1) = \alpha x_2 + x_3 > 0$, and hence $x_2 > x_1$.

First, we assume that $w_p w_{p+1}$ is a special edge of F_n, then $x_p = x_{p+1}$ and $p \leqslant \lfloor \frac{1}{2}(n-3) \rfloor$. In this case, we have $p \geqslant 2$ by $x_2 > x_1$. Let $G_1 = F_n + w_{p-1}w_{n-p-1} + w_p w_{n-p} - w_{p-1}w_p - w_{n-p-1}w_{n-p}$. Then, $G_1 \cong F_n$. By (3.1) and Lemma 3.1,

$$0 = \Theta(G_1) - \Theta(F_n) \geqslant 2(x_{p-1} - x_{n-p})(x_{n-p-1} - x_p) = 0,$$

and hence $\mathbf{x}$ is also a Perron vector of G_1. In this case, $x_{p-1} = x_{n-p} = x_p = x_{p+1}$. Now, let $G_2 = F_n + w_{p-2}w_{n-p-1} + w_{p-1}w_{n-p} - w_{p-2}w_{p-1} - w_{n-p-1}w_{n-p}$. Then, $G_2 \cong F_n$. Similarly, we have $x_{p-2} = x_{p-1} = x_p = x_{p+1}$ (since $x_{p-1} = x_{p+1} = x_{n-1-p}$). By repeating the above process, we have $x_1 = x_2$, a contradiction. Thus, we can conclude that F_n contains no special edge.

Secondly, we assume that w_p is a special vertex of F_n, then $x_p = x_{p-2} = x_{n-p} = x_{n+2-p}$ and $x_{p-1} = x_{n+1-p}$, where $p \leqslant \lfloor \frac{1}{2}(n-1) \rfloor$. Since $p \leqslant \lfloor \frac{1}{2}(n-1) \rfloor$, $w_p \neq w_{n-p}$. Let $G_3 = F_n + w_{p-1}w_{n+1-p} + w_{n-p}w_{p-2} - w_{p-1}w_{p-2} - w_{n+1-p}w_{n-p}$. Then, $G_3 \cong F_n$. By Lemma 3.1,

$$0 = \Theta(G_3) - \Theta(F_n) \geqslant 2(x_{p-1} - x_{p-2})^2 \geqslant 0,$$

and hence $x_{p-1} = x_{p-2}$. Now, $w_{p-1}w_{p-2}$ is a special edge of F_n, a contradiction. □

P r o o f of Theorem 3.1. In the proof of this result, we rewrite $K_1 \vee (C_b \cup P_{n-b-1})$ as G. Without loss of generality, we suppose that n is even, as the case of n being odd can be dealt with by a similar method.

Let $n-1 = 2k+1$, where k is a positive integer. By Lemma 3.2, $x_{k+1-j} = x_{k+j+1}$ holds for any $j \in \{1, 2, \ldots, k\}$. If $b = 2s+1$ (s is a positive integer), then $k \geqslant s+1$ due to $n - b \geqslant 3$. It is easy to see that $G \cong F_n + w_{k+1-s}w_{k+s+1} + w_{k-s}w_{k+s+2} - w_{k+1-s}w_{k-s} - w_{k+s+1}w_{k+s+2}$. By Lemma 3.2, $x_{k+1-s} \neq x_{k-s}$. Now, $\Theta(G) - \Theta(F_n) \geqslant \mathbf{x}^\top(A(G) + \alpha D(G))\mathbf{x} - \mathbf{x}^\top(A(F_n) + \alpha D(F_n))\mathbf{x} = 2(x_{k+1-s} - x_{k-s})^2 > 0$ by Lemma 3.1.

Otherwise, $b = 2s$. In this case, since $n - b \geqslant 3$, we have $k \geqslant s+1$ as both k and s are positive integers. Thus it is easy to see that $G \cong F_n + w_{k+1-s}w_{k+s} + w_{k-s}w_{k+s+1} - w_{k+1-s}w_{k-s} - w_{k+s}w_{k+s+1}$. In this case, $\Theta(G) - \Theta(F_n) \geqslant \mathbf{x}^\top(A(G) + \alpha D(G))\mathbf{x} - \mathbf{x}^\top(A(F_n) + \alpha D(F_n))\mathbf{x} = 0$ by Lemma 3.1. From Lemma 3.1, if $\Theta(G) = \Theta(F_n)$, then $\mathbf{x}$ is also a Perron vector of $\Theta(G)$. Since $\Theta(G)x_{k+1-s} = \Theta(F_n)x_{k+1-s}$, we have $x_{k-s} = x_{k+s} = x_{k+2-s}$. In this case, w_{k+2-s} is a special vertex of F_n, against Lemma 3.2. This completes the proof of the theorem. □

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Extremal Results for Cacti

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Abstract
In this paper, we determine the unique maximum (or minimum) extremal graph for general spectral radius, zeroth-order general Randić index, general sum-connectivity index, general Platt index, second Zagreb index and multiplicative Zagreb indices in the class of cacti with $n \geq 4$ vertices and $k \geq 0$ cycles. By applying our new result, we demonstrate the unique maximum extremal graph for general spectral radius, zeroth-order general Randić index, general sum-connectivity index, general Platt index, second Zagreb index and second multiplicative Zagreb index in the class of cacti with $n \geq 4$ vertices. Furthermore, we also determine the unified maximum extremal graphs for general spectral radius, zeroth-order general Randić index and the second multiplicative Zagreb index in the class of cacti with $n \geq 4$ vertices and $k \geq 1$ pendant vertices.

Keywords Extremal graph · Zeroth-order general Randić index · General sum-connectivity index · General Platt index · Cactus graph

Mathematics Subject Classification 05C07 · 05C35 · 05C90

1 Introduction

Throughout this paper, we only concern with simple undirected connected graphs. Let $N(u)$ and $d(u)$ denote the neighbor set and degree of the vertex u of a graph G,

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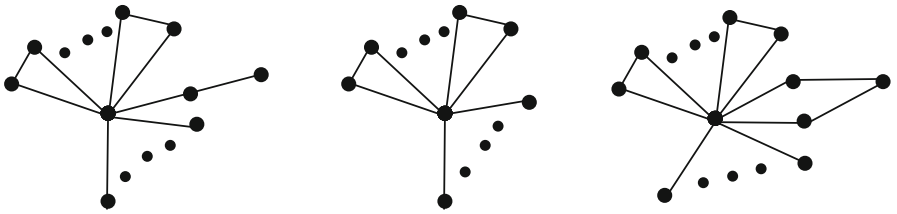


Fig. 1 The cacti $F^0_{n,k}$, $F^1_{n,k}$ and $F^2_{n,k}$, where $k \geq 1$

respectively. When G needs to be indicated, we replace $N(u)$ and $d(u)$ by $N_G(u)$ and $d_G(u)$, respectively. A vertex with degree k will be referred as a *k-vertex*. Particularly, a 1-vertex will be referred as a *pendant vertex* in the sequel. If $u \in V(G)$ and $G - u$ are not connected, then u is called a *cut-vertex* of G. Similarly, if $uv \in E(G)$ and $G - uv$ is not connected, then uv is called a *cut-edge* of G.

As usual, a cycle, a path and a star with n vertices are denoted by C_n, P_n and $K_{1,n-1}$, respectively. A *cactus graph* G, or *cactus* for short, is a connected graph in which each block of G is either an edge or a cycle. For a cactus G and a block B of G, if B contains exactly one cut-vertex, then B is called a *pendant block* of G. Let $C_{n,k}$ be a special cactus obtained from the star $K_{1,n-1}$ by adding k (≥ 0) independent edges among those pendant vertices of $K_{1,n-1}$. As shown in Fig. 1, we let $F^0_{n,k}$, $F^1_{n,k}$ and $F^2_{n,k}$ be three special cacti with n vertices and k (≥ 1) pendant vertices. Denote by $\mathbb{C}(n,k)$ the class of cacti with n vertices and k (≥ 0) cycles, and let $\mathbb{W}(n,k)$ be the class of cacti with n vertices and k (≥ 1) pendant vertices. From these definitions, it follows that $C_{n,k} \in \mathbb{C}(n,k)$ and $C_{n,k}$ contain exactly $2k$ vertices of degrees two. Furthermore, we let $\mathbb{C}(n)$ be the class of cacti with n vertices.

In this paper, we shall give unified extremal results of cacti for general graph spectrum and some topological indices, and we need to introduce some concepts on graph spectrum and topological indices. Let $R_\alpha(G)$ and $R^0_\alpha(G)$ be the *general Randić index* and *zeroth-order general Randić index* of G, where

$$R_\alpha(G) = \sum_{uv \in E(G)} \big(d(u)d(v)\big)^\alpha \text{ and } R^0_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha.$$

Denote by $\chi_\alpha(G)$ and $Pl_\alpha(G)$ the *general sum-connectivity index* and *general Platt index* of G, respectively, where

$$\chi_\alpha(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^\alpha, \text{ and } Pl_\alpha(G) = \sum_{uv \in E(G)} \big(d(u) + d(v) - 2\big)^\alpha.$$

For basic mathematical properties of general sum-connectivity index, including various lower and upper bounds, see [6,26,28]. The concept of general Randić index was constructed by Bollobás and Erdős [3], the zeroth-order general Randić index was firstly put forward by Li and Zheng [11], the general sum-connectivity index was

raised by Zhou and Trinajstić [28], and the general Platt index of G was introduced by Ali and Dimitrov [2]. Actually, $R_\alpha(G)$, $R^0_\alpha(G)$, $\chi_\alpha(G)$ and $Pl_\alpha(G)$ are the general cases of many popular topological indices. For instance, $M_1(G) = R^0_2(G)$ is known as the *first Zagreb index* [7], $M_2(G) = R_1(G)$ is known as the *second Zagreb index* [7], $R^0_{-1}(G)$ is called the *inverse degree* $ID(G)$ of G (see [23]), $R_{-\frac{1}{2}}(G)$ is always referred as the *Randić index* of G [17], $\chi_{-\frac{1}{2}}(G)$ is famous as the *sum-connectivity index* of G [27], and $Pl_2(G)$ is known as the *reformulated first Zagreb index* of G [16]. Furthermore, Hollas [8] extended $R_\alpha(G)$, $\chi_\alpha(G)$ and $Pl_\alpha(G)$ to $BID(G)$, and Yao et al. [24] generalized $R^0_\alpha(G)$ to $H_f(G)$, where

$$BID(G) = \sum_{uv\in E(G)} \varphi\big(d(u), d(v)\big) \text{ and } H_f(G) = \sum_{v\in V(G)} f\big(d(v)\big).$$

In some literature, $BID(G)$ was called the *bond incident degree index* [2] or the *connectivity function* [20] of G, and $H_f(G)$ was called the *vertex-degree-function index* of G [24]. In 2010, Todeschini et al. [19] put forward the concepts of *multiplicative Zagreb indices* for graph G, that is

$$\prod\nolimits_1(G) = \prod_{u\in V(G)} \big(d(u)\big)^2, \text{ and } \prod\nolimits_2(G) = \prod_{u\in V(G)} \big(d(u)\big)^{d(u)}.$$

Similarly, $\prod^1(G)$ was also generalized to $\prod^\alpha(G)$ by two of the present authors and their collaborators [24], where

$$\prod\nolimits_\alpha(G) = \prod_{u\in V(G)} \big(d(u)\big)^\alpha.$$

Let $A(G)$ and $D(G)$, respectively, be the adjacency matrix and the diagonal matrix of G. Then, $M_\beta(G) = A(G) + \beta D(G)$ is called the *general matrix* of G and we use $\Theta(G, \beta)$ to denote the *general spectral radius*, namely the largest eigenvalue of $A(G)+\beta D(G)$ [13]. It is easy to see that $A(G)+\beta D(G)$ is a general case of the adjacency matrix and *signless Laplacian matrix* $Q(G)$ of G, where $Q(G) = D(G)+A(G)$. Hereafter, let $\rho(G)$ and $\mu(G)$ be the largest eigenvalues of $A(G)$ and $Q(G)$, respectively, and we call $\rho(G)$ and $\mu(G)$ the *spectral radius* and *signless Laplacian spectral radius* of G, respectively. When G is connected and $\beta \geq 0$, $M_\beta(G)$ is a nonnegative irreducible matrix; by the famous Perron–Frobenius theorem for nonnegative irreducible matrix (see [13]), there exists a unique unit positive eigenvector $\mathbf{f_G}$ such that $M_\beta(G)\mathbf{f_G} = \Theta(G, \beta)\mathbf{f_G}$. Hereafter, this eigenvector $\mathbf{f_G}$ is called the *Perron vector* of G.

As observed in some literature, for many graph categories, extremal graphs with respect to some prescribed topological indices or spectral invariants are the same. Therefore, it is natural for us to consider the following interesting problem:

Problem 1 *How to determine a unified extremal graph in a given graph category for as many topological and spectral invariants as possible.*

Recently, more and more extremal results of topological indices or spectral invariants in the class of cacti have been determined by other scholars [4,5,9,10,12,14,21,22,25], and it was shown that, in the class of cacti with n vertices and k cycles, $C_{n,k}$ is the unique extremal graph with maximal spectral radius [4], maximal Merrifield–Simmons index [12], minimum Hosoya index [12], minimal Wiener index [12], minimal Randić index [14] and maximum signless Laplacian spectral radius [5]. Similarly, in the class of cacti with n vertices and k pendant vertices, Li et al. determined the unique extremal cactus with maximum signless Laplacian spectral radius [10], they also identified the extremal cactus with maximum first and second Zagreb indices [9], Ahmed et al. deduced the unique extremal cactus with maximum zeroth-order general Randić index for $\alpha > 1$ [1], and Wang et al. determined the extremal minimum and maximum first (resp., second) multiplicative Zagreb index [22]. Extremal problem was also considered within the class of cacti with n vertices. For instance, in the class of cacti with $n \geq 4$ vertices, the maximum first and second Zagreb indices were determined in [9], and maximum signless Laplacian spectral radius was identified in [18].

In this paper, we shall provide a unified method to determine the unique extremal graph for general spectral radius and some topological indices among the class of cacti with $n \geq 4$ vertices, that is,

Theorem 1.1 *In the class of cacti with $n \geq 4$ vertices and $k \geq 0$ cycles, $C_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, maximum $\chi_\alpha(G)$ and maximum $Pl_\alpha(G)$ for $\alpha > 1$, maximum $R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, minimum $R^0_\alpha(G)$ for $0 < \alpha < 1$, minimum $\prod^\alpha(G)$ for $\alpha > 0$, maximum $\prod^\alpha(G)$ for $\alpha < 0$, and maximum $M_2(G)$ and maximum $\prod_2(G)$.*

It is easily checked that Theorem 1.1 extends the corresponding results of [4,5]. By applying Theorem 1.1, we shall identify the unique maximum extremal graph for general spectral radius and some topological indices among the class of cacti with $n \geq 4$ vertices, and our results will extend the corresponding results of [9,18].

Theorem 1.2 *In the class of cacti with $n \geq 4$ vertices, C_{n,k_0} uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, maximum $\chi_\alpha(G)$ and maximum $Pl_\alpha(G)$ for $\alpha > 1$, maximum $R^0_\alpha(G)$ for $\alpha > 1$, maximum $M_2(G)$ and maximum $\prod_2(G)$, where $k_0 = \lfloor \frac{n-1}{2} \rfloor$.*

Furthermore, we will present a very simple method to determine the maximum extremal graphs for the general spectral radius, the second multiplicative Zagreb index and the zeroth-order general Randić index, which will extend the corresponding results of [1,10,22].

Theorem 1.3 *In the class of cacti with n vertices and $k \geq 1$ pendant vertices, (i) if $n - k \equiv 1 \pmod 2$, then $F^1_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, maximum $R^0_\alpha(G)$ for $\alpha > 1$ and maximum $\prod_2(G)$. (ii) if $n - k \equiv 0 \pmod 2$, then $F^0_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$; (iii) if $n - k \equiv 0 \pmod 2$, then $R^0_\alpha(G) \leq k + (n-2)^\alpha + (n-k-1)2^\alpha$ for $\alpha > 1$ and $\prod_2(G) \leq (n-2)^{n-2}2^{2(n-k-1)}$, where each equality holds if and only if $G \in \{F^0_{n,k}, F^2_{n,k}\}$.*

In what follows (including all results), **for the sake of simplification**, unless special indicated, β always defines a nonnegative real number, G is a connected graph with

$\mathbf{f_G}$ as its Perron vector, and $f_G(u)$ defines the corresponding value of f_G on the vertex u. Furthermore, $f(x)$ and $\varphi(x, y)$ are two functions defined on $x \geq 1$ and $y \geq 1$, and $\mathcal{G}$ defines a given graph category.

2 Some Preliminaries

Let $\mathbf{s} = (s_1, s_2, \ldots, s_n)$ and $\mathbf{t} = (t_1, t_2, \ldots, t_n)$ be two non-increasing sequences of real numbers. We write $\mathbf{s} \trianglelefteq \mathbf{t}$ if and only if $\sum_{i=1}^{n} s_i = \sum_{i=1}^{n} t_i$, and $\sum_{i=1}^{j} s_i \leq \sum_{i=1}^{j} t_i$ for all $j = 1, 2, \ldots, n$. Furthermore, we write $\mathbf{s} \triangleleft \mathbf{t}$ if and only if $\mathbf{s} \trianglelefteq \mathbf{t}$ and $\mathbf{s} \neq \mathbf{t}$. The ordering $\mathbf{s} \trianglelefteq \mathbf{t}$ is always referred to as *majorization* [13,15]. Among all majorization theorems, the following one was discovered long time ago, and it is not restricted to graphical invariants.

Theorem 2.1 [15] *Let $\mathbf{s} = (s_1, s_2, \ldots, s_n)$ and $\mathbf{t} = (t_1, t_2, \ldots, t_n)$ be two non-increasing sequences of real numbers. If $\mathbf{s} \triangleleft \mathbf{t}$, then for any strictly convex function $g(x)$, we have $\sum_{i=1}^{n} g(s_i) < \sum_{i=1}^{n} g(t_i)$.*

Theorem 2.2 *If $H_f(G)$ is maximum $\big($resp., minimum$\big)$ in $\mathcal{G}$ for any strictly convex $\big($resp., concave$\big)$ function $f(x)$, then $\prod^{\alpha}(G)$ is maximum for $\alpha < 0$ $\big($resp., minimum for $\alpha > 0\big)$ in $\mathcal{G}$.*

Proof Let $f(x) = \alpha \ln x$. Then, $H_f(G) = \sum_{j=1}^{n} \alpha \ln d_j$. It is easy to see that $\prod^{\alpha}(G) < \prod^{\alpha}(G')$ if and only if $H_f(G) < H_f(G')$. When $x \geq 1$, since $f''(x) = -\frac{\alpha}{x^2}$, we conclude that $f(x)$ is a strictly convex function for $\alpha < 0$, and it is a strictly concave function for $\alpha > 0$. This completes the proof of this result. □

Theorem 2.3 *If $H_f(G)$ is maximum among all graphs in $\mathcal{G}$ for any strictly convex $\big($and strictly increasing$\big)$ function $f(x)$, then $\prod_2(G)$ is maximum in $\mathcal{G}$.*

Proof Let $f(x) = x \ln x$ and let $H_f(G) = \sum_{i=1}^{n} d_i \ln d_i$. Then, $\prod_2(G) < \prod_2(G')$ if and only if $H_f(G) < H_f(G')$. When $x \geq 1$, since $f''(x) = \frac{1}{x} > 0$ and $f'(x) = 1 + \ln x > 0$, $f(x)$ is both a strictly convex and strictly increasing function. This completes the proof of this result. □

With the similar reason as Theorems 2.2 and 2.3 , let $f(x) = x^{\alpha}$. Then, we have

Theorem 2.4 *If $H_f(G)$ is maximum $\big($resp., minimum$\big)$ in $\mathcal{G}$ for any strictly convex $\big($resp., concave$\big)$ function $f(x)$, then $R_{\alpha}^{0}(G)$ is maximum for $\alpha > 1$ or $\alpha < 0$ $\big($resp., minimum for $0 < \alpha < 1\big)$ in $\mathcal{G}$. Furthermore, if $H_f(G)$ is maximum in $\mathcal{G}$ for any strictly convex and strictly increasing function $f(x)$, then $R_{\alpha}^{0}(G)$ is also maximum in $\mathcal{G}$ for $\alpha > 1$.*

Hereafter, let G be a connected graph, and let u and v be two vertices of G such that $\{w_1, w_2, \ldots, w_s\} \subseteq N(v) \backslash \big(N(u) \cup \{u\}\big)$, where $1 \leq s \leq d(v)$. Denote by

$$G^* = G - vw_1 - vw_2 - \cdots - vw_s + uw_1 + uw_2 + \cdots + uw_s.$$

Theorem 2.5 *If $d_G(u) \geq d_G(v)$, then $H_f(G^*) > H_f(G)$ when $f(x)$ is a strictly convex function, and $H_f(G^*) < H_f(G)$ when $f(x)$ is a strictly concave function.*

Proof Since $\big(d(u), d(v)\big) \lhd \big(d(u)+s, d(v)-s\big)$ and in view of

$$H_f(G^*) - H_f(G) = f\big(d(u)+s\big) + f\big(d(v)-s\big) - f\big(d(u)\big) - f\big(d(v)\big),$$

the result follows from Theorem 2.1. □

Corollary 2.6 *If $f(x)$ is a strictly convex and strictly increasing function, then $H_f(G^*) > H_f(G)$ when $d_G(u) \geq d_G(v)$, and $H_f(G) > H_f(H)$ when H is a proper subgraph of G.*

Proof In view of Theorem 2.5 and since $f(x)$ is strictly increasing, the desired result holds. □

Theorem 2.7 [13] *If $\beta \geq 0$, then $\Theta(G^*, \beta) > \Theta(G, \beta)$ when $f_G(u) \geq f_G(v)$, and $\Theta(G, \beta) > \Theta(H, \beta)$ when H is a proper subgraph of G.*

3 The Proof of Theorem 1.1

This section will be dedicated to the proof of Theorem 1.1. Actually, we shall prove a more general result, that is, Theorem 3.3, and we shall need to introduce the following definition.

Definition 3.1 A symmetric bivariate function $\varphi(x, y)$ is called *good escalating* (resp., *de-escalating*) if $\varphi(x, y)$ is symmetric and satisfying the following (i)–(v):

(i) If $x_1 + y_1 \geq x_2 + y_2$, then $\varphi(x_1, y_1) \geq$ (resp., $\leq$) $\varphi(x_2, y_2)$, where the inequality is strict if $x_1 + y_1 > x_2 + y_2$;
(ii) If $s \in \{1, 2\}$, then $\varphi(x_1 + s, x_2) + \varphi(x_1 - s, x_2) \geq$ (resp., $\leq$) $2\varphi(x_1, x_2)$;
(iii) If $s \in \{1, 2\}$, then $\varphi(x_1 + s, y_1 - s) + \varphi(x_1 - s, y_1 + s) \geq$ (resp., $\leq$) $2\varphi(x_1, y_1)$;
(iv) If $x_1 \geq 3$ and $y_1 \geq 2$, then $\varphi(x_1, y_1) + \varphi(2, 1) >$ (resp. $<$) $\varphi(y_1, 2) + \varphi(x_1, 1)$;
(v) If $p \geq 1$ and $x_1 \geq 2$, then $\varphi\big(x_1 + p, 2\big) + \varphi\big(2, 2\big) \geq$ (resp., $\leq$) $\varphi\big(p + 2, 2\big) + \varphi\big(x_1, 2\big)$.

Lemma 3.2 *If $\alpha > 1$, then $\chi_\alpha(G)$ and $Pl_\alpha(G)$ are good escalating functions.*

Proof We only prove the case of $\chi_\alpha(G)$, as the case of $Pl_\alpha(G)$ can be shown by a similar method. Let $\varphi(x, y) = (x + y)^\alpha$ and let $f(z) = z^\alpha$, where $\min\{x, y, z\} \geq 1$ and $x + y \geq 3$. In view of $\alpha > 1$, and since $f'(z) = \alpha z^{\alpha-1}$ and $f''(z) = \alpha(\alpha-1)z^{\alpha-2}$, $f(z)$ is a strictly convex and strictly increasing function for $z \geq 1$. Thus, $\varphi(x, y)$ satisfies (i) and (iii) of Definition 3.1.
If $s \in \{1, 2\}$, since $\varphi(x, y)$ is defined on $x \geq 1$ and $y \geq 1$, we have $x_1 + s + x_2 > x_1 + x_2$ and so Theorem 2.1 implies that $\varphi(x_1 + s, x_2) + \varphi(x_1 - s, x_2) = \big(x_1 + s + x_2\big)^\alpha + \big(x_1 - s + x_2\big)^\alpha \geq 2\big(x_1 + x_2\big)^\alpha = 2\varphi(x_1, x_2)$. Thus, Definition 3.1 (ii) holds.
If $x_1 \geq 3$ and $y_1 \geq 2$, then Theorem 2.1 implies that $\varphi(x_1, y_1) + \varphi(2, 1) = (x_1 + y_1)^\alpha + 3^\alpha > (y_1 + 2)^\alpha + (x_1 + 1)^\alpha = \varphi(y_1, 2) + \varphi(x_1, 1)$, and so Definition 3.1 (iv)

holds, as $x_1 + y_1 > \max\{x_1 + 1, y_1 + 2\}$. With the similar reason, Definition 3.1 (v) also holds. □

In view of Theorems 2.2–2.4 and Lemma 3.2, to prove Theorem 1.1, it suffices to show

Theorem 3.3 *In the class of cacti with $n \geq 4$ vertices and $k \geq 0$ cycles, $C_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, the maximum (resp., minimum) $BID(G)$ when $\varphi(x, y)$ is a good escalating (resp., de-escalating) function, the maximum (resp., minimum) $H_f(G)$ when $f(x)$ is a strictly convex (resp., concave) function, and the maximum $M_2(G)$.*

Throughout this section, for simplification, we call G as an *extremal graph* if G is an extremal graph as defined in Theorem 3.3.

Lemma 3.4 *If $n \geq 4$ and $k \geq 0$, then C_n is not an extremal graph of $\mathbb{C}(n, k)$.*

Proof By contradiction, we prove this result. For this, we assume that $G \cong C_n$ is an extremal graph of $\mathbb{C}(n, k)$. Since $n \geq 4$, we may suppose that $uv \in E(G)$ with $f_G(u) \geq f_G(v)$. In this case, there exists a vertex w such that $w \in N_G(v) \backslash N_G(u)$ and $w \notin \{u, v\}$. Let $G_1 = G - vw + uw$. Then, $\Theta(G_1, \beta) > \Theta(G, \beta)$ by Theorem 2.7, and so $G \cong C_n$ is not an extremal graph of $\mathbb{C}(n, k)$ for general spectral radius. With the similar reason, by Theorem 2.5, G is also not an extremal graph of $\mathbb{C}(n, k)$ for vertex-degree-function index.

We now suppose that $G \cong C_n$ is an extremal graph of $\mathbb{C}(n, k)$ for bond incident degree index. Without loss of generality, we may suppose that $\varphi(x, y)$ is a good escalating function. Since $n \geq 4$ and $G \cong C_n$, we have $k = 1$ and hence

$$\begin{aligned} &BID\big(C_{n,1}\big) - BID\big(C_n\big) \\ &= \big((n-3)\varphi(n-1,1) + 2\varphi(n-1,2) + \varphi(2,2)\big) - n\varphi(2,2) \\ &= (n-3)\varphi(n-1,1) + 2\varphi(n-1,2) - (n-1)\varphi(2,2) \\ &> (n-1)\big(\varphi(n-1,1) - \varphi(2,2)\big) \geq 0, \end{aligned}$$

a contradiction. Combining this with

$$M_2\big(C_{n,1}\big) - M_2\big(C_n\big) = (n-1)(n-3) > 0,$$

C_n is not an extremal graph of $\mathbb{C}(n, k)$ for bond incident degree index or the second Zagreb index. □

Lemma 3.5 *Let G be an extremal graph of $\mathbb{C}(n, k)$ for the general spectral radius (resp., vertex-degree-function index). If $n \geq 4$ and $k \geq 0$, then G contains exactly one cut-vertex.*

Proof Since G is a cactus and in view of Lemma 3.4, G contains at least one cut-vertex. By contradiction, we prove this result. For this, we assume that u_0 and v_0 are two cut-vertices such that the distance between u_0 and v_0 is as large as possible.

If G is an extremal graph of $\mathbb{C}(n,k)$ for general spectral radius, then we may suppose that $f_G(u_0) \geq f_G(v_0)$ and B is a pendant block of G with cut-vertex v_0. Let $G_1 = G + \{u_0z : z \in N(v_0) \cap B\} - \{v_0z : z \in N(v_0) \cap B\}$. By Theorem 2.7, it follows that $\Theta(G_1, \beta) > \Theta(G, \beta)$, which contradicts the fact $G_1 \in \mathbb{C}(n,k)$ and the choice of G. With a similar reason and in view of Theorem 2.5, G is also not an extremal graph of $\mathbb{C}(n,k)$ for vertex-degree-function index. □

Lemma 3.6 *Let G be an extremal graph of $\mathbb{C}(n,k)$ for bond incident degree index (resp., the second Zagreb index). If $n \geq 4$ and $k \geq 0$, then G contains exactly one cut-vertex.*

Proof Since G is a cactus graph and in view of Lemma 3.4, G contains at least one cut-vertex. By contradiction we prove this result. For this we assume that G contains at least two cut-vertices. Here, we can choose u_0 and v_0 as two cut-vertices of G such that u_0 and v_0 are the cut-vertices of the pendant blocks B_1 and B_2, respectively. Without loss of generality, we may suppose that $\varphi(x,y)$ is a good escalating function. In what follows, we set $b = 0$ if $u_0v_0 \notin E(G)$ and $b = 1$ if $u_0v_0 \in E(G)$.

Case 1 Both B_1 and B_2 are cycles. In this case, we may suppose that $B_1 : u_0u_1 \cdots u_su_0$ and $B_2 : v_0w_1 \cdots w_tv_0$ are two cycles. Let $G_1 = G - v_0w_1 - v_0w_t + u_0w_1 + u_0w_t$ and let $G_2 = G - u_0u_1 - u_0u_s + v_0u_1 + v_0u_s$. By an elementary computation, it follows that

$$\begin{aligned}
&BID(G_1) - BID(G)\\
&= \sum_{w\in N_G(v_0)\setminus\{u_0\}} \Big(\varphi\big(d_G(v_0)-2, d_G(w)\big) - \varphi\big(d_G(v_0), d_G(w)\big)\Big)\\
&\quad + \sum_{z\in N_G(u_0)\setminus\{v_0\}} \Big(\varphi\big(d_G(u_0)+2, d_G(z)\big) - \varphi\big(d_G(u_0), d_G(z)\big)\Big)\\
&\quad +2\varphi\big(d_G(u_0)+2, 2\big) - 2\varphi\big(d_G(v_0)-2, 2\big)\\
&\quad +b\Big(\varphi\big(d_G(u_0)+2, d_G(v_0)-2\big) - \varphi\big(d_G(u_0), d_G(v_0)\big)\Big), \text{ and}\\
&BID(G_2) - BID(G) = \sum_{w\in N_G(v_0)\setminus\{u_0\}} \Big(\varphi\big(d_G(v_0)+2, d_G(w)\big)\\
&\quad -\varphi\big(d_G(v_0), d_G(w)\big)\Big)\\
&\quad + \sum_{z\in N_G(u_0)\setminus\{v_0\}} \Big(\varphi\big(d_G(u_0)-2, d_G(z)\big) - \varphi\big(d_G(u_0), d_G(z)\big)\Big)\\
&\quad +2\varphi\big(d_G(v_0)+2, 2\big) - 2\varphi\big(d_G(u_0)-2, 2\big)\\
&\quad +b\Big(\varphi\big(d_G(v_0)+2, d_G(u_0)-2\big) - \varphi\big(d_G(v_0), d_G(u_0)\big)\Big).
\end{aligned}$$

Recall that $\varphi(x,y)$ is a good symmetric function. Thus,

$$\varphi\big(d_G(v_0)-2,d_G(w)\big)+\varphi\big(d_G(v_0)+2,d_G(w)\big)-2\varphi\big(d_G(v_0),d_G(w)\big)\geq 0,$$
$$\varphi\big(d_G(u_0)-2,d_G(z)\big)+\varphi\big(d_G(u_0)+2,d_G(z)\big)-2\varphi\big(d_G(u_0),d_G(z)\big)\geq 0,$$
$$\varphi\big(d_G(u_0)+2,2\big)+\varphi\big(d_G(v_0)+2,2\big)-\varphi\big(d_G(v_0)-2,2\big)-\varphi\big(d_G(u_0)-2,2\big)>0$$
and $\varphi\big(d_G(u_0)+2,d_G(v_0)-2\big)+\varphi\big(d_G(v_0)+2,d_G(u_0)-2\big)$
$-2\varphi\big(d_G(u_0),d_G(v_0)\big)\geq 0,$

which is contrary with

$$BID(G_1)+BID(G_2)-2BID(G)\leq 0.$$

With the similar reason, we have

$$M_2(G_1)+M_2(G_2)-2M_2(G)=32-8b>0,\ \text{a contradiction.}$$

Case 2 Both B_1 and B_2 are pendant edges. In this case, we may suppose that $B_1 : u_0z_0$ and $B_2 : v_0w_0$ are two pendant edges. (Recall that u_0 and v_0 are two cut-vertices.) Let $G_3 = G - v_0w_0 + u_0w_0$ and let $G_4 = G - u_0z_0 + v_0z_0$. By an elementary computation, it easily follows that

$$\begin{aligned}
&BID(G_3)-BID(G)\\
&=\sum_{w\in N_G(v_0)\setminus\{u_0\}}\Big(\varphi\big(d_G(v_0)-1,d_G(w)\big)-\varphi\big(d_G(v_0),d_G(w)\big)\Big)\\
&\quad+\sum_{z\in N_G(u_0)\setminus\{v_0\}}\Big(\varphi\big(d_G(u_0)+1,d_G(z)\big)-\varphi\big(d_G(u_0),d_G(z)\big)\Big)\\
&\quad+\varphi\big(d_G(u_0)+1,1\big)-\varphi\big(d_G(v_0)-1,1\big)\\
&\quad+b\Big(\varphi\big(d_G(u_0)+1,d_G(v_0)-1\big)-\varphi\big(d_G(u_0),d_G(v_0)\big)\Big),\ \text{and}\\
&BID(G_4)-BID(G)=\sum_{w\in N_G(v_0)\setminus\{u_0\}}\Big(\varphi\big(d_G(v_0)+1,d_G(w)\big)\\
&\quad-\varphi\big(d_G(v_0),d_G(w)\big)\Big)\\
&\quad+\sum_{z\in N_G(u_0)\setminus\{v_0\}}\Big(\varphi\big(d_G(u_0)-1,d_G(z)\big)-\varphi\big(d_G(u_0),d_G(z)\big)\Big)\\
&\quad+\varphi\big(d_G(v_0)+1,1\big)-\varphi\big(d_G(u_0)-1,1\big)\\
&\quad+b\Big(\varphi\big(d_G(v_0)+1,d_G(u_0)-1\big)-\varphi\big(d_G(v_0),d_G(u_0)\big)\Big).
\end{aligned}$$

Recall that $\varphi(x, y)$ is a good symmetric function. Thus,

$$\varphi\big(d_G(v_0)-1,d_G(w)\big)+\varphi\big(d_G(v_0)+1,d_G(w)\big)-2\varphi\big(d_G(v_0),d_G(w)\big)\geq 0,$$
$$\varphi\big(d_G(u_0)-1,d_G(z)\big)+\varphi\big(d_G(u_0)+1,d_G(z)\big)-2\varphi\big(d_G(u_0),d_G(z)\big)\geq 0,$$
$$\varphi\big(d_G(u_0)+1,1\big)+\varphi\big(d_G(v_0)+1,1\big)-\varphi\big(d_G(v_0)-1,1\big)-\varphi\big(d_G(u_0)-1,1\big)>0,$$

$$\text{and} \quad \varphi\big(d_G(u_0)+1, d_G(v_0)-1\big)+\varphi\big(d_G(v_0)+1, d_G(u_0)-1\big) -2\varphi\big(d_G(u_0), d_G(v_0)\big) \geq 0,$$

which is contrary with

$$BID(G_3)+BID(G_4)-2BID(G) \leq 0.$$

With the similar reason, we have

$$M_2(G_3)+M_2(G_4)-2M_2(G)=4-2b>0, \text{ a contradiction.}$$

Case 3 B_1 **is a pendant edge and** B_2 **is a cycle**. In this case, by **Case 1** and **Case 2**, we may suppose that each pendant block with cut-vertex u_0 is a pendant edge and each pendant block with cut-vertex v_0 is a cycle. Furthermore, if we let u_0 and v_0 be such two cut-vertices with largest distance in G, then u_0 and v_0 are all the cut-vertices of G adjacent with pendant blocks. (Otherwise, **Case 1** or **Case 2** happens.) Thus, we may suppose that $v_1, v_2, \ldots, v_p$ are all the pendant vertices being adjacent with u_0 and let x_0 be the cut-vertex of G such that the distance of u_0 and x_0 is as small as possible, where $x_0 = v_0$ is also permitted. Let $G_6 = G + x_0v_1 + x_0v_2 + \cdots + x_0v_p - u_0v_1 - u_0v_2 - \cdots - u_0v_p$. Then, $G_6 \in \mathbb{C}(n,k)$. As before, we suppose that $B_1 : u_0z_0$ and $B_2 : v_0w_1w_2\cdots w_tv_0$. We firstly prove the following claim:

Claim 1 If u_0 lies on a cycle C_q, then $q=3$ and so $u_0x_0 \in E(G)$.

Proof of Claim 1 By contradiction, we prove this result. For this, we assume that $q \geq 4$ and we suppose that $C_q = u_0z_1z_2\cdots z_{q-1}u_0$, where $v_0 \in V(C_q)$ is also permitted. In this case, as u_0 and v_0 are all the cut-vertices of G adjacent with pendant blocks, we can conclude that except for exactly two vertices of C_q, each of the other vertex is a 2-vertex. Now, we may suppose that $d_G(z_1)=2$ and let $G_5 = G - z_1z_2 - u_0z_0 + z_0z_1 + u_0z_2$. Then, $G_5 \in \mathbb{C}(n,k)$. Since $d_G(u_0) \geq 3$ and $d_G(z_2) \geq 2$, we have

$$\begin{aligned} BID(G_5)-BID(G) &= \varphi(d_G(u_0), d_G(z_2)) \\ &\quad + \varphi(2,1) - \varphi(d_G(z_2),2) - \varphi(d_G(u_0),1) > 0 \end{aligned}$$

and

$$M_2(G_5)-M_2(G) = \big(d_G(u_0)-2\big)\big(d_G(z_2)-1\big) > 0, \text{ a contradiction.}$$

This completes the proof of our claim. □

By **Claim** 1, we can conclude that $u_0x_0 \in E(G)$ and either $N(u_0) \cap N(x_0) = \emptyset$ (if u_0x_0 is a cut-edge) or $N(u_0) \cap N(x_0) = \{y_0\}$ (if u_0x_0 is on one cycle), where $d_G(y_0)=2$.

Subcase 3.1 $N(u_0) \cap N(x_0) = \{y_0\}$, **where** $d_G(y_0) = 2$. Since x_0 is a cut-vertex of G, we have $d_G(x_0) \geq 3$ and so $\varphi\big(d_G(x_0)+p, 1\big) > \varphi\big(p+2, 1\big)$. Combining this with $d_G(u_0) = p+2$, it follows that

$$\begin{aligned} BID(G_6) - BID(G) &= p\varphi\big(d_G(x_0)+p, 1\big) + 2\varphi\big(d_G(x_0)+p, 2\big) + \varphi\big(2, 2\big) \\ &\quad + \sum_{z\in N_G(x_0)\setminus\{u_0, y_0\}} \varphi\big(d_G(x_0)+p, d_G(z)\big) - p\varphi\big(p+2, 1\big) - \varphi\big(p+2, 2\big) \\ &\quad - \varphi\big(d_G(x_0), p+2\big) - \varphi\big(d_G(x_0), 2\big) - \sum_{z\in N_G(x_0)\setminus\{u_0, y_0\}} \varphi\big(d_G(x_0), d_G(z)\big) \\ &> 2\varphi\big(d_G(x_0)+p, 2\big) + \varphi\big(2, 2\big) - \varphi\big(p+2, 2\big) - \varphi\big(d_G(x_0), p+2\big) \\ &\quad - \varphi\big(d_G(x_0), 2\big) \geq \varphi\big(d_G(x_0)+p, 2\big) + \varphi\big(2, 2\big) - \varphi\big(p+2, 2\big) - \varphi\big(d_G(x_0), 2\big) \geq 0 \end{aligned}$$

and

$$\begin{aligned} M_2(G_6) - M_2(G) &> p\big(d_G(x_0)-2\big) + 4\big(d_G(x_0)+p\big) \\ &\quad + 4 - 2\big(p+2\big) - d_G(x_0)\big(p+4\big) = 0, \end{aligned}$$

a contradiction.

Subcase 3.2 $N(u_0) \cap N(x_0) = \emptyset$. Since x_0 is a cut-vertex of G, we have $d_G(x_0) \geq 2$ and so $\varphi\big(d_G(x_0)+p, 1\big) > \varphi\big(p+1, 1\big)$. Combining this with $d_G(u_0) = p+1$, it follows that

$$\begin{aligned} &BID(G_6) - BID(G) \\ &= (p+1)\varphi\big(d_G(x_0)+p, 1\big) + \sum_{z\in N_G(x_0)\setminus\{u_0\}} \varphi\big(d_G(x_0)+p, d_G(z)\big) \\ &\quad - p\varphi\big(p+1, 1\big) - \varphi\big(d_G(x_0), p+1\big) - \sum_{z\in N_G(x_0)\setminus\{u_0\}} \varphi\big(d_G(x_0), d_G(z)\big) \\ &> (p+1)\varphi\big(d_G(x_0)+p, 1\big) - p\varphi\big(p+1, 1\big) - \varphi\big(d_G(x_0), p+1\big) \\ &> \varphi\big(d_G(x_0)+p, 1\big) - \varphi\big(d_G(x_0), p+1\big) \geq 0 \end{aligned}$$

and

$$M_2(G_6) - M_2(G) > (p+1)\big(d_G(x_0)+p\big) - p\big(p+1\big) - d_G(x_0)\big(p+1\big) = 0,$$

a contradiction. □

Proof of Theorem 3.3 By Lemmas 3.5 and 3.6, the results hold if $k = 0$ and so we may suppose that $k \geq 1$. Now, it suffices to show that each cycle of G is a triangle. By contradiction, we prove this result. For this, we assume that G contains a cycle with length being at least four, and we may suppose that $w_1w_2\cdots w_qw_1$ is such a cycle, where w_1 is the maximum degree vertex of G and $q \geq 4$. Let $G_1 = G + w_1w_{q-1} - w_{q-1}w_q$. Then, $G_1 \in \mathbb{C}(n, k)$.

Since $d_G(w_1) \geq 3$ by Lemma 3.4 and $k \geq 1$, we have $\big(d_G(w_1), 2\big) \lhd \big(d_G(w_1) + 1, 1\big)$. In view of Theorem 2.5 and

$$H_f(G_1) - H_f(G) = f(d_G(w_1) + 1) + f(1) - f(d_G(w_1)) - f(2),$$

we get a contradiction if G is an extremal graph of $\mathbb{C}(n, k)$ for the vertex-degree-function index. Note that $d_G(w_1) \geq 3$ by Lemma 3.4. Thus,

$$\begin{aligned} M_2(G_1) - M_2(G) &> \Big(d_G(w_1) + 1\Big) + 2\Big(d_G(w_1) + 1\Big) \\ &\quad -2d_G(w_1) - 4 = d_G(w_1) - 1 > 0, \end{aligned}$$

and so G is not an extremal graph of $\mathbb{C}(n, k)$ for the second Zagreb index.

Now, we suppose that G is an extremal graph of $\mathbb{C}(n, k)$ for the general spectral radius. If $f_G(w_1) \geq f_G(w_q)$, then Theorem 2.7 implies that $\Theta(G_1, \beta) > \Theta(G, \beta)$, which is contrary with the choice of G. Otherwise, $f_G(w_1) < f_G(w_q)$. In the latter case, let $G_2 = G - \big\{w_1x : x \in N_G(w_1)\backslash\{w_q\}\big\} + \big\{w_qx : x \in N_G(w_1)\backslash\{w_q\}\big\}$. Now, $G_2 \in \mathbb{C}(n, k)$ and $\Theta(G_2, \beta) > \Theta(G, \beta)$ by Theorem 2.7, a contradiction.
The last possibility is that G is an extremal graph of $\mathbb{C}(n, k)$ for the bond incident degree index. Without loss of generality, we suppose that $\varphi(x, y)$ is a good escalating function. Since $d_G(w_1) \geq 3$ by Lemma 3.4 and $k \geq 1$, we have

$$\begin{aligned} BID(G_1) - BID(G) &= \varphi\big(d_G(w_1) + 1, 1\big) + \varphi\big(d_G(w_1) + 1, 2\big) \\ &\quad - \varphi\big(2, 2\big) - \varphi\big(d_G(w_1), 2\big) \\ &\quad + \sum_{z \in N_G(w_1)\backslash\{w_q\}} \varphi\big(d_G(w_1) + 1, d_G(z)\big) \\ &\quad - \sum_{z \in N_G(w_1)\backslash\{w_q\}} \varphi\big(d_G(w_1), d_G(z)\big) \\ &> \varphi\big(d_G(w_1) + 1, 1\big) - \varphi\big(2, 2\big) > 0, \end{aligned}$$

a contradiction. □

4 The Proof of Theorem 1.2

In view of Theorems 2.3–2.4 and Lemma 3.2, to prove Theorem 1.2, it suffices to show the following result:

Theorem 4.1 *In the class of cacti with $n \geq 4$ vertices, C_{n,k_0} uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, the maximum $BID(G)$ when $\varphi(x, y)$ is a good escalating function with $\varphi(2, 2) \geq 0$, the maximum $H_f(G)$ when $f(x)$ is a strictly convex and strictly increasing function, and the maximum $M_2(G)$, where $k_0 = \lfloor \frac{n-1}{2} \rfloor$.*

Proof Suppose that G is an extremal graph as defined in Theorem 4.1. We may suppose that $G \in \mathbb{C}(n, k)$. From Theorem 3.3, it follows that $G \cong C_{n,k}$, where $k \geq 0$. By

contradiction, we prove this result. For this, we assume that $k < \lfloor \frac{n-1}{2} \rfloor$. It is easily checked that

$$\begin{aligned} &H_f(C_{n,k+1}) - H_f(C_{n,k}) = 2\big(f(2) - f(1)\big) > 0, \\ &BID(C_{n,k+1}) - BID(C_{n,k}) = 2\varphi(n-1,2) + \varphi(2,2) - 2\varphi(n-1,1) \\ &\quad \geq 2\varphi(n-1,2) - 2\varphi(n-1,1) > 0 \end{aligned}$$

and

$$M_2(C_{n,k+1}) - M_2(C_{n,k}) = 2(n+1) > 0.$$

Combining this with Theorem 2.7, we complete the proof of this theorem. □

5 The Proof of Theorem 1.3

From Theorems 2.3 and 2.4 , to show Theorem 1.3, it suffices to prove the following result:

Theorem 5.1 *Let $f(x)$ be a strictly convex and strictly increasing function. In the class of cacti with $n \geq 4$ vertices and $k \geq 1$ pendant vertices, (i) if $n - k \equiv 1 \ (mod\ 2)$, then $F^1_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$, and maximum $H_f(G)$. (ii) if $n - k \equiv 0 \ (mod\ 2)$, then $F^0_{n,k}$ uniquely has the maximum $\Theta(G, \beta)$ for $\beta \geq 0$; (iii) if $n - k \equiv 0 \ (mod\ 2)$, then $H_f(G) \leq kf(1) + f(n-2) + (n-k-1)f(2)$, where the equality holds if and only if $G \in \{F^0_{n,k}, F^2_{n,k}\}$.*

Throughout this section, we may suppose that G_0 is an extremal graph of $\mathbb{W}(n, k)$ as defined in Theorem 5.1. A path $P_s : u_1u_2 \cdots u_s$ with $s \geq 2$ is called a *pendant path* of G if $d_G(u_s) = 1 < 2 = d_G(u_{s-1}) = d_G(u_{s-2}) = \cdots = d_G(u_2) = 2 < d_G(u_1)$, and u_1 is called the *initial vertex* of P_s. We have the following result:

Lemma 5.2 *If P_s is a pendant path with the largest length of G_0, then $s \leq 3$.*

Proof If $s \geq 4$, then we let $G_1 = G_0 + u_1u_3$, and so G_0 is a proper subgraph of G_1. Therefore, $G_1 \in \mathbb{W}(n, k)$, contrary with Theorems 2.5 and 2.7. Hence, we get the required result. □

An *internal path* joining the vertices w_1 and w_t ($w_1 = w_t$ is also permitted) of G is a path $Q_t : w_1w_2 \cdots w_t$ such that $d_G(w_1) \geq 3$, $d_G(w_t) \geq 3$ and $d_G(w_i) = 2$ (if exist) for $2 \leq i \leq t-1$. An *internal path* $Q_t : w_1w_2 \cdots w_t$ is called an *internal cut path* if $t \geq 2$, $w_1 \neq w_t$, and each edge of Q_t is a cut-edge of G.

Lemma 5.3 *G_0 contains no internal cut path.*

Proof By contradiction, we prove this result. For this, we assume that $Q_t : w_1w_2 \cdots w_t$ is an internal cut path of G_0. If $t \geq 3$, then let $G_1 = G_0 + w_1w_t$, and so G_0 is a proper subgraph of G_1 with $G_1 \in \mathbb{W}(n, k)$, contrary with Theorems 2.5 and 2.7 . Therefore, $t = 2$.

Without loss of generality, we may suppose that $f_{G_0}(w_2) \geq f_{G_0}(w_1)$. Let $G_2 = G_0 - w_1u + w_2u$, where $u \in N_{G_0}(w_1)\backslash\big(N_{G_0}(w_2) \cup \{w_2\}\big)$. Since $d_{G_0}(w_1) \geq 3$, we have $G_2 \in \mathbb{W}(n,k)$. By Theorem 2.7, it follows that $\Theta(G_2,\beta) > \Theta(G_0,\beta)$, and so G_0 is not an extremal graph of $\mathbb{W}(n,k)$ for general spectral radius, a contradiction. In view of Theorem 2.5, we can conclude that G_0 is also not an extremal graph of $\mathbb{W}(n,k)$ for vertex-degree-function index, a contradiction. □

Lemma 5.4 *All the pendant paths of G_0 have the same initial vertex.*

Proof Again by contradiction, we prove this result. For this, we assume that $P : u_1u_2\cdots u_s$ and $P' : w_1w_2\cdots w_t$ are two pendant paths of G_0 with initial vertices u_1 and w_1, respectively, where $u_1 \neq w_1$. By the definitions of u_1 and w_1, we have

$$\min\big\{d_{G_0}(u_1),\ d_{G_0}(w_1)\big\} \geq 3.$$

Without loss of generality, we may suppose that $f_{G_0}(u_1) \geq f_{G_0}(w_1)$. Let $G_1 = G_0 - w_1w_2 + u_1w_2$. Then, $G_1 \in \mathbb{W}(n,k)$, contrary with Theorem 2.7. Similarly, by Theorem 2.5 we can also deduce a contradiction for vertex-degree-function index. □

Hereafter, by Lemma 5.4, we let v_0 be the unique initial vertex with degree being at least three (if exists) of G_0.

Lemma 5.5 *v_0 is the unique cut-vertex of G_0 with degree being at least three.*

Proof Since $k \geq 1$, v_0 must be one cut-vertex of G_0. By contradiction, we prove this result. For this, we assume that u_0 is another cut-vertex of G_0 with degree being at least three such that the distance between u_0 and v_0 is as large as possible. In view of Lemma 5.4 and the choice of u_0 and v_0, there exists a pendant block B and vertex v such that B is a cycle with $u_0 \in B$ and vv_0 is a cut-edge in a pendant path. We suppose that $N_{G_0}(u_0) \cap V(B) = \{u, w\}$. Let $G_1 = G_0 + u_0v - vv_0$ and $G_2 = G_0 + v_0u + v_0w - uu_0 - wu_0$. By Lemma 5.3, G_0 contains no internal cut path and hence $G_1 \in \mathbb{W}(n,k)$ and $G_2 \in \mathbb{W}(n,k)$.

Case 1 The general spectral radius. If $f_{G_0}(u_0) \geq f_{G_0}(v_0)$, then $\Theta\big(G_1,\beta\big) > \Theta\big(G_0,\beta\big)$ by Theorem 2.7, a contradiction. Otherwise, $f_{G_0}(u_0) < f_{G_0}(v_0)$ and so once again Theorem 2.7 implies that $\Theta\big(G_2,\beta\big) > \Theta\big(G_0,\beta\big)$, a contradiction.

Case 2 The vertex-degree-function index. If $d_{G_0}(u_0) \geq d_{G_0}(v_0)$, then $H_f\big(G_1\big) > H_f\big(G_0\big)$ by Theorem 2.5, a contradiction. Otherwise, $d_{G_0}(u_0) < d_{G_0}(v_0)$ and so $H_f\big(G_2\big) > H_f\big(G_0\big)$ follows from Theorem 2.5, a contradiction. □

Let G be a connected graph with $uv \in E(G)$, and let $G_{u,v}$ be the graph obtained from G by subdividing the edge uv, i.e., adding a new vertex w and edges uw, wv in $G - uv$.

Lemma 5.6 [13] *Let G be a connected graph with at least one cycle. If uv is an edge of some internal path of G and $\beta \geq 0$, then $\Theta(G,\beta) > \Theta(G_{u,v},\beta)$.*

Proof of Theorem 5.1 For $n = 4$, since $k \geq 1$, it is easily checked that the result holds. Thus, we may suppose that $n \geq 5$ in the following. If $G_0 \cong P_n$, then $k = 2$ and so

$G_0 \in \mathbb{W}(n, 2)$. However, we can construct a cactus G_1 obtained from G_0 by adding one edge to G_0 such that $G_1 \in \mathbb{W}(n, 2)$ and G_0 is a proper subgraph of G_1, contrary with Theorems 2.5 and 2.7 .

Otherwise, $G_0 \ncong P_n$. Combining this with $k \geq 1$, Lemma 5.5 implies that v_0 is the unique cut-vertex of G_0 with degree being at least three. Hereafter, let $P_s : v_0u_1u_2 \cdots u_{s-1}$ be a longest pendant path of G_0.

Claim 2 If $k \geq 2$, then each of the pendant paths except P_s is a pendant edge.

Proof of Claim 2 By contradiction, we prove **Claim** 2. For this, we assume that $P_t : v_0z_1z_2$ is another pendant path of length two by Lemmas 5.2 and 5.4 . Let $G_2 = G_0 + z_1u_1$. By the choice of P_s, $G_2 \in \mathbb{W}(n, k)$ and G_0 is a proper subgraph of G_2, which is contrary with Theorems 2.5 and 2.7. This completes the proof of the claim. □

If G_0 is a tree, then by Lemmas 5.2, 5.4 and 5.5 with **Claim** 2 it follows that $G_0 \in \{F^0_{n,k}, F^1_{n,k}\}$ as $G_0 \ncong P_n$. Hence, the result holds. Otherwise, G_0 contains at least one cycle. Since v_0 is the unique cut-vertex of G_0 with degree being at least three, by Lemmas 5.3–5.5, G_0 is obtained from a rose graph (a rose graph is a graph with several cycles that all meet in one vertex) by attaching some paths (maximum path length is 2) to the maximum degree vertex v_0 of the rose graph. Denote $C_q : v_0w_1w_2 \cdots w_{q-1}v_0$ as a cycle with the largest length among all the cycles of G_0. If $q = 3$, then $G_0 \in \{F^0_{n,k}, F^1_{n,k}\}$ by **Claim** 2, and so the result holds. Otherwise, we assume that $q \geq 4$ in the following. We now consider the following two cases:

Case 1 The general spectral radius. Let $G_3 = G_0 - w_1w_2 - w_2w_3 + w_1w_3$ and let $G_4 = G_3 + w_2u_{s-1}$. (Recall that u_{s-1} is the pendant vertex of G_0.) Then, $G_4 \in \mathbb{W}(n, k)$. Since G_3 is a proper subgraph of G_4, we have $\Theta(G_4, \beta) > \Theta(G_3, \beta) > \Theta(G_0, \beta)$ by Lemma 5.6 and Theorem 2.7, a contradiction.

Case 2 The vertex-degree-function index. By Lemma 5.2, we have $s \leq 3$. For $s = 3$, let $G_5 = G_0 + v_0w_2 - w_1w_2$ and let $G_6 = G_5 + w_1u_1$ (see the definition of P_s). Then, $G_6 \in \mathbb{W}(n, k)$. Since G_5 is a proper subgraph of G_6 with $d_{G_0}(v_0) \geq d_{G_0}(w_1)$, we have $H_f(G_6) > H_f(G_5) > H_f(G_0)$ by Corollary 2.6, a contradiction.

Otherwise, $s = 2$. By Lemma 5.2, P_s is a pendant edge. One can easily check that $H_f(G_4) = H_f(G_0)$. The length of the longest pendant path of G_4 is equal to two. By the choice of G_0 and the discussion of $s = 3$, we can conclude that except for C_q, each other cycle of G_0 is a triangle and $q = 4$. Hence, $G_0 \cong F^2_{n,k}$. □

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SHORT COMMUNICATION

Some Properties of Algebraic Connectivity

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Abstract In this paper, we obtain two methods to compare the algebraic connectivity of two graphs, and we also give some graph operations that increase or decrease the algebraic connectivity of a graph.

Keywords Algebraic connectivity · Graph operation · Fiedler vector

Mathematics Subject Classification 05C35 · 05C75 · 05C05

Introduction

Throughout this paper, G is a simple undirected graph. For a vertex v of the graph G, we use $N(v)$ and $d(v)$ to denote the neighbor set and degree of v in G, respectively. If $d(u) = 1$, then we call u a *pendant vertex*. Suppose that P is a path. If one end vertex of P is a pendant vertex while all the internal vertices of P are vertices with degrees two, then P is called a *pendant path*. As usual, C_n and P_n define, respectively, the cycle and path on n vertices. Suppose v is a vertex of G, and $P_s = w_1w_2\cdots w_s$, where $V(P_s) \cap V(G) = \emptyset$. If we obtain a new graph G' from G and P_s by adding one edge vw_1, then we say that G' is obtained from G by *attaching* the pendant vertex w_1 of P_s to v of G.

If G is a connected graph with n vertices and $n-1$ (respectively, n) edges, then G is called a tree (respectively, a unicyclic graph). Hereafter, let $P_{n-\Delta+1} = x_1x_2\cdots x_{n-\Delta+1}$ and let $B(n,\Delta)$ be a tree with n vertices and maximum degree Δ obtained from $P_{n-\Delta+1}$ by attaching $\Delta-1$ pendent vertices (say $x_n, x_{n-1}, \ldots, x_{n-\Delta+2}$) to the vertex $x_{n-\Delta+1}$ of $P_{n-\Delta+1}$. Let Z_{x_k} be the tree with n vertices obtained from $B(n-p,\Delta)$ by attaching p pendant vertices to x_k of $B(n-p,\Delta)$, where $p \geq 1$.

The *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$, where $D(G)$ and $A(G)$ are the diagonal matrix of vertex degrees and adjacency matrix of G, respectively. Since $L(G)$ is positive semidefinite matrix with all row sums being equal to zero [1], we can use $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0$ to denote the eigenvalues of $L(G)$. As early as in 1973, Fiedler [2] revealed the relation between Laplacian spectrum and structure of G via proving that "G is connected if and only if $\lambda_{n-1}(G) > 0$." From then on, $\lambda_{n-1}(G)$ is also called the *algebraic connectivity* of G. In the following, we always use the symbol $\alpha(G)$ in place of $\lambda_{n-1}(G)$, and call an eigenvector corresponding to $\alpha(G)$ a *Fiedler vector* of G.

Eichinger et al. [3, 4] presented that the eigenvalues of the Laplacian matrix of a molecular graph determine the distribution function of the so-called radius of gyration of the molecule and that the nonzero eigenvalues and their eigenvectors can be used efficiently to compute the

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scattering functions for Gaussian molecules. It is worth mentioning that the asymptotic behavior of the distribution function of the radius of gyration of a molecule depends mostly upon the magnitude and multiplicity of $\alpha(G)$ [3]. Maas showed in [5] that the Laplacian eigenvalues of the underlying graph determine the kinematic behavior of a liquid flowing through a system of communicating pipes. It turns out that the algebraic connectivity $\alpha(G)$ determines the basic behavior of the flow (e.g., whether the flow is of periodic or aperiodic type).

Let $J_{s\times t}$ and $O_{s\times t}$ be the matrices of all ones and zeros with s rows and t columns, respectively. Specially, O_n defines a square matrix of all zeros of order n. By the famous Courant–Fisher theorem [6], for any unit column vector orthogonal to $J_{1\times n}$, we have $\alpha(G) \le \varphi^{\mathrm{T}} L(G)\varphi$ with equality holding if and only if φ is a Fiedler vector of G. Hereafter, we use $\chi = (\chi(v_1), \chi(v_2), \ldots, \chi(v_n))^{\mathrm{T}}$ to define a Fiedler vector of G. From the definition,

$$\alpha(G)\chi(v) = (L(G)\chi)_v \tag{1}$$

holds for any $v \in V(G)$.

Some graph operations play a crucial role on the solution to extremal problems of algebraic connectivity, and hence received more and more attentions [7–10]. In this paper, we present two methods to compare the algebraic connectivity of two graphs, and we also determine some graph operations that increase or decrease the algebraic connectivity of a graph.

Suppose v is a vertex of a connected graph G with at least two vertices. Let $G_{s,t}$ $(t \ge s \ge 1)$ be the graph obtained from G and two new paths $P_s = w_1 w_2 \cdots w_s$ and $P_t = u_1 u_2 \cdots u_t$, by adding the edges vw_1 and vu_1. Let $G_{s-1,t+1} = G_{s,t} - w_{s-1}w_s + u_t w_s$.

Lemma 1 [7]*Let G be a connected graph with at least two vertices. If $t \ge s \ge 1$, then $\alpha(G_{s,t}) \ge \alpha(G_{s-1,t+1})$. Furthermore, the inequality is strict if either $\chi(w_s) \ne 0$or $\chi(u_t) \ne 0$,where χ is a Fiedler vector.*

Lemma 2 [10]*Let v be a vertex of a connected graph G. Suppose that $w_1, w_2, \ldots, w_s$ are pendant vertices of G, which are adjacent to v. Let G' be the graph obtained from G by adding any t $\left(1 \le t \le \frac{s(s-1)}{2}\right)$ edges among $w_1, w_2, \ldots, w_s$. If $\alpha(G) \ne 1$, then $\alpha(G) = \alpha(G')$.*

Suppose that χ is a Fiedler vector and v is a vertex of G. In the sequel, we call $\chi(v)$ the *weight* of v. Furthermore, we call v a *positive vertex* (or *negative vertex*) if $\chi(v) > 0$ (or $\chi(v) < 0$), and we call v a *zero vertex* if $\chi(v) = 0$. For Fiedler vector, one of the famous results is the following:

Lemma 3 [11] *Let G be a connected graph with χ being a Fiedler vector, and let v be a cut vertex of G. If $\chi(v) > 0$, then exactly one component of $G - v$ contains at least one negative vertex, while all the vertices in the remaining components of $G - v$ are positive vertices with weight being larger than $\chi(v)$.*

When M is a symmetric real matrix of order n, we use the symbol $\theta_1(M) \ge \theta_2(M) \ge \cdots \ge \theta_n(M)$ to denote the eigenvalues of M, and we use $\tau(M)$ to denote the minimum eigenvalue of M, namely $\tau(M) = \theta_n(M)$. The following lemma is always called *interlacing theorem* [6].

Lemma 4 [6] *If M is a symmetric real matrix of order n with N being its principal submatrix of order s, then $\theta_{n-s+i}(M) \le \theta_i(N) \le \theta_i(M)$ holds for any $i \in \{1, 2, \ldots, s\}$.*

From Lemma 4, Bapat et al. proved the following relation between algebraic connectivity and the minimum eigenvalues of some principal submatrices of $L(G)$.

Lemma 5 [12] *Let G be a connected graph, and let W be a set of vertices of G such that $G - W$ is disconnected. Let G_1 and G_2 be two arbitrary components of $G - W$, and let L_1 and L_2 be the principal submatrices of $L(G)$ corresponding to G_1 and G_2, respectively. If $\tau(L_1) \le \tau(L_2)$, then either $\tau(L_2) > \alpha(G)$ or $\tau(L_1) = \tau(L_2) = \alpha(G)$.*

For the relation between $\alpha(G)$ and $\alpha(G - v)$, the following properties are famous.

Lemma 6 *Let G be a connected graph with n vertices and $v \in V(G)$. (1) [13] If v is a cut vertex of G, then $\alpha(G) \le 1$ with equality holding if and only if $d(v) = n - 1$. (2) [9, 14] If v is a pendant vertex of G, then $\alpha(G) \le \alpha(G - v)$.*

In the following, we let B_k be the matrix of order k obtained from $L(P_{k+1})$ by deleting the row and column corresponding to one pendant vertex of P_{k+1}.

Lemma 7 [7] *Let $P_{k+1} = w_1 w_2 \cdots w_{k+1}$ be a pendant path of the graph G such that $d(w_1) = 1$ and $d(w_{k+1}) \ge 1$. If χ is a Fiedler vector of G, then $\chi(w_i) = \chi(w_1) \prod_{j=1}^{i-1} \big(\theta_j(B_{i-1}) - \alpha(G)\big)$ holds for any $i \in \{2, 3, \ldots, k+1\}$.*

Let G_1 and G_2 be two disjoint graphs with $|V(G_i)| = n_i \ge 2$ and $u_i \in V(G_i)$, where $i \in \{1, 2\}$. Let $Z(G_1(u_1), G_2(u_2))$ be the graph obtained from G_1 and G_2 by identifying the vertices u_1 and u_2.

Lemma 8 [15] *Let G_1 and G_2 be two disjoint connected graphs with $|V(G_i)| = n_i \ge 2$, where $i \in \{1, 2\}$. Suppose that χ is a Fiedler vector of $Z(G_1(u_1), G_2(u_2))$, $\{u_1, w_1\} \subseteq V(G_1)$, and $u_2 \in V(G_2)$. If $(\chi(w_1) - \chi(u_1)) \sum_{y \in V(G_2)\setminus\{u_2\}} \chi(y) \ge 0$, then $\alpha(Z(G_1(u_1), G_2(u_2))) \ge \alpha(Z(G_1(w_1), G_2(u_2)))$. Furthermore, if $\chi(w_1) \ne \chi(u_1)$, then the inequality is strict.*

How to compare the algebraic connectivity of two graphs is a difficult problem [8–10, 14]. In this section, we shall give two methods to compare the algebraic

connectivity of two graphs. Let $\Phi(B,x)=\det(xI-B)$ denote the characteristic polynomial of a square matrix B. In particular, we always simply write $\Phi(L(G),x)$ as $\Phi(G,x)$.

Lemma 9 (1) *For any* $1\le j\le t$, *we have* $\theta_j(B_t)=\lambda_{2j}(P_{2t+1})$; (2) *If* $t>s\ge 1$, *then* $\theta_s(B_s)>\theta_t(B_t)$, $\theta_{s-1}(B_s)>\theta_{t-1}(B_t)$, $\theta_{s-1}(B_s)>\theta_s(B_s)$ *and* $\alpha(P_s)>\alpha(P_t)$.

Proof Suppose that $P_{2t+1}=w_1w_2\cdots w_{2t+1}$. Let M denote the submatrix of $L(P_{2t+1})$ by deleting the row and column corresponding to the vertex w_{t+1}. By Lemma 4, $\theta_j(B_t)=\theta_{2j}(M)\le\lambda_{2j}(P_{2t+1})\le\theta_{2j-1}(M)=\theta_j(B_t)$. Thus, $\theta_j(B_t)=\lambda_{2j}(P_{2t+1})$, which implies that (1) holds.

It is well known that the eigenvalues of $L(P_n)$ are $2+2\cos(\frac{i\pi}{n})$, where $j=1,2,\ldots,n$. When $1\le x\le k$, since $\psi(x)=2\big(1+\cos\big(\frac{\pi}{k}x\big)\big)$ is strictly decreasing, we have

$$\theta_j(B_t)=\lambda_{2j}(P_{2t+1})=2\left(1+\cos\left(\frac{2j}{2t+1}\pi\right)\right) \tag{2}$$

for any $j\in\{1,2,\ldots,t\}$.

By Eq. (2), $\theta_t(B_t)<\theta_s(B_s)$, $\theta_{s-1}(B_s)>\theta_{t-1}(B_t)$ and $\theta_{s-1}(B_s)>\theta_s(B_s)$. Note that $\alpha(P_t)=2\big(1-\cos\frac{\pi}{t}\big)<2\big(1-\cos\frac{\pi}{s}\big)=\alpha(P_s)$. Thus, the result follows. □

Corollary 1 *If* T *is a tree and* $\alpha(T)=\theta_k(B_k)$, *then the length of longest path of* T *is at most* $2k+1$.

Proof Suppose that the longest path of T is P_q. By contradiction, assume that $q\ge 2k+2$. Now, Lemma 6 (2) and Lemma 9 imply that $\alpha(T)\le\alpha(P_q)<\alpha(P_{2k+1})=\theta_k(B_k)$, a contradiction. Thus, $q\le 2k+1$. □

Lemma 10 *Let* G *and* G' *be two connected graphs with* n *vertices such that* $\Phi(G,x)-\Phi(G',x)=\psi_1(x)\Phi(P_k,x)+\psi_2(x)\Phi(B_k,x)$ *and* $\alpha(G)\le\lambda_{n-2}(G')$. *Then,* $\alpha=\alpha(G)<\alpha(G')$ *if one of the following four cases happens*: (1) $\theta_k(B_k)\le\alpha\le\alpha(P_{k+1})$, $(-1)^{n-k}\psi_1(\alpha)<0$ *and* $(-1)^{n-k}\psi_2(\alpha)\le 0$. (2) $\theta_k(B_k)<\alpha<\alpha(P_{k+1})$, $(-1)^{n-k}\psi_1(\alpha)\le 0$ *and* $(-1)^{n-k}\psi_2(\alpha)<0$. (3) $\alpha<\alpha(P_k)$, $\psi_2(\alpha)=0$ *and* $(-1)^{n-k}\psi_1(\alpha)<0$. (4) $\theta_k(B_k)<\alpha<\theta_{k-1}(B_k)$, $\psi_1(\alpha)=0$ *and* $(-1)^{n-k}\psi_2(\alpha)<0$.

Proof Here, we only prove (1), since the other cases can be proved similarly. By Lemma 9, we have $\alpha\le\alpha(P_{k+1})<\alpha(P_k)$, and hence

$$(-1)^k\Phi(P_k,\alpha)=\prod_{i=1}^{k}(\lambda_i(P_k)-\alpha)<0. \tag{3}$$

By Lemma 4, we have $\alpha\le\alpha(P_{k+1})\le\theta_{k-1}(B_k)$. Since $\theta_k(B_k)\le\alpha$, it follows that

$$(-1)^k\Phi(B_k,\alpha)=\prod_{i=1}^{k}(\theta_i(B_k)-\alpha)\le 0. \tag{4}$$

Note that $\Phi(G,\alpha)=0$ and $\alpha>0$. If (1) holds, then by (3) and (4) we have

$$\begin{aligned}\alpha\prod_{i=1}^{n-1}(\lambda_i(G')-\alpha)&=(-1)^{n-1}\Phi(G',\alpha)\\&=(-1)^n(\psi_1(\alpha)\Phi(P_k,\alpha)+\psi_2(\alpha)\Phi(B_k,\alpha))>0.\end{aligned}$$

Since $\alpha(G)\le\lambda_{n-2}(G')$, we have $\alpha(G')=\lambda_{n-1}(G')>\alpha$. □

The following lemma is very similar to Lemma 10, so we omit the proof.

Lemma 11 *Let* G *and* G' *be two connected graphs with* n *vertices such that* $\Phi(G',x)-\Phi(G,x)=\psi_1(x)\Phi(P_k,x)+\psi_2(x)\Phi(B_k,x)$ *and* $\alpha(G')\le\lambda_{n-2}(G)$. *Then,* $\alpha=\alpha(G')>\alpha(G)$ *if one of the following four cases happens*: (1) $\theta_k(B_k)\le\alpha\le\alpha(P_{k+1})$, $(-1)^{n-k}\psi_1(\alpha)>0$ *and* $(-1)^{n-k}\psi_2(\alpha)\ge 0$. (2) $\theta_k(B_k)<\alpha<\alpha(P_{k+1})$, $(-1)^{n-k}\psi_1(\alpha)\ge 0$ *and* $(-1)^{n-k}\psi_2(\alpha)>0$. (3) $\alpha<\alpha(P_k)$, $\psi_2(\alpha)=0$ *and* $(-1)^{n-k}\psi_1(\alpha)>0$. (4) $\theta_k(B_k)<\alpha<\theta_{k-1}(B_k)$, $\psi_1(\alpha)=0$ *and* $(-1)^{n-k}\psi_2(\alpha)>0$.

By employing Lemmas 10 and 11, sometimes we can easily determine the relation of algebraic connectivity between two graphs. For instance, the following two results were proved by complex methods, and we shall present a simple proof to each of them.

As shown in Fig. 1, let $U_n^+(k)$ be the graph obtained by attaching one isolated vertex x_{n-2} and the pendant vertex x_{n-5} of a path $P_{n-5}=x_1x_2\cdots x_{n-5}$ to two adjacent vertices, say x_{n-3} and x_{n-4}, of C_3, respectively, and then attaching one isolated vertex x_n to the vertex x_k, where $V(C_3)=\{x_{n-1},x_{n-3},x_{n-4}\}$.

Theorem 1 [8] *If* $n\ge 9$, *then* $\alpha(U_n^+(2))<\alpha(U_n^+(n-4))$.

Proof It is easy to see that (see [8]) $\Phi(U_n^+(n-4),x)-\Phi(U_n^+(2),x)=\psi_1(x)\Phi(P_{n-6},x)$, where $\psi_1(x)=-x(x^3-6x^2+10x-6)$. Now, Lemmas 2 and 6 imply that $\alpha(U_n^+(n-4))\le\alpha(P_{n-3})\le\alpha(P_6)<0.27$, $\alpha(P_{n-3})\le\alpha(P_{n-6})$, and $\alpha(U_n^+(n-4))\le\alpha(U_n^+(n-4)-x_n)=\lambda_{n-2}(U_n^+(n-4)-x_nx_{n-4})=\lambda_{n-2}(U_n^+(2)-x_nx_2)\le\lambda_{n-2}(U_n^+(2))$. Since $0<\alpha(U_n^+(n-4))<0.27$, we have $\psi_1(\alpha)>0$. Thus, the result follows from Lemma 11(iii). □

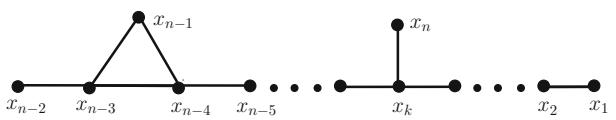


Fig. 1 The unicyclic graph $U_n^+(k)$

Suppose that b is a real number. Let $\mathrm{sgn}(b) = 1, 0, -1$, if $b > 0$, $b = 0$, or $b < 0$, respectively. Let $Z(G; P_k^{(s)})$ be the graph obtained from a connected graph G by attaching the pendant vertex w_{i1} of the i-th path $P_k^{(i)} = w_{i1}w_{i2}\cdots w_{ik}$ to the vertex v of G, where $i \in \{1, 2, \ldots, s\}$ and $|V(G)| \geq 2$.

Lemma 12 *Let χ be a Fiedler vector of $Z(G; P_k^{(s)})$. If $\alpha(Z(G; P_k^{(s)})) \neq \theta_k(B_k)$ and $s \geq 2$, then $0 < \alpha(Z(G; P_k^{(s)})) < \theta_k(B_k)$, $\mathrm{sgn}(\chi(w_{11})) = \mathrm{sgn}(\chi(w_{12})) = \cdots = \mathrm{sgn}(\chi(w_{1k})) = \mathrm{sgn}(\chi(v))$ and $\chi(w_{1j}) = \chi(w_{2j}) = \cdots = \chi(w_{sj})$ holds for any $j \in \{1, 2, \ldots, k\}$.*

Proof By Lemma 5 and $\alpha(Z(G; P_k^{(s)})) \neq \theta_k(B_k)$, we have $0 < \alpha(G) < \theta_k(B_k)$. Furthermore, Lemmas 7 and 9 imply that $\mathrm{sgn}(\chi(w_{11})) = \mathrm{sgn}(\chi(w_{12})) = \cdots = \mathrm{sgn}(\chi(w_{1k})) = \mathrm{sgn}(\chi(v))$ and $\chi(w_{1j}) = \chi(w_{2j}) = \cdots = \chi(w_{sj})$ holds for any $j \in \{1, 2, \ldots, k\}$. □

Lemma 13 *Let u and v be two vertices of a connected graph G, and let $G^* \cong Z(G; P_k^{(s)}) + uw_{11} + uw_{21} + \cdots + uw_{s1} - vw_{11} - vw_{21} - \cdots - vw_{s1}$. Suppose that χ is a Fiedler vector of $Z(G; P_k^{(s)})$ and $s \geq 2$. If $\chi(u) \geq \chi(v) \geq 0$ and $\alpha(Z(G; P_k^{(s)})) \neq \theta_k(B_k)$, then $\alpha(Z(G; P_k^{(s)})) \geq \alpha(G^*)$. Furthermore, if $\chi(u) \neq \chi(v)$, then the inequality is strict.*

Proof Since $\alpha(Z(G; P_k^{(s)})) \neq \theta_k(B_k)$ and $s \geq 2$, by Lemmas 3 and 12, $\chi(y) \geq \chi(v) \geq 0$ holds for any $y \in V(Z(G; P_k^{(s)})) \backslash V(G)$. Now, the result follows from Lemma 8. □

The following result improves Corollary 2.11 of [15].

Corollary 2 *Let u and v be two vertices of a connected graph G,* and let $w_1, w_2, \ldots, w_s$ *be $s \geq 1$ pendant vertices adjacent with v in G. Let $G^* \cong G + uw_1 + uw_2 + \cdots + uw_s - vw_1 - vw_2 - \cdots - vw_s$. (1) If $\alpha(G) = 1$, then $\alpha(G) \geq \alpha(G^*)$. Furthermore, if $d_{G^*}(u) < |V(G^*)| - 1$, then the inequality is strict. (2) If $\alpha(G) \neq 1$, χ is a Fiedler vector of G and $\chi(u) \geq \chi(v) \geq 0$, then $\alpha(G) \geq \alpha(G^*)$. Furthermore, if $\chi(u) \neq \chi(v)$, then the inequality is strict.*

Proof Since $s \geq 1$, v is a cut vertex of G^*. If $\alpha(G) = 1$, then $\alpha(G^*) \leq 1 = \alpha(G)$ follows from Lemma 6 (1). Once again, by Lemma 6 (1) we have $\alpha(G^*) < \alpha(G)$ if $d_{G^*}(u) < |V(G^*)| - 1$. Thus, (1) holds. Now, we turn to prove (2). If $s \geq 2$, by Lemma 13, (2) holds. If $s = 1$, by Eq. (1), we have $(1 - \alpha)\chi(w_1) = \chi(v) \geq 0$. Note that $0 < 1 - \alpha < 1$ by Lemma 6 (1). Thus, $\chi(w_1) \geq 0$. By Lemma 8, (2) follows. □

Definition 1 Let $G_0 \cong Z(P_1; P_{k_1}, P_{k_2}, \ldots, P_{k_s})$ be the graph obtained by attaching k paths $P_{k_1}, P_{k_2}, \ldots, P_{k_s}$ to the isolated vertex w, and let $Z(G_0; P_{q_1}, P_{q_2}, \ldots, P_{q_t})$ be the graph obtained from G_0 by attaching t paths $P_{q_1}, P_{q_2}, \ldots, P_{q_t}$ to the pendant vertex w_1 of P_{k_1} in G_0.

Lemma 14 *Let G_0 and $Z(G_0; P_{q_1}, P_{q_2}, \ldots, P_{q_t})$ be the graphs as defined in Definition 1, and let $q_1 = \max\{q_1, q_2, \ldots, q_t, k_2, k_3, \ldots, k_s\}$. If $t \geq 2$ and $s \geq 2$, then $\alpha(Z(G_0; P_{q_1}, P_{q_2}, \ldots, P_{q_t})) > \alpha(Z(G_0; P_{q_1+1}, P_{q_2-1}, \ldots, P_{q_t}))$.*

Proof Let $G' \cong Z(G_0; P_{q_1}, P_{q_2}, \ldots, P_{q_t})$, $G'' \cong Z(G_0; P_{q_1+1}, P_{q_2-1}, \ldots, P_{q_t})$, and also let $\alpha = \alpha(G')$. Suppose that χ is a Fiedler vector of G', and suppose that $k_2 = \max\{k_i : 2 \leq i \leq s\}$. Since w and w_1 are two cut vertices of G', $0 < \alpha < 1$ follows from Lemma 6 (1).

Case 1. $\alpha \neq \theta_{q_1}(B_{q_1})$. Let x and y be the pendant vertices of P_{q_1} and P_{q_2} in G', respectively. Suppose that $\chi(x) = 0$ and $\chi(y) = 0$. In this case, by Lemma 7, $\chi(w_1) = 0$ and $\chi(v) = 0$ holds for any $v \in V(P_{q_1}) \cup V(P_{q_2})$. By Lemmas 5 and 9, $\alpha < \min\{\theta_{q_i}(B_{q_i}) : 2 \leq i \leq t\}$. Note that $\chi(w_1) = 0$. By Lemma 7, $\chi(v) = 0$ holds for any $v \in V(P_{q_i})$, where $1 \leq i \leq t$.

Since $\chi(w_1) = 0$, by Eq. (1), $\chi(v) = 0$ holds for any vertex $v \in V(P_{k_1}) \cup \{w\}$. Let L_1 be the principal submatrix of $L(G)$ corresponding to the vertex set of the component containing w_1 in $G - w$, and suppose that L_1 is a square matrix of order p. If $\alpha \geq \theta_{k_2}(B_{k_2})$, then $\theta_{k_2}(B_{k_2}) \leq \alpha \leq \theta_p(L_1)$ follows from Lemma 5. Note that B_{q_1} is the principal submatrix of L_1. By Lemmas 4 and 9, $\theta_p(L_1) \leq \theta_{q_1}(B_{q_1}) \leq \theta_{k_2}(B_{k_2})$. Thus, $\alpha = \theta_{q_1}(B_{q_1})$, a contradiction. Once again, Lemma 9 implies that $\alpha < \theta_{k_2}(B_{k_2}) = \min\{\theta_{k_i}(B_{k_i}) : 2 \leq i \leq s\}$.

Now, from Lemma 7 and $\chi(w) = 0$, we can conclude that $\chi(v) = 0$ holds for any $v \in V(P_{k_i})$, where $2 \leq i \leq s$. Thus, $\chi = O_{n\times 1}$, a contradiction. Therefore, either $\chi(x) \neq 0$ or $\chi(y) \neq 0$. By Lemma 1, the result follows.

Case 2. $\alpha = \theta_{q_1}(B_{q_1})$. Suppose that $q_1 = q_2 = \cdots = q_j > q_{j+1} \geq \cdots \geq q_t$, where $1 \leq j \leq t$. If there exists some pendant vertex of P_{q_i} $(1 \leq i \leq j)$ in G' being not a zero vertex, then the result follows from Lemma 1. Otherwise, all pendant vertices of $P_{q_1}, P_{q_2}, \ldots, P_{q_j}$ are zero vertices in G'. By Lemma 7, $\chi(v) = 0$ holds for any $v \in V(P_{q_i}) \cup \{w_1\}$, where $1 \leq i \leq j$. By Lemma 9, $\alpha = \theta_{q_1}(B_{q_1}) < \theta_{q_{j+1}}(B_{q_{j+1}}) \leq \cdots \leq \theta_{q_t}(B_{q_t})$. Note that $\chi(w_1) = 0$. By Lemma 7, we can conclude that $\chi(v) = 0$ holds for any $v \in V(P_{q_i})$, where $j + 1 \leq i \leq t$. Now, since $0 < \alpha < 1$ and Eq. (1), $\chi(v) = 0$ holds for any $v \in V(P_{k_1}) \cup \{w\}$.

By Lemma 9, $\alpha = \theta_{q_1}(B_{q_1}) \leq \theta_{k_2}(B_{k_2}) = \min\{\theta_{k_i}(B_{k_i}) : 2 \leq i \leq s\}$. If $\theta_{q_1}(B_{q_1}) < \theta_{k_2}(B_{k_2})$, since $\chi(w) = 0$, we have $\chi = O_{n\times 1}$ by Lemma 7, a contradiction. Thus, $\theta_{q_1}(B_{q_1}) = \theta_{k_2}(B_{k_2})$. Once again, Lemma 9 implies that $k_2 = q_1$, and hence G' contains a path $P_{2q_1+1+k_1}$, which contradicts Corollary 1. □

Corollary 3 If $q_1 = \max\{q_1, q_2, \ldots, q_{s-1}\}$ and $s \geq 3$, then $\alpha(Z(P_1; P_{q_1}, P_{q_2}, \ldots, P_{q_s})) > \alpha(Z(P_1; P_{q_1+1}, P_{q_2-1}, \ldots, P_{q_s}))$.

Proof We may suppose that $q_3 \geq q_4 \geq \cdots \geq q_s$. If $q_3 \geq 2$, then the result follows from Lemma 14 with $s = 2$ and $k_2 = 1$. Otherwise, $q_3 = q_4 = \cdots = q_s = 1$.

Let $G^* \cong Z(P_1; P_{q_1}, P_{q_2}, \ldots, P_{q_s})$ and also let $\alpha = \alpha(G^*)$. If $q_1 = 1$, then the result follows from Lemma 6 (1). Otherwise, $q_1 \geq 2$. Then, $0 < \alpha < 1$ by Lemma 6 (1). Let χ be a Fiedler vector of G^*, and also let x and y be the pendant vertices of P_{q_1} and P_{q_2} in G^*, respectively. If $\chi(x) = \chi(y) = 0$, then by Lemma 7 and Eq. (1) we have $\chi = O_{n\times 1}$, a contradiction. Therefore, either $\chi(x) \neq 0$ or $\chi(y) \neq 0$. Now, the result follows from Lemma 1. □

Definition 2 Let G be a connected graph with $n - s - p \geq 2$ vertices, and let G' be the graph obtained from G by attaching the pendant vertex x_s of a path $P_s = x_1 x_2 \cdots x_s$ to the vertex x_{s+1} of G. Let $G^*(x_k)$ be the graph with n vertices obtained from G' by attaching $p \geq 1$ isolated vertices to x_k of G', and let χ be a Fiedler vector of $G^*(x_k)$.

Lemma 15 Let G and $G^*(x_k)$ be the graphs as defined in Definition 2. Suppose that $\alpha(G^*(x_k)) \leq \alpha(P_{q+1})$ and $\chi(x_{s+1}) = 0$ indicates $\chi(v) = 0$ holds for any vertex $v \in V(G)$. (1) If $2 \leq k \leq \lfloor \frac{q+1}{2} \rfloor \leq s + 1$, then $\alpha(G^*(x_k)) > \alpha(G^*(x_{k-1}))$. (2) If $\lfloor \frac{n}{2} \rfloor + 1 \leq k \leq s \leq q$, then $\alpha(G^*(x_k)) > \alpha(G^*(x_{k+1}))$. (3) If $2 \leq k \leq s$, then either $\alpha(G^*(x_k)) > \alpha(G^*(x_{k-1}))$ or $\alpha(G^*(x_k)) > \alpha(G^*(x_{k+1}))$.

Proof Set $\alpha = \alpha(G^*(x_k))$. Since $G^*(x_k)$ is a connected graph with n vertices, by Lemma 6 (1) we may suppose that $0 < \alpha < 1$. If $\chi(x_1) = 0$, by Eq. (1) and $0 < \alpha < 1$, $\chi(u) = \chi(x_{s+1}) = 0$ holds for any $u \in V(G^*(x_k)) \backslash V(G)$. In this case, we have $\chi = O_{n\times 1}$, a contradiction. Thus, $\chi(x_1) \neq 0$. Since $-\chi$ is also a Fiedler vector of $G^*(x_k)$, we may suppose that $\chi(x_1) > 0$. It is well known that P_n uniquely minimizes the algebraic connectivity in the class of connected graphs with n vertices [10]. Thus, $\alpha(P_n) < \alpha \leq \alpha(P_{q+1})$, since $G^*(x_k) \ncong P_n$. By Lemma 9,

$$\theta_{\lfloor \frac{n}{2} \rfloor}\left(B_{\lfloor \frac{n}{2} \rfloor}\right) < \alpha < \theta_{\lfloor \frac{q-1}{2} \rfloor}\left(B_{\lfloor \frac{q-1}{2} \rfloor}\right). \tag{5}$$

We first prove (1). If $k = 2$, by Eq. (1) we have $\chi(x_1) > \chi(x_2) > 0$. Since $0 < \alpha < 1$, (1) follows from Corollary 2 (2). In the following, we suppose that $k \geq 3$. Since $k \leq \lfloor \frac{q+1}{2} \rfloor$, by Lemma 9 and inequality (5) it follows that $\theta_{k-1}(B_{k-1}) > \alpha$ holds for any $3 \leq k \leq \lfloor \frac{q+1}{2} \rfloor$. By Lemma 7, $\chi(x_j) > 0$ holds for any $j \in \{1, 2, \ldots, k\}$. Thus, $\chi(x_{k-1}) > \chi(x_k) > 0$ follows from Lemma 3. By Corollary 2 (2), (1) holds.

In the following, we prove (2). Since $\alpha \leq \alpha(P_{q+1})$, by Lemmas 4 and 9, for any $3 \leq k \leq q$ we have

$$\alpha \leq \alpha(P_{q+1}) \leq \theta_{q-1}(B_q) < \theta_{q-2}(B_{q-1}) < \cdots < \theta_{k-2}(B_{k-1}). \tag{6}$$

By inequality (5) and Lemma 9, $\alpha > \theta_{k-1}(B_{k-1})$ holds for any $\lfloor \frac{n}{2} \rfloor + 1 \leq k \leq q$. Since $\chi(x_1) > 0$, by Lemma 7 and inequality (6) we have $\chi(x_k) < 0$. Note that $-\chi$ is also a Fiedler vector of $G^*(x_k)$. Thus, $-\chi(x_k) > 0$ and $-\chi(x_1) < 0$. By Lemma 3, $-\chi(x_{k+1}) > -\chi(x_k) > 0$. Since $0 < \alpha < 1$, (2) follows from Corollary 2 (2).

Now, we turn to prove (3). If $\chi(x_k) = \chi(x_{k-1}) = 0$, since $0 < \alpha < 1$, we can conclude that $\chi(z) = 0$ holds for any pendant vertex z, which is adjacent with x_k in $G^*(x_k)$. By Eq. (1), we have $\chi = O_{n\times 1}$, a contradiction. Therefore, either $\chi(x_k) \neq 0$ or $\chi(x_{k-1}) \neq 0$.

We first consider the case $\chi(x_k) \neq 0$. If $\chi(x_k) < 0$, since $-\chi$ is also a Fiedler vector of $G^*(x_k)$ and $-\chi(x_1) < 0$, $-\chi(x_{k+1}) > -\chi(x_k) > 0$ follows from Lemma 3. Thus, $\alpha(G^*(x_k)) > \alpha(G^*(x_{k+1}))$ follows from Corollary 2 (2). If $\chi(x_k) > 0$, by Lemma 3, either $\chi(x_{k+1}) > \chi(x_k) > 0$ or $\chi(x_{k-1}) > \chi(x_k) > 0$. By Corollary 2 (2), either $\alpha(G^*(x_k)) > \alpha(G^*(x_{k+1}))$ or $\alpha(G^*(x_k)) > \alpha(G^*(x_{k-1}))$ holds.

In the following, we suppose that $\chi(x_k) = 0$, and hence $\chi(x_{k-1}) \neq 0$. Since $-\chi$ is also a Fiedler vector of $G^*(x_k)$, we may suppose that $\chi(x_{k-1}) > \chi(x_k) = 0$. By Corollary 2 (2), $\alpha(G^*(x_k)) > \alpha(G^*(x_{k-1}))$. □

Theorem 2 Let Z_{x_k} be the graph as defined in Section 1. Suppose that $\Delta \geq 3$, $p \geq 1$ and $n - \Delta - p \geq 2$. (1) If $2 \leq k \leq \lfloor \frac{n-\Delta-p}{2} \rfloor + 1$, then $\alpha(Z_{x_k}) > \alpha(Z_{x_{k-1}})$. (2) If $\lfloor \frac{n}{2} \rfloor + 1 \leq k \leq n - \Delta - p$, then $\alpha(Z_{x_k}) > \alpha(Z_{x_{k+1}})$. (3) If $2 \leq k \leq n - \Delta - p$, then either $\alpha(Z_{x_k}) > \alpha(Z_{x_{k-1}})$ or $\alpha(Z_{x_k}) > \alpha(Z_{x_{k+1}})$.

Proof By Lemma 6 (1), we may suppose that $0 < \alpha(Z_{x_k}) < 1$. Let χ be a Fiedler vector of Z_{x_k}. If $\chi(x_{n-p-\Delta+1}) = 0$, by Eq. (1) it follows that $\chi(u) = 0$ holds for $u \in \{x_{n-p-\Delta+1}, x_{n-p-\Delta+2}, \ldots, x_n\}$. By Lemma 6 (2), $\alpha(Z_{x_k}) \leq \alpha(P_{n-p-\Delta+2})$. Now, the result follows from Lemma 15. □

Conclusion

The algebraic connectivity of graphs is probably the most important information contained in the spectrum of a graph. This eigenvalue is related to several important graph invariants, and it has been extensively investigated. Recently, the algebraic connectivity has received much more attention on applications of hard problems in graph theory: the expanding properties of graphs, weighted graphs, isoperimetric number, genus and other invariants of a graph; applications on combinatorial optimization problems: the problem of certain flowing process, the maximum cut problem and the traveling salesman problem. Fiedler [2] calls $\alpha(G)$ as the algebraic connectivity of the graph G.

This is influenced by its relation to the classical connectivity parameters of the graph—the vertex connectivity $v(G)$ and the edge connectivity $\eta(G)$. Moreover, Fiedler [2] explored the properties of the eigenvector χ associated with $\alpha(G)$. This eigenvector χ, known as the Fiedler vector, is used in graph bipartition. In this paper, we present two methods for comparing the relationship of algebraic connectivity between two graphs, and we also obtain some properties for the algebraic connectivity.

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ORIGINAL PAPER

Unified Spectral Hamiltonian Results of Balanced Bipartite Graphs and Complementary Graphs

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Abstract
There have been researches on sufficient spectral conditions for Hamiltonian properties and path-coverable properties of graphs. Utilizing the Bondy–Chvátal closure, we provide a unified approach to study sufficient graph eigenvalue conditions for these properties and sharpen several former spectral Hamiltonian results on balanced bipartite graphs and complementary graphs.

Keywords Hamiltonian graphs · Traceable graphs · (Almost)balanced bipartite graphs · complementary graphs · (Signless Laplacian)spectral radius

Mathematics Subject Classification 05C50 · 15A18 · 15A36

1 Introduction

We study simple undirected graphs, with undefined terms and notation following [3]. As in [3], $\delta(G)$, $\kappa(G)$, $\kappa'(G)$ and $\overline{G}$ denote the minimum degree, the connectivity, the edge-connectivity and the complement of a graph G, respectively. For an integer k, a graph G is *k-connected* (resp. *k-edge-connected*) if $\kappa(G) \geq k$

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(resp. $\kappa'(G) \geq k$). Throughout this paper, for an integer $s \geq 1$, let sK_1 be the edgeless graph with s vertices. Let $S \subseteq V(G)$ be a subset. For any vertex $u \in V(G)$, define $N_S(u) = \{v \in S : uv \in E(G)\}$. If H is a subgraph of G, then we use $N_H(u)$ for $N_{V(H)}(u)$. In particular, $N_G(u) = \{v \in V(G) : uv \in E(G)\}$ and $d_G(u) = |N_G(u)|$. We often use $N(u)$ and $d(u)$ for $N_G(u)$ and $d_G(u)$, respectively, when G is understood from the context. A graph G is *nontrivial* if it has at least one edge. As in [3], G is *Hamiltonian* (resp., *traceable*) if G contains a spanning cycle (resp., spanning path), and is *Hamilton-connected* if any pair of distinct vertices are joined by a spanning path.

Definition 1.1 Let $q \geq 0$ be an integers and let G be a graph.

(i) G is *q-traceable* (resp. *q-Hamiltonian*, *q-Hamilton-connected*) if any removal of at most q vertices from G results in a traceable graph (resp., a Hamiltonian graph, a Hamilton-connected graph).

(ii) G is *q-edge-Hamiltonian* if any collection of vertex-disjoint paths with at most q edges altogether must belong to a Hamiltonian cycle in G.

(iii) G is *q-path-coverable* if $V(G)$ can be covered by no more than q vertex-disjoint paths.

Following [3], we use $G[X]$ to denote the subgraph of G induced by X. By Definition 1.1(i), a q-Hamiltonian graph is also a $(q+1)$-traceable graph. However, a $(q+1)$-traceable graph is not necessarily a q-Hamiltonian graph. For instance, the Petersen graph is 1-traceable, but not 0-Hamiltonian. Moreover, a traceable graph is a 0-traceable graph, and a Hamiltonian graph is both a 0-Hamiltonian and a 1-traceable graph. If G is Hamilton-connected, then for any pair of vertices $\{u, v\}$ of G, there is a Hamiltonian path connecting u and v. Thus, $G\big[V(G)\backslash\{u, v\}\big]$ contains a Hamiltonian path, and hence G is 2-traceable.

As in [3], the *join* $G \vee H$ of two disjoint graphs G and H is defined by $V(G \vee H) = V(G) \cup V(H)$ and $E(G \vee H) = E(G) \cup E(H) \cup \big\{xy : x \in V(G)$ and $y \in V(H)\big\}$. A *k-regular* graph is a graph with $d_G(u) = k$ for each vertex $u \in V(G)$. For two different nonnegative integers p and q, a *(p, q)-semi-regular bipartite* graph is a bipartite graph G with vertex bipartition (U, V) such that $d_G(u) = p$, $\forall u \in U$ and $d_G(v) = q$, $\forall v \in V$. As usual, let K_n, C_n and $K_{k,n-k}$ be the complete graph, cycle and complete bipartite graph with n vertices, respectively. Following [15], for nonnegative integers n, k and s satisfying $s \leq k \leq \frac{1}{2}(n + s - 2)$, define the graph $M_n^{k,s}$ with n vertices and minimum degree k as follows:

$$M_n^{k,s} = K_s \vee \big(K_{n-k-1} \cup K_{k+1-s}\big).$$

In order to characterize the exceptional graphs in our main results, we introduce several graph families in the following.

Definition 1.2 Let n, k, p, q, r be five nonnegative integers, and s be an integer.

(i) Define $\mathbb{B}_{n,k,s,r} = \left\{\overline{G_1} \vee G_2 : G_1 = (U,V) \text{ is a connected } (k-s, n-k-1)\text{-semi-regular bipartite graph with } n-s-1+r \text{ vertices and } G_2 \text{ is a spanning subgraph of } K_{s+1-r}, \text{ where } 0 \le r \le s+1 \text{ and } r \ne 1\right\}$. In particular, $\mathbb{B}_{n,k,-1,0} = \left\{M_n^{k,0}\right\} = \left\{K_{n-k-1} \cup K_{k+1}\right\}$.

(ii) Define $\mathbb{C}_{n,s,r} = \left\{\overline{G_1} \vee G_2 : G_1 \text{ is a connected } (p, n-s-1-p)\text{-semi-regular bipartite graph with } n-s-1+r \text{ vertices and } G_2 \text{ is a spanning subgraph of } K_{s+1-r}, \text{ where } 0 \le r \le s+1,\ r \ne 1 \text{ and } 1 \le p \le \frac{n-s-1}{2}\right\}$. In particular, $\mathbb{C}_{n,-1,0} = \left\{K_p \cup K_{n-p} : \text{where } 1 \le p \le \frac{n}{2}\right\}$.

(iii) Suppose that $n = 2k+1-s$ and $s \le 1$. Define $\mathbb{H}_{n,k,s,r} = \left\{G_1 \vee G_2 : G_1 \text{ is a } r\text{-regular graph with } n-k+r \text{ vertices and } G_2 \text{ is a spanning subgraph of } K_{k-r}, \text{ where } 0 \le r \le k\right\}$. In particular, $\mathbb{H}_{n,k,s,k}$ is the set of all k-regular graphs with n vertices.

(iv) Let $\mathbb{D}_{n,s,r} = \left\{\left(\overline{G_1} \vee \overline{G_2}\right) \vee G_3 : G_1 \text{ and } G_2 \text{ are two connected } \frac{n-s-1}{2}\text{-regular graphs with } |V(G_1)| + |V(G_2)| = n-r \text{ and } G_3 \text{ is a spanning subgraph of } K_r \text{ with } \mu\left(\overline{G_3}\right) \le n-s-1, \text{ where } 0 \le r \le s-1\right\}$. In particular, $\mathbb{D}_{n,1,0} = \left\{K_{\frac{n}{2},\frac{n}{2}}\right\}$.

(v) Let $\mathbb{W}_{n,s,r} = \left\{\overline{G_1} \vee G_2 : G_1 \text{ is a connected } \frac{n-s-1}{2}\text{-regular graph with } n-r \text{ vertices and } G_2 \text{ is a spanning subgraph of } K_r \text{ with } \mu\left(\overline{G_2}\right) \le n-s-1, \text{ where } 0 \le r \le \frac{n+s-1}{2}\right\}$. In particular, $\mathbb{W}_{n,-1,0}$ is the set of $\left(\frac{n}{2}-1\right)$-regular graphs.

(vi) Suppose that $n > k \ge 0$, $p \ge k+1$, and let (X, Y) be the vertex bipartition of $K_{n,p+q}$ with $|X| = n$ and $|Y| = p+q$. Let $X_1 \subset X$ be a subset with $|X_1| = n-k$, $Y_1 \subset Y$ be a subset with $|Y_1| = q \ge 1$ and $K = K_{n,p+q}[X_1 \cup Y_1]$ be the induced subgraph. Define $B_{k,n-k;p,q} = K_{n,p+q} - E(K)$. When k is understood from the context, we often write $B_{k,n-k;p,q}$ as $Z_{p,q}$ and define $Z_{p,q}^0 = Z_{p,q} - e$, where $e = uv \in E(Z_{p,q})$ satisfying $d_{Z_{p,q}}(u) = n$ and $d_{Z_{p,q}}(v) = p$. To simplify the notation in the proofs, we define

$$F_{n,k,s} = Z_{n+s-k-1,k+1-s} \text{ and } F_{n,k,s}^0 = Z_{n+s-k-1,k+1-s}^0. \tag{1.1}$$

As examples, let $L_1, L_2, \ldots, L_6$ be the six graphs depicted in Fig. 1. By setting $G_1 = K_{2,4}$ in Definition 1.2 (i)–(ii), we have $L_1 \in \mathbb{B}_{9,4,2,0} \cap \mathbb{C}_{9,2,0}$. By taking $G_1 = C_7$ in Definition 1.2 (iii), we have $L_2 \in \mathbb{H}_{9,4,0,2}$. Let $G_1 = G_2 = K_3$ and $G_3 = K_{1,2}$ in Definition 1.2 (iv), it follows that $L_3 \in \mathbb{D}_{9,4,3}$. As $\overline{L_4} = C_6 \cup K_3$, by Definition

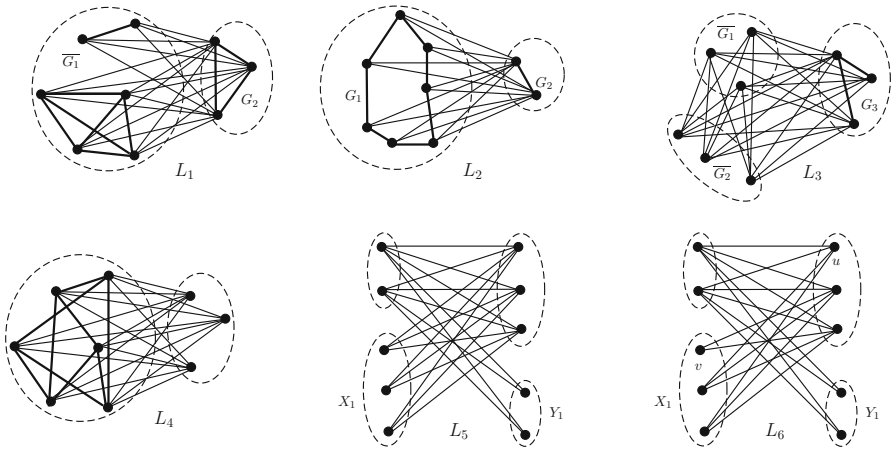


Fig. 1 The graphs $L_1, L_2, \ldots, L_6$

1.2(v), we have $L_4 \in \mathbb{W}_{9,4,3}$. Letting $n = 5$, $k = 2$ and $s = 1$ in Definition 1.2 (vi), we observe that $L_5 = B_{2,3;3,2} = Z_{3,2} = F_{5,2,1}$ and $Z^0_{3,2} = F^0_{5,2,1} = L_6$.

Following [3], we use $G = \left[U, V\right]$ to denote a bipartite graph with vertex bipartition (U, V); and G is *balanced* (respectively, *almost balanced*) if $|U| = |V|$ (respectively, if $|U| - |V| \in \{1, -1\}$). Let p and q be two nonnegative integers. A bipartite graph $G = [U, V]$ is *(p, q)-traceable* if for any subset $S \subset G$ satisfying $|S \cap U| = p$, $|S \cap V| = q$ and $|(|U| - p) - (|V| - q)| \leq 1$, $G - S$ is traceable; and $G = [U, V]$ is *(p, q)-Hamiltonian* if for any subset $S \subset G$ satisfying $|S \cap U| = p$, $|S \cap V| = q$ and $|U| - p = |V| - q$, $G - S$ is Hamiltonian.

For two graphs G and H, we write $H \subseteq G$ if H is a subgraph of G. For nonnegative integers n and k, let $\mathbb{G}_n$ be the class of graphs with n vertices, and define the *k-closure* of a graph G following [4], denoted by $\mathscr{C}_k(G)$, to be the graph obtained from G by recursively joining pairs of nonadjacent vertices whose degree sum is at least k until no such pair remains nonadjacent. By definition, $G \subseteq \mathscr{C}_k(G)$. A graphical property P is *k-stable* if for any graph $G \in \mathbb{G}_n$, G has Property P if and only if $\mathscr{C}_k(G)$ has Property P. It is worth noting that this definition of k-stable is a slightly different from that in [2].

There is also a closure concept for bipartite graphs [2]. Let $k > 0$ be an integer and $G = [U, V]$ be a bipartite graph. The *bipartite closure graph* $\mathscr{B}_k(G)$ of G is the bipartite graph obtained from G by recursively joining pairs of nonadjacent vertices u, v with $u \in U$ and $v \in V$ whose degree sum is at least k until no such pair remains nonadjacent. By definition, $G \subseteq \mathscr{B}_k(G)$.

Let $A(G)$ and $D(G)$, respectively, be the adjacency matrix and the diagonal degree matrix of G. The *signless Laplacian matrix* of G is defined to be $Q(G) = D(G) + A(G)$. The *spectral radius* of G, denoted by $\rho(G)$, is the largest eigenvalue of $A(G)$, and the *signless Laplacian spectral radius* of G, denoted by $\mu(G)$, is the largest eigenvalue of $Q(G)$. Throughout this paper, let α be a

nonnegative real number and define $\Theta(G,\alpha)$ be the largest eigenvalue of the matrix $A(G)+\alpha D(G)$. By definition, $\Theta(G,0)=\rho(G)$ and $\Theta(G,1)=\mu(G)$.

There have been lots of studies on graphical properties warranted by various kind of graph spectral conditions. Our current research is motivated by these studies, as revealed in the subsections in this section. We will have brief literature reviews on the relationship between graphical properties and the eigenvalues of the complement of a graph in Sect. 1.1, and those of balanced and almost balanced bipartite graphs in Sect. 1.2. As the properties involved are possessed by complete graphs or complete balanced bipartite graphs, and are stable under taking the corresponding Bondy–Chvátal closures, we in this paper investigate the relationship between different types of graph eigenvalues and the property when a related Bondy–Chvátal closure of the graph is a complete graph or a complete balanced bipartite graph. Our main results, as shown in Sects. 1.1 and 1.2, present unified conclusions that generalize several former results in a number of different problems.

1.1 Spectral Results of Complement Graphs on Hamiltonian Problem

There have been researches on describing the Hamiltonian properties of a graph G in terms of the eigenvalues of $\overline{G}$. The following are the related pioneer results.

Theorem 1.3 *Let G be a graph on n vertices.*

(i) (Fiedler and Nikiforov [8]) If $\rho(\overline{G})\le\sqrt{n-1}$, then G is traceable unless $G=M_n^{0,0}$.

(ii) (Fiedler and Nikiforov [8]) If $\rho(\overline{G})\le\sqrt{n-2}$, then G is Hamiltonian unless $G=M_n^{1,1}$.

(iii) (Yu and Fan [18]) If $n\ge 4$ and if $\rho(\overline{G})\le\sqrt{\frac{(n-2)^2}{n}}$, then G is Hamilton-connected.

(iv) (Li and Ning [12]) Suppose that $n\ge 2k+2$ and $\delta(G)\ge k\ge 0$. If $\rho(\overline{G})\le\rho\left(\overline{M_n^{k,0}}\right)$, then G is traceable unless $G\in\mathbb{B}_{n,k,-1,0}$ or $G\in\mathbb{H}_{n,k,-1,0}$.

(v) (Li and Ning [12]) Suppose that $n\ge 2k+1$ and $\delta(G)\ge k\ge 1$. If $\rho(\overline{G})\le\rho\left(\overline{M_n^{k,1}}\right)$, then G is Hamiltonian unless $G\in\mathbb{B}_{n,k,0,0}$ or $G\in\mathbb{H}_{n,k,0,0}$.

Extensions of some of the results stated in Theorem 1.3 have been obtained by several researchers, as seen in the theorem below.

Theorem 1.4 *Let G be a connected graph on n vertices.*

(i) (Yu et al. [20]) Suppose that $n\ge 2k+1$ and $\delta(G)\ge k\ge q+1\ge 1$. If $\rho(\overline{G})\le\sqrt{(k-q)(n-k-1)}$, then G is q-Hamiltonian and q-edge-Hamiltonian unless $G\in\mathbb{B}_{n,k,q,r}$ or $G\in\mathbb{H}_{n,k,q,r}$.

(ii) (Yu et al. [19], Chen and Zhang [5]) Suppose that $n\ge 2k$ and $\delta(G)\ge k\ge 2$. If $\rho(\overline{G})\le\sqrt{(k-1)(n-k-1)}$, then G is Hamilton-connected unless $G\in\mathbb{B}_{n,k,1,0}$ or $G\in\mathbb{H}_{n,k,1,r}$.

Analogous adjacency and signless Laplacian spectral conditions of the completeness of a graph to warrant similar or other properties have also been investigated. The following results come from Theorems 3.1, 3.4 and Corollary 3.2 of Yu et al. [20].

Theorem 1.5 (*Yu et al.* [20]) *Let G be a graph on n vertices.*

(i) Suppose that $n \geq 2k+1$, $\delta(G) \geq k \geq \max\{q-1, 1\}$ and $q \geq 1$. If $\rho(\overline{G}) \leq \sqrt{(k-q+2)(n-k-1)}$, then G is q-connected and q-edge-connected unless $G \in \mathbb{B}_{n,k,q-2,r}$ or $G \in \mathbb{H}_{n,k,q-2,r}$.

(ii) Suppose that $n \geq 2k+q+1$, $\delta(G) \geq k \geq 1$ and $q \geq 1$. If $\rho(\overline{G}) \leq \sqrt{(k+q)(n-k-1)}$, then G is q-path-coverable unless $G \in \mathbb{H}_{n,k,-q,r}$ or $G = K_{k+1} \cup K_{n-k-1}$ when $q = 1$.

Theorem 1.6 *Let G be a graph with n vertices.*

(i) (Zhou [21]) If $\mu(\overline{G}) \leq n$, then G is traceable unless $G \in \mathbb{C}_{n,-1,0}$ or $G \in \mathbb{W}_{n,-1,r}$.

(ii) (Zhou [21]) If $\mu(\overline{G}) \leq n-1$ and $n \geq 3$, then G is Hamiltonian unless $G \in \mathbb{C}_{n,0,0}$ or $G \in \mathbb{W}_{n,0,r}$, where $1 \leq r \leq \frac{n-1}{2}$.

(iii) (Yu and Fan [18]) If $\mu(\overline{G}) \leq n-2$ and $n \geq 6$, then G is Hamilton-connected unless $G \in \mathbb{C}_{n,1,0}$ or $G \in \mathbb{D}_{n,1,0}$ or $G \in \mathbb{W}_{n,1,r}$, where $1 \leq r \leq \frac{n}{2}$.

It is observed that in the theorems above, all the graphical properties warranted by the various spectral properties satisfy certain level of stability, as shown in the result of Bondy and Chvátal below.

Theorem 1.7 *Let n and q be two integers with $n \geq 3$ and $q \geq 0$. Each of the following holds for a graph on n vertices.*

(i) (Bondy and Chvátal [2]) The property that "G is q-connected" is $(n+q-2)$-stable.

(ii) (Bondy and Chvátal [2]) The property that "G is q-edge-connected" is $(n+q-2)$-stable.

(iii) (Bondy and Chvátal [2]) The property that "G is q-path-coverable" is $(n-q)$-stable.

(iv) (Bondy and Chvátal [2]) The property that "G is q-edge-Hamiltonian" is $(n+q)$-stable.

(v) (Bondy and Chvátal [2]) The property that "G is q-Hamiltonian connected" is $(n+q+1)$-stable.

(vi) (Bondy and Chvátal [2]) The property that "G is q-Hamiltonian" is $(n+q)$-stable.

(vii) (Liu et al. [15]) The property that "G is q-traceable" is $(n+q-1)$-stable.

These motivate our current study. The main result of this paper is the following.

Theorem 1.8 *Let n, k and s be three integers and let G be a graph on n vertices.*

(i) Suppose that $n \geq \max\{2k, 2k+1-s\}$ and $\delta(G) \geq k \geq \max\{s, 1\}$. If $\rho(\overline{G}) \leq \sqrt{(k-s)(n-k-1)}$, then either $\mathscr{C}_{n+s}(G) = K_n$ or $G \in \mathbb{B}_{n,k,s,r} \cup \mathbb{H}_{n,k,s,r}$, or both $s = k-1$ and $G = \overline{K_{1,k-1}} \vee \overline{K_{1,k-1}}$.

(ii) Suppose that $n \geq 3s+2$. If $\mu(\overline{G}) \leq n-s-1$, then either $\mathscr{C}_{n+s}(G) = K_n$, or $G \in \mathbb{C}_{n,s,r} \cup \mathbb{D}_{n,s,r} \cup \mathbb{W}_{n,s,r}$.

Since K_n is q-traceable for any $0 \leq q \leq n$, the corollary below follows immediately from Theorem 1.7(vii) and Theorem 1.8 with $s = q-1$.

Corollary 1.9 *Let n, k and q be three nonnegative integers and G be a graph with $|V(G)| = n$.*

(i) Suppose that $n \geq \max\{2k, 2k+2-q\}$ and $\delta(G) \geq k \geq \max\{q-1, 1\}$. If $\rho(\overline{G}) \leq \sqrt{(k+1-q)(n-k-1)}$, then G is q-traceable, unless $G \in \mathbb{B}_{n,k,q-1,r} \cup \mathbb{H}_{n,k,q-1,r}$ or both $G = \overline{K_{1,k-1}} \vee \overline{K_{1,k-1}}$ and $q = k$.

(ii) Suppose that $n \geq 3q-1$. If $\mu(\overline{G}) \leq n-q$, then G is q-traceable unless $G \in \mathbb{C}_{n,q-1,r} \cup \mathbb{D}_{n,q-1,r} \cup \mathbb{W}_{n,q-1,r}$.

As the complete graph has all the properties listed in Theorems 1.7 and 1.8 generalizes the corresponding results in Theorems 1.3, 1.4, 1.5 and 1.6, when s is taking different appropriate values. Motivated by Theorem 1.6, it is natural to consider whether the possibility that "$G \in \mathbb{W}_{n,q-1,r}$" can be removed from the statement of Corollary 1.9(ii). The following example suggests that the answer is negative.

Example 1.10 Let n and q be two integers such that $q \geq 2$, $n \geq 3q-5$ and $n+q$ is even. If G_1 is a $(q-2)$-regular graph with $\frac{n+q-2}{2}$ vertices, then $G = G_1 \vee \left(\frac{n-q+2}{2}\right)K_1$ is $\frac{n+q-2}{2}$-regular, and hence $G \in \mathbb{W}_{n,q-1,r}$. Note that any deletion of q vertices from G_1 to G results in a non-traceable graph. Thus, G is not q-traceable.

1.2 Spectral Results of Balanced Bipartite Graphs on Hamilton Problem

Researches on predicting traceable and Hamiltonian bipartite graphs by graph spectral conditions have been attracted many researchers, as seen in [9, 12, 14, 16, 17], among others. The following theorem displays some of the spectral results on Hamiltonian properties of balanced bipartite graphs.

Theorem 1.11 *Let G be a balanced bipartite graph on $2n$ vertices.*

(i) (Liu et al. [16]) If $n \geq 3$, $\delta(G) \geq 1$ and $\rho(G) \geq \sqrt{n^2-2n+3}$, then G is traceable.

(ii) (Li and Ning [13]) If $n \geq (k+2)^2$, $\delta(G) \geq k \geq 2$ and either $\rho(G) \geq \rho(F_{n,k,0})$ or $\mu(G) \geq \mu(F_{n,k,0})$, then G is traceable unless $G = F_{n,k,0}$.

(iii) (Jiang et al. [10]) If $n \geq \max\{(k+2)^2, \frac{k^2(k+1)}{2} + k + 3\}$, $\delta(G) \geq k \geq 2$ and $\rho(G) \geq \sqrt{n(n-k-1)}$, then G is traceable unless $G = F_{n,k,0}$.

(vi) (Liu et al. [16]) If $n \geq 4$, $\delta(G) \geq 2$ and $\rho(G) \geq \sqrt{n^2 - 2n + 4}$, then G is Hamiltonian unless $G = B_{2,n-2;n-2,2}$.

(v) (Li and Ning [12]) If $n \geq (k+1)^2$, $\delta(G) \geq k \geq 1$ and $\rho(G) \geq \rho\left(Z_{n-k,k}\right)$, then G is Hamiltonian unless $G = Z_{n-k,k}$.

(vi) (Ge and Ning [9]) If $n \geq k^3 + 2k + 4$, $\delta(G) \geq k \geq 1$ and $\rho(G) \geq \sqrt{n(n-k)}$, then G is Hamiltonian unless $G = Z_{n-k,k}$.

(vii) (Jiang et al. [10]) If $n \geq \max\{(k+1)^2, \frac{k^3}{2} + k + 3\}$, $\delta(G) \geq k \geq 1$ and $\rho(G) \geq \sqrt{n(n-k)}$, then G is Hamiltonian unless $G = Z_{n-k,k}$.

(viii) (Li and Ning [12]) If $n \geq (k+1)^2$, $\delta(G) \geq k \geq 1$ and $\mu(G) \geq \mu\left(Z_{n-k,k}\right)$, then G is Hamiltonian unless $G = Z_{n-k,k}$.

Our current research is also motivated by the results in Theorem 1.11. The following is a useful tool.

Theorem 1.12 (*Bondy and Chvátal* [2]) *A balanced bipartite graph G with $2n$ vertices is Hamiltonian if and only if $\mathscr{B}_{n+1}(G)$ is Hamiltonian.*

To extend results in Theorem 1.11, we need a more general form of Theorem 1.12 in our arguments, as stated in the following Proposition 1.13.

Proposition 1.13 *Let G be a balanced bipartite graph with $2n$ vertices and $q \geq 0$ be an integer,*

(i) G is (q, q)-Hamiltonian if and only if $\mathscr{B}_{n+q+1}(G)$ is (q, q)-Hamiltonian.
(ii) G is (q, q)-traceable if and only if $\mathscr{B}_{n+q+1}(G)$ is (q, q)-traceable.

The main result in this subsection is to find a unified approach as a generalization of all the former results stated in Theorem 1.11, as shown in the following theorem.

Theorem 1.14 *Let k and s be two nonnegative integers and let G be a balanced bipartite graph with $|V(G)| = 2n \geq 8k(k+1)$ and $\delta(G) \geq k \geq \max\{s, 1\}$. If either $\rho(G) \geq \rho\left(F^0_{n,k,s}\right)$ or $\mu(G) \geq \mu\left(F^0_{n,k,s}\right)$, then $\mathscr{B}_{n+s}(G) = K_{n,n}$ unless $G \in \left\{F_{n,k,s}, F^0_{n,k,s}\right\}$.*

Since $K_{n,n}$ is (q, q)-Hamiltonian for $0 \leq q \leq n-2$, from Proposition 1.13(i) and Theorem 1.14 we deduce the following result.

Corollary 1.15 *Let q and k be two nonnegative integers and let G be a balanced bipartite graph with $|V(G)| = 2n \geq 8k(k+1)$. If $\delta(G) \geq k \geq q+1$ and if either $\rho(G) \geq \rho\left(F^0_{n,k,q+1}\right)$ or $\mu(G) \geq \mu\left(F^0_{n,k,q+1}\right)$, then G is (q, q)-Hamiltonian unless $G \in \left\{F_{n,k,q+1}, F^0_{n,k,q+1}\right\}$.*

Theorem 1.16 *Let q and k be two nonnegative integers and let G be a balanced bipartite graph with $|V(G)| = 2n \geq \max\{6k(k+1), 4(k+2)^2\}$ and $\delta(G) \geq k \geq 2$. If either $\rho(G) \geq \rho(F^0_{n,k,0})$ or $\mu(G) \geq \mu(F^0_{n,k,0})$, then G is traceable unless $G \in \{F_{n,k,0}, F^0_{n,k,0}\}$.*

With Proposition 1.17 below, Corollary 1.15 and Theorem 1.16 extend Theorem 1.11 for sufficiently large n.

Proposition 1.17 *Let n, k and s be three nonnegative integers. If $n \geq \max\{\frac{1}{2}(k^2+4)(k+1), (k+1)(k-s+2)+2\}$ and $k \geq \max\{s, 1\}$, then $\rho(F^0_{n,k,s}) < \sqrt{n(n+s-k-1)}$.*

In [15], studies have been done on the relationship between Hamiltonian properties of a graph G and the value of $\Theta(G, \alpha)$, the largest eigenvalue of the matrix $A(G) + \alpha D(G)$ for a real number α. To further the studies in [15], we in this paper will show a lower bound to $\Theta(G, \alpha)$ that assures a balanced bipartite graph G to be (q, q)-traceable as well as to be (q, q)-Hamiltonian. Towards this aim, for integers k, n, s and a real number α, we define

$$\begin{aligned} \varepsilon_0(s) =& n(n+s-k-2) + (k+1)(k+2-s), \text{ and} \\ \Theta_0(s) =& \alpha\left(\frac{\varepsilon_0(s)}{n} + n\right) + (1-\alpha)\sqrt{\varepsilon_0(s)}. \end{aligned} \tag{1.2}$$

Theorem 1.18 *Let k and $s \geq -2$ be two integers and let G be a balanced bipartite graph with $|V(G)| = 2n \geq 6k+8$ and $\delta(G) \geq k \geq \max\{|s|, 1\}$. If $\Theta(G, \alpha) > \Theta_0(s)$ and $0 \leq \alpha \leq 1$, then either $\mathscr{B}_{n+s}(G) = K_{n,n}$ or $G \subseteq F_{n,k,s}$.*

As $K_{n,n}$ is (q, q)-Hamiltonian for $0 \leq q \leq n-2$, Corollary 1.19 follows immediately from Proposition 1.13(i) and Theorem 1.18.

Corollary 1.19 *Let q and k be two nonnegative integers and let G be a balanced bipartite graph with $|V(G)| = 2n \geq 6k+8$. If $\delta(G) \geq k \geq q+1$ and if both $\Theta(G, \alpha) > \Theta_0(q+1)$ and $0 \leq \alpha \leq 1$, then G is (q, q)-Hamiltonian unless $G \subseteq F_{n,k,q+1}$.*

The following theorem summarizes some of the former results using the spectral radius $\rho(G)$ or the signless Laplacian spectral radius $\mu(G)$ to study the traceability of an almost balanced bipartite graph G.

Theorem 1.20 *Let $G[U, V]$ be an almost balanced bipartite graph with $|V(G)| = 2n-1$.*

(i) (Liu et al. [16]) Suppose that $n \geq 4$, $\delta(G) \geq 1$, and for any $v \in V$, $d_G(v) \geq 2$. If $\rho(G) \geq \sqrt{n^2 - 3n + 4}$, then G is traceable unless $G \in \{B_{2,n-2;n-3,2}, B_{2,n-2;n-2,1}\}$.

(ii) (Yu et al. [19]) Suppose that $n \geq \max\left\{\frac{1}{2}(k^3+2k+4), (k+1)^2\right\}$ and $\delta(G) \geq k \geq 1$. If $\rho(G) > \sqrt{n(n-k-1)}$, then G is traceable unless $G = Z_{n-k-1,k}$.

(iii) (Yu et al. [19]) Suppose that $n \geq (k+1)^2$ and $\delta(G) \geq k \geq 1$. If $\mu(G) > 2n-k-2+\frac{(k+1)^2}{n}$, then G is traceable unless $G \subseteq Z_{n-k-1,k}$.

This also motivates our research along the same line. For a real number α, define

$$\begin{aligned}\Omega(\alpha) =& \alpha\left(2n+q-k-2+\frac{(k+1)(k+1-q)}{n}\right)\\ &+(1-\alpha)\sqrt{n(n+q-k-2)+(k+1)(k+1-q)}.\end{aligned} \tag{1.3}$$

Our main result in this direction is Theorem 1.21, which generalizes Theorem 1.20 when n is sufficiently large.

Theorem 1.21 *Let q and k be two nonnegative integers and let G be an almost balanced bipartite graph with $|V(G)| = 2n-1$ and $\delta(G) \geq k \geq q+1$.*

(i) If $n \geq 3k+4$, $0 \leq \alpha \leq 1$, and $\Theta(G,\alpha) > \Omega(\alpha)$, then G is (q, q)-traceable unless $G \subseteq Z_{n+q-k-1,k-q}$.

(ii) If $n \geq 4k(k+1)$, and if either $\rho(G) \geq \rho\left(Z^0_{n+q-k-1,k-q}\right)$ or $\mu(G) \geq \mu\left(Z^0_{n+q-k-1,k-q}\right)$, then G is (q, q)-traceable unless $G \in \left\{Z_{n+q-k-1,k-q}, Z^0_{n+q-k-1,k-q}\right\}$.

The organization of this paper is as follows. In Sect. 2, we present the proof to Theorem 1.8. Proposition 1.13 will be justified in Sect. 3. Section 4 is denoted to the verification of Theorem 1.18. Utilizing Theorem 1.18, we then present the proof of Theorem 1.14 in Sect. 5. In Sect. 6, we prove Theorem 1.16 and Proposition 1.17, and then we complete the proof of Theorem 1.21 in Sect. 7.

2 The proof of Theorem 1.8

We start with a few additional lemmas, which are needed in our arguments.

Lemma 2.1 *Let G be a graph with $|E(G)| > 0$. Each of the following holds*:

(i) (Cvetković et al. [7]) $\mu(G) \geq \min\{d(u)+d(v) : uv \in E(G)\}$. Moreover, if G is connected, then equality holds if and only if G is regular or semi-regular bipartite.

(ii) (Li and Ning [12]) $\rho(G) \geq \min\{\sqrt{d(u)d(v)} : uv \in E(G)\}$. Moreover, if G is connected, then equality holds if and only if G is regular or semi-regular bipartite.

Lemma 2.2 *Let p and q be integers with $p \geq q \geq 1$. If G is a (p, q)-semi-regular bipartite graph, then $|V(G)| \neq q + p + 1$.*

Proof By contradiction, let $G = [U, V]$ be a (p, q)-semi-regular bipartite graph with $|V(G)| = q + p + 1$. By the definition of a (p, q)-semi-regular bipartite graph, we have

$$|U| + |V| = p + q + 1,\ p|U| = q|V|,\ |U| \geq q \geq 1, \text{ and } |V| \geq p \geq 1.$$

Since the order of a (p, q)-semi-regular bipartite graph $[U, V]$ is $p + q + 1$, either $(|U|, |V|) = (q, p + 1)$ or $(|U|, |V|) = (q + 1, p)$, but, as $p > 0$ and $q > 0$, neither of the two possibilities is consistent with $p|U| = q|V|$. □

Proof of Theorem 1.8 For the sake of notational simplicity, throughout the proof, we let $H = \mathscr{C}_{n+s}(G)$. Our argument is to assume that $H \neq K_n$ to prove that in Theorem 1.8 (i), $G \in \mathbb{B}_{n,k,s,r} \cup \mathbb{H}_{n,k,s,r}$ unless $G = \overline{K_{1,k-1}} \vee \overline{K_{1,k-1}}$ and $s = k - 1 \geq 2$, and in Theorem 1.8 (ii), $G \in \mathbb{C}_{n,s,r} \cup \mathbb{D}_{n,s,r} \cup \mathbb{W}_{n,s,r}$.

Since $H \neq K_n$, $\overline{H}$ contains at least one non-trivial component. We shall let F denote a non-trivial component of $\overline{H}$. For any $u, v \in V(H)$ with $uv \notin E(H)$ and $d_H(u) \geq d_H(v)$, as $H = \mathscr{C}_{n+s}(G)$, we conclude that $d_H(u) + d_H(v) \leq n + s - 1$, and so for any edge $uv \in E(\overline{H})$,

$$d_{\overline{H}}(u) + d_{\overline{H}}(v) \geq 2(n - 1) - (n + s - 1) = n - s - 1. \tag{2.1}$$

□

Proof of Theorem 1.8 (i) Our proof of Theorem 1.8 (i) takes an approach similar to those in the justifications of Theorem 1.6(ii) in [12] and of Theorem 3.1 in [20]. Here, for the completeness of the proof, we present it in detail. By (2.1), we have

$$d_{\overline{H}}(u) d_{\overline{H}}(v) \geq d_{\overline{H}}(u)\big(n - s - 1 - d_{\overline{H}}(u)\big). \tag{2.2}$$

Since $\delta(H) \geq \delta(G) \geq k$, we have $d_{\overline{H}}(v) \leq n - k - 1$. This, together with (2.1), implies that $d_{\overline{H}}(v) \geq d_{\overline{H}}(u) \geq n - s - 1 - d_{\overline{H}}(v) \geq k - s$. Hence for each $uv \in E(\overline{H})$, we have

$$k - s \leq d_{\overline{H}}(u) \leq d_{\overline{H}}(v) \leq n - k - 1.$$

Let $\Phi(x) = x(n - s - 1 - x)$ with $k - s \leq x \leq n - k - 1$. The concavity of quadratic functions implies that

$$\Phi(x) \geq \min\big\{\Phi(k - s), \Phi(n - k - 1)\big\} = (k - s)(n - k - 1). \tag{2.3}$$

By Lemma 2.1(ii), and by (2.2) and (2.3), we have

$$\begin{aligned}\sqrt{(k - s)(n - k - 1)} &\leq \min\Big\{\sqrt{d_{\overline{H}}(u) d_{\overline{H}}(v)} : uv \in E(F)\Big\} \\ &\leq \rho(\overline{H}) \leq \rho(\overline{G}) \leq \sqrt{(k - s)(n - k - 1)}.\end{aligned}$$

Claim 1 below follows from Lemma 2.1(ii). □

Claim 1 For any nontrivial component F of $\overline{H}$, each of the following holds.

(i) F is either regular or semi-regular bipartite.
(ii) For any edge $uv \in E(F)$, we have $d_{\overline{H}}(u) = k - s \le n - k - 1 = d_{\overline{H}}(v)$.
(iii) $n - k \le |V(F)| \le n$.

We shall complete the proof of Theorem 1.8(i) by examining the following two cases.

Case 1. $\overline{H}$ contains at least two non-trivial components.

Let F_1 and F_2 be two non-trivial components of $\overline{H}$. By Claim 1, each of F_1 and F_2 is either regular or semi-regular bipartite, and for any edge $uv \in E(\overline{H})$, $d_{\overline{H}}(u) = k - s \le n - k - 1 = d_{\overline{H}}(v)$. By Claim 1 (iii), we have $2(n-k) \le n$, and so $2k \le \max\{2k+1-s, 2k\} \le n \le 2k$. Thus $n = 2k$, $s \ge 1$ and $\overline{H}$ must have exactly two non-trivial components F_1 and F_2 with $|V(F_1)| = |V(F_2)| = k$. Pick an $F_i \in \{F_1, F_2\}$.

If F_i is regular, then $k - s = n - k - 1 = k - 1$, and so $s = 1$. As $|V(F_1)| = |V(F_2)| = k$ and by Claim 1(ii), $F_1 = F_2 = K_k$. Since $\rho(\overline{G}) = \rho(\overline{H}) = k - 1$ and $\overline{H} \subseteq \overline{G}$, we have $\overline{G} = K_k \cup K_k$, and so $G \in \mathbb{H}_{n,k,1,0}$.

If F_i is semi-regular bipartite, then $d_{\overline{H}}(v) = n - k - 1 = k - 1 = |V(F_i)| - 1$, and so $F_i = K_{1,k-1}$ and $1 = d_{\overline{H}}(u) = k - s$. As $s = k - 1$ and by Claim 1(ii), it follows that $F_1 = F_2 = K_{1,k-1}$. Since $\rho(\overline{G}) = \rho(\overline{H}) = \sqrt{k-1}$ and $\overline{H} \subseteq \overline{G}$, we have $\overline{G} = K_{1,k-1} \cup K_{1,k-1}$, and so $G = \overline{K_{1,k-1}} \vee \overline{K_{1,k-1}}$, as desired.

Case 2. $\overline{H}$ contains only one non-trivial component.

Let F denote this only nontrivial component of $\overline{H}$. By Claim 1(i), F is a regular or semi-regular bipartite graph. Assume first that F is a semi-regular bipartite graph. By Claim 1(ii), F is a connected $(n-k-1, k-s)$-semi-regular bipartite graph, and so for some integer r with $0 \le r \le k$, $|V(F)| = n - s - 1 + r$. It follows that $\overline{H} = F \cup (s+1-r)K_1$. Since $\rho(\overline{H}) = \rho(\overline{G})$ and $\overline{H}$ is a spanning subgraph of $\overline{G}$, we have $F \cup (s+1-r)K_1 \subseteq \overline{G} \subseteq F \cup K_{s+1-r}$, and so $\overline{F} \vee (s+1-r)K_1 \subseteq G \subseteq \overline{F} \vee K_{s+1-r}$. By Lemma 2.2, this implies that $G \in \mathbb{B}_{n,k,s,r}$.

Hence we may assume that F is regular. By Claim 1 (ii), $k - s = n - k - 1$ and so $2k + 1 - s = n \ge 2k$, implying $s \le 1$. By Claim 1 (iii), we conclude that $|V(F)| = n - k + r$, for some integer r with $0 \le r \le k$. It follows that $\overline{H} = F \cup (k-r)K_1$. As $\rho(\overline{H}) = \rho(\overline{G})$ and $\overline{H}$ is a spanning subgraph of $\overline{G}$, we have $F \cup (k-r)K_1 \subseteq \overline{G} \subseteq F \cup K_{k-r}$, and so $\overline{F} \vee (k-r)K_1 \subseteq G \subseteq \overline{F} \vee K_{k-r}$. Since $\overline{F}$ is a r-regular graph with $|V(\overline{F})| = n + r - k$, by Definition 1.2(ii), $G \in \mathbb{H}_{n,k,s,r}$.

This completes the proof of Theorem 1.8 (i). □

Proof of Theorem 1.8 (ii) By (2.1) and Lemma 2.1(i), we conclude that, for each nontrivial component F of $\overline{H}$, $n - s - 1 \le \mu(F) \le \mu(\overline{H}) \le \mu(\overline{G}) \le n - s - 1$, F is either a regular or a semi-regular bipartite graph, and for any $uv \in E(\overline{H})$,

$$\mu(F) = \mu(\overline{H}) = \mu(\overline{G}) = d_{\overline{H}}(u) + d_{\overline{H}}(v) = n - s - 1. \quad (2.4)$$

Similar to the proof of Theorem 1.8 (i), we justify Theorem 1.8 (ii) by a case analysis. □

Claim 2 If $\overline{H}$ has a semi-regular bipartite component, then $\overline{H}$ has exactly one nontrivial component.

Assume that F is a semi-regular bipartite component of $\overline{H}$. By (2.4), $|V(F)| \geq n - s - 1$. If $\overline{H} - V(F)$ contains a nontrivial component F', then by (2.4), $|V(F')| \geq \frac{1}{2}(n - s + 1)$. It follows from $n - s - 1 + \frac{n-s+1}{2} \leq n$ that $n \leq 3s + 1$, contrary to the assumption that $n \geq 3s + 2$. Hence F is the unique non-trivial component of $\overline{H}$. This validates the claim.

Case 1. $\overline{H}$ has a semi-regular bipartite component.

We assume that F is a semi-regular bipartite component of $\overline{H}$. By Claim 2, F is the only nontrivial component of $\overline{H}$. We may assume that F is a connected (p, q)-semi-regular graph with $1 \leq p \leq q$, and for some integer r with $0 \leq r \leq s + 1$, $|V(F)| = n - s - 1 + r$. Thus $s \geq -1$, $\overline{H} = F \cup (s + 1 - r)K_1$, and $1 \leq p \leq \frac{1}{2}(n - s - 1)$ by (2.4).

Since $\mu(\overline{G}) = \mu(\overline{H})$ and $\overline{H}$ is a spanning subgraph of $\overline{G}$, we have $F \cup (s + 1 - r)K_1 \subseteq \overline{G} \subseteq F \cup K_{s+1-r}$, and so $\overline{F} \vee (s + 1 - r)K_1 \subseteq G \subseteq \overline{F} \vee K_{s+1-r}$. By Lemma 2.2, we conclude that $G \in \mathbb{C}_{n,s,r}$. This proves Theorem 1.8 (ii) if Case 1 occurs.

Case 2. $\overline{H}$ does not have a semi-regular bipartite component.

By Lemma 2.1(i) and the assumption of Case 2, every non-trivial component of $\overline{H}$ is regular. Let F denote a component of $\overline{H}$. Then for any vertex $u \in V(F)$, by (2.4), $d_{\overline{H}}(u) = \frac{1}{2}(n - s - 1)$, and so $|V(F)| \geq \frac{1}{2}(n - s + 1)$.

If $\overline{H}$ contains at least three non-trivial components, then $\frac{3(n-s+1)}{2} \leq n$, implying $n \leq 3(s - 1)$, contrary to the assumption that $n \geq 3s + 2$. Hence $\overline{H}$ contains at most two nontrivial components. Let F' denote the possible nontrivial component of $\overline{H} - V(F)$, if it exists.

We first suppose that H is regular, and so $\overline{H}$ is $\frac{1}{2}(n - s - 1)$-regular. In this case, either $\overline{H} = F$ or $\overline{H} = F \cup F'$, where F and F' are both connected $\frac{1}{2}(n - s - 1)$-regular. Since $\overline{H} \subseteq \overline{G}$ and $\mu(\overline{G}) = \mu(\overline{H})$, it follows that $\overline{H} = \overline{G}$, and so $G = H \in \mathbb{W}_{n,s,0}$ for $\overline{H} = F$ or $G = H \in \mathbb{D}_{n,s,0}$ for $\overline{H} = F \cup F'$.

Hence we may assume that H is not regular, and so $\overline{H} \neq F$. Assume first that F and F' are two nontrivial components of $\overline{H}$ containing $\frac{1}{2}(n - s + 1) + r_1$ and $\frac{1}{2}(n - s + 1) + r_2$ vertices, respectively. Thus $\overline{H} = F \cup F' \cup (s - 1 - r_1 - r_2)K_1$. Since $\mu(\overline{G}) = \mu(\overline{H})$ and since $\overline{H}$ is a spanning subgraph of $\overline{G}$, we conclude that $\overline{F} \vee \left(\overline{F'} \vee (s - 1 - r_1 - r_2)K_1\right) \subseteq G \subseteq \overline{F} \vee \left(\overline{F'} \vee K_{s-1-r_1-r_2}\right)$, and so $G \in \mathbb{D}_{n,s,r}$, where $1 \leq r \leq s - 1$.

Therefore, we may assume that F is the only non-trivial component of $\overline{H}$, and so $\overline{H} = F \cup rK_1$, where $r = |V(G) \backslash V(F)|$. Since F is $\frac{1}{2}(n - s - 1)$-regular, we have $\frac{1}{2}(n - s + 1) \leq |V(F)| \leq n - 1$. Since $\mu(\overline{G}) = \mu(\overline{H})$ and since $\overline{H}$ is a spanning

subgraph of $\overline{G}$, it follows that $F \cup rK_1 \subseteq \overline{G} \subseteq F \cup K_r$, and so $\overline{F} \vee rK_1 \subseteq G \subseteq \overline{F} \vee K_r$. This implies that $G \in \mathbb{W}_{n,s,r}$, where $1 \leq r \leq \frac{1}{2}(n+s-1)$. □

3 The Proof of Proposition 1.13

The following result initiated the study of the Bondy–Chvátal closure concept for balanced bipartite graphs.

Lemma 3.1 (*Lemma* 7.3.5 *of* [1]) *Let $G = [U, V]$ be a balanced bipartite graph with $2n$ vertices. Let $u \in U$ and $v \in V$ be two non-adjacent vertices with $d_G(u) + d_G(v) \geq n + 1$. Then G is Hamiltonian if and only if $G + uv$ is Hamiltonian.*

To prove Proposition 1.13, it suffices to prove the following two lemmas.

Lemma 3.2 *Let $G = [U, V]$ be a balanced bipartite graph with $2n$ vertices and q be a nonnegative integer. Let $w_1 \in U$ and $w_2 \in V$ be two vertices satisfying $w_1w_2 \notin E(G)$ and $d_G(w_1) + d_G(w_2) \geq n + q + 1$. Then the following are equivalent.*

(i) G is (q, q)-Hamiltonian.
(ii) $G' = G + w_1w_2$ is (q, q)-Hamiltonian.

Proof As (i) implies (ii) by definition, it remains to show that (ii) implies (i). Let $S \subset V(G)$ satisfying $|S \cap U| = |S \cap V| = q$ and $G_1 = G\big[V(G)\backslash S\big]$. We are to show that G_1 has a Hamilton cycle.

Since G' is (q, q)-Hamiltonian, $G'\big[V(G)\backslash S\big]$ contains a Hamilton cycle C. If C is not a Hamilton cycle of G_1, then $w_1w_2 \in E(C)$, and so this Hamilton cycle C can be expressed as $C = w_1w_2 \ldots w_{2n-2q}w_1$. Since $w_1 \in U$ and $w_2 \in V$, we observe that $|N_S(w_1)| + |N_S(w_2)| \leq |S| = 2q$. As $d_G(w_1) + d_G(w_2) \geq n + q + 1$, we have $d_{G_1}(w_1) + d_{G_1}(w_2) \geq n - q + 1$.

Note that G_1 is a balanced bipartite graph with $2(n - q)$ vertices. By Lemma 3.1, G_1 is Hamiltonian if and only if $G_1 + w_1w_2$ is Hamiltonian. □

Lemma 3.3 *Let $G = [U, V]$ be a balanced bipartite graph with $2n$ vertices and q be a nonnegative integer. Let $w_1 \in U$ and $w_2 \in V$ be two vertices satisfying $w_1w_2 \notin E(G)$ and $d_G(w_1) + d_G(w_2) \geq n + q + 1$. Then the following are equivalent.*

(i) G is (q, q)-traceable.
(ii) $G' = G + w_1w_2$ is (q, q)-traceable.

Proof By definition, we observe that (i) implies (ii), and so it suffices to show that (ii) implies (i). Let $S \subset V(G)$ satisfying $|S \cap U| = |S \cap V| = q$ and $G_1 = G\big[V(G)\backslash S\big]$. We are to show that G_1 has a Hamilton path. Since G' is (q, q)-traceable, $G_1 + w_1w_2$ contains a Hamilton path P.

If P is not a Hamilton path of G_1, then $w_1w_2 \in E(P)$. We suppose that $P = u_1u_2 \cdots u_{2n-2q}$, where $w_1 = u_i$ and $w_2 = u_{i+1}$. As $G'[U, V]$ is bipartite with

$u_i \in U$ and $u_{i+1} \in V$, we observe that $|N_S(u_i)| + |N_S(u_{i+1})| \le |S| = 2q$. By the assumption that $d_G(u_i) + d_G(u_{i+1}) \ge n + q + 1$, we conclude that

$$d_{G_1}(u_i) + d_{G_1}(u_{i+1}) \ge n - q + 1. \tag{3.1}$$

Case 1. $u_1 \in U$.

Then, as $u_i \in U$, i is odd. If $u_i u_{2n-2q} \in E(G)$, then $P - \{u_i u_{i+1}\} + \{u_i u_{2n-2q}\}$ is a Hamilton path of G_1. Hence we may assume that $u_i u_{i+1}, u_i u_{2n-2q} \notin E(G)$. Similarly, we have $u_{i+1} u_1 \notin E(G)$.

Claim 1. There is an index j with either $i + 3 \le j \le 2n - 2q - 2$ or $2 \le j \le i - 3$, such that $u_i u_j$, $u_{i+1} u_{j+1} \in E(G_1)$.

Since G is bipartite, we may suppose that $N_{G_1}(u_i) = \{u_{s_1}, u_{s_2}, \ldots, u_{s_p}\}$, where $2n - 2q \notin \{s_1, s_2, \ldots, s_p\} = \emptyset$ and for $t \in \{1, 2, \ldots, p\}$, s_t is even. If Claim 1 fails, then $N_{G_1}(u_{i+1}) \subseteq \{u_1, u_3, u_5, \ldots, u_{2n-2q-1}\} \setminus \{u_{s_1+1}, u_{s_2+1}, \ldots, u_{s_p+1}\}$. Thus, $d_{G_1}(u_{i+1}) \le n - q - p$ and so by (3.1), $n - q + 1 \le d_{G_1}(u_i) + d_{G_1}(u_{i+1}) \le p + (n - q - p) = n - q$, a contradiction. This completes the proof of Claim 1.

By Claim 1, either for some j with $2 \le j \le i - 3$, both $u_i u_j \in E(G_1)$ and $u_{i+1} u_{j+1} \in E(G_1)$, whence $u_1 u_2 \ldots u_j u_i u_{i-1} \ldots u_{j+1} u_{i+1} u_{i+2} \cdots u_{2n-2q}$ is a Hamiltonian path of $G[V(G) \setminus S]$; or for some j with $i + 3 \le j \le 2n - 2q - 2$, both $u_i u_j \in E(G_1)$ and $u_{i+1} u_{j+1} \in E(G_1)$, whence $u_1 u_2 \ldots u_i u_j u_{j-1} \ldots u_{i+1} u_{j+1} u_{j+2} \ldots u_{2n-2q}$ is a Hamiltonian path of $G[V(G) \setminus S]$. This proves that Lemma 3.3 (ii) implies Lemma3.3 (i) in this case.

Case 2. $u_1 \in V$.

As $u_i \in U$, i is even. We first justify the following claim.

Claim 2. There is an index j with either $i + 3 \le j \le 2n - 2q - 1$ or $1 \le j \le i - 3$, such that $u_i u_j$ and $u_{i+1} u_{j+1} \in E(G_1)$.

Since G is bipartite, we may suppose that $N_{G_1}(u_i) = \{u_{s_1}, u_{s_2}, \ldots, u_{s_p}\}$, where s_t is odd for $t \in \{1, 2, \ldots, p\}$. If Claim 1 fails, then $N_{G_1}(u_{i+1}) \subseteq \{u_2, u_4, u_6, \ldots, u_{2n-2q}\} \setminus \{u_{s_1+1}, u_{s_2+1}, \ldots, u_{s_p+1}\}$. Thus, by (3.1), $n - q + 1 \le d_{G_1}(u_i) + d_{G_1}(u_{i+1}) \le p + (n - q - p) = n - q$, a contradiction. This completes the proof of Claim 2.

By Claim 2, either for some j with $1 \le j \le i - 3$, both $u_i u_j \in E(G_1)$ and $u_{i+1} u_{j+1} \in E(G_1)$, whence $u_1 u_2 \ldots u_j u_i u_{i-1} \ldots u_{j+1} u_{i+1} u_{i+2} \cdots u_{2n-2q}$ is a Hamiltonian path of $G[V(G) \setminus S]$; or for some j with $i + 3 \le j \le 2n - 2q - 1$, both $u_i u_j \in E(G_1)$ and $u_{i+1} u_{j+1} \in E(G_1)$, whence $u_1 u_2 \ldots u_i u_j u_{j-1} \ldots u_{i+1} u_{j+1} u_{j+2} \ldots u_{2n-2q}$ is a Hamiltonian path of $G[V(G) \setminus S]$. Thus in any case, Lemma3.3 holds always. □

4 The Proof of Theorem 1.18

Following the notation in [3], if A, B are disjoint subsets of $V(G)$, then define $E_G[A, B] = \{xy \in E(G) : x \in A \text{ and } y \in B\}$ and $e_G(A, B) = |E_G[A, B]|$. The functions $\varepsilon_0(s)$ and $\Theta_0(s)$, defined in (1.2), will be used in the arguments in this section.

Throughout this section, let k, n and s be integers, and unless otherwise stated, we always assume that $G = [U, V]$ is a balanced bipartite graph with $|V(G)| = 2n$ and $H = \mathscr{B}_{n+s}(G)$. By definition, we have

$$\begin{aligned} &\delta(H) \geq \delta(G),\ |E(H)| \geq |E(G)|, \\ &\quad \text{and } \forall u \in U,\ v \in V \text{ with } uv \notin E(H),\ d_H(u) + d_H(v) \leq n + s - 1. \end{aligned} \tag{4.1}$$

Lemma 4.1 *If $n \geq 3k + 4$, $s \geq -2$, $\delta(G) \geq k \geq \max\{|s|, 1\}$, and $|E(G)| > \varepsilon_0(s)$, then $\mathscr{B}_{n+s}(G) = K_{n,n}$ unless $K_{n,n+s-k-1} \subseteq \mathscr{B}_{n+s}(G)$.*

Proof We assume that $H \neq K_{n,n}$ to prove that $K_{n,n+s-k-1}$ must be a subgraph of H. Define

$$\begin{aligned} U_0 &= \Big\{w \in U : d_G(w) \geq \frac{1}{2}(n+s)\Big\}, n_U = |U_0|, \\ V_0 &= \Big\{w \in V : d_G(w) \geq \frac{1}{2}(n+s)\Big\} \text{ and } n_V = |V_0|. \end{aligned}$$

Claim 1. $n_U \geq k + s + 3$ and $n_V \geq k + s + 3$.

By symmetry, it suffices to prove $n_U \geq k + s + 3$. Direct counting yields that

$$\begin{aligned} |E(G)| \leq |E(H)| &= \sum_{v \in U} d_H(v) = \sum_{v \in U_0} d_H(v) \\ &\quad + \sum_{v \in U - U_0} d_H(v) \leq n n_U + \frac{1}{2}(n + s - 1)(n - n_U). \end{aligned} \tag{4.2}$$

It follows by (4.2) and by $|E(G)| > \varepsilon_0(s)$ that

$$\begin{aligned} n_U &\geq \frac{2|E(G)|}{n+1-s} - \frac{n(n+s-1)}{n+1-s} \\ &> \frac{2n(n+s-k-2) + 2(k+1)(k+2-s) - n(n+s-1)}{n+1-s} \\ &= \frac{n^2 - (2k+3-s)n + 2(k+1)(k-s+2)}{n+1-s} \\ &= k + s + 2 + \frac{\Phi(n)}{n+1-s}, \end{aligned} \tag{4.3}$$

where $\Phi(n) = n^2 - (2k+3-s)n + 2(k+1)(k-s+2) - (n+1-s)(k+s+2) = n^2 - (3k+5)n + 2k^2 - ks + 5k + s^2 - s + 2$.

Since $n \geq 3k + 4$, we have $\Phi'(n) = 2n - (3k+5) > 0$, and so $\Phi(n) \geq \Phi\big(3k+4\big) = k(2k-s) + 2(k-1) + s(s-1) > 0$. It follows by (4.3) that Claim 1 holds.

Let p_0 and q_0 be two positive integers such that $p_0 \geq q_0$ and $p_0 + q_0 = \max\{p + q, \text{ where } K_{p,q} \subseteq H\}$. By Claim 1, we may assume that $p_0 \geq q_0 \geq k + s + 3$. Let $U' \subseteq U$ and $V' \subseteq V$ such that $H\big[U' \cup V'\big] = K_{p_0,q_0}$ with $|U'| = p_0$ and $|V'| = q_0$. For any $v \in V \backslash V'$, if v will be adjacent with every vertex of U', then a violation to the maximality of $p_0 + q_0$ occurs. Hence v is not adjacent to

at least one vertex in U'. By the definition of the $(n+s)$-closure of G and by symmetry, we have

$$\forall v \in V\backslash V',\ d_H(v) \le n+s-q_0-1 \text{ and } \forall u \in U\backslash U',\ d_H(u) \le n+s-p_0-1. \tag{4.4}$$

Claim 2. $q_0 \ge n+s-k-2$.

Assume that Claim 2 does not hold. Then $k+s+3 \le q_0 \le n+s-k-3$. Define $\Phi_1(x) = x^2-(n+s-1)x+n(n+s-1)$. Since H is bipartite, and by (4.4), we have

$$\begin{aligned}|E(H)| &= \sum_{v\in V} d_H(v) = \sum_{v\in V'} d_H(v) + \sum_{v\in V-V'} d_H(v)\\ &\le nq_0 + \big(n-q_0\big)\big(n+s-q_0-1\big)\\ &= q_0^2-(n+s-1)q_0+n(n+s-1) = \Phi_1(q_0).\end{aligned}$$

As $k+s+3 \le q_0 \le n+s-k-3$, we have

$$\Phi_1(q_0) \le \max\Big\{\Phi_1\big(k+s+3\big),\ \Phi_1\big(n+s-k-3\big)\Big\}.$$

Since $n \ge 3k+4$, we have both $\varepsilon_0(s)-\Phi_1\big(n+s-k-3\big) = n-(2k-s+4) \ge k+s \ge 0$, and $\varepsilon_0(s)-\Phi_1\big(k+s+3\big) = (s+2)(n-2k-5) \ge 0$. Thus, $\varepsilon_0(s) < |E(G)| \le |E(H)| \le \Phi_1(q_0) \le \varepsilon_0(s)$, a contradiction. This completes the proof of Claim 2.

Claim 3. $p_0+q_0 \ge 2n+s-k-1$.

Assume that Claim 3 fails, and so $p_0+q_0 \le 2n+s-k-2$. By Claim 2, we have $p_0 \ge q_0 \ge n+s-k-2$. By (4.4),

$$\begin{aligned}|E(H)| &\le e_H\big(U',\ V'\big) + e_H\big(U\backslash U',\ V\big) + e_H\big(U,\ V\backslash V'\big)\\ &\le p_0q_0 + (n+s-1-p_0)(n-p_0) + (n+s-1-q_0)(n-q_0).\end{aligned} \tag{4.5}$$

If $p_0 \ge n+s-k$, then as $\delta(G) \ge k$, it follows from the definition of the $(n+s)$-closure of G that each vertex of V' must be adjacent to every vertex of U, and so $p_0 = n$ and $q_0 = n+s-k-2$. It follows by (4.5) that $\varepsilon_0(s) < |E(G)| \le |E(H)| \le n(n+s-k-2)+(k+1)(k+2-s) = \varepsilon_0(s)$, a contradiction. Hence we may assume that $n+s-k-2 \le q_0 \le p_0 \le n+s-k-1$.

If $p_0 = q_0 = n+s-k-1$, then by (4.5) we have $|E(H)| \le (n+s-k-1)^2 + 2k(k+1-s)$. As $n \ge 3k+4$, this leads to

$$\begin{aligned}&\varepsilon_0(s) - |E(H)|\\ &\ge \varepsilon_0(s) - \big((n+s-k-1)^2 + 2k(k+1-s)\big)\\ &= (k-s)(n+s-2k-1)+1 \ge (k-s)((3k+4)+s-2k-1)+1\\ &= (k-s)(k+s+3)+1 > 0.\end{aligned}$$

Hence $|E(G)| \le |E(H)| < \varepsilon_0(s)$, contrary to the assumption of the lemma.

If $p_0 = n+s-k-1$ and $q_0 = n+s-k-2$, then by (4.5) and $n \ge 3k+4$ we

have $|E(G)| \le (n+s-k-1)(n+s-k-2)+k(k+1-s)+(k+1)(k+2-s) < \varepsilon_0(s)$, again a contradiction.

If $p_0 = n+s-k-2 = q_0$, then by (4.5) and $n \ge 3k+4$ we have $|E(G)| \le (n+s-k-2)^2 + 2(k+1)(k+2-s) < \varepsilon_0(s)$, contrary to the assumption of the lemma, and so Claim 3 is justified.

If $p_0 = n$, then the lemma follows from Claim 3. Assume that $p_0 \le n-1$, and so $q_0 \ge n+s-k$ by Claim 3. As $\delta(G) \ge k$, we conclude that every vertex of U' must be adjacent to all vertices of V, implying that $p_0 \ge q_0 = n$, contrary to the assumption that $H \ne K_{n,n}$. □

Theorem 4.2 *If $n \ge 3k+4$, $s \ge -2$, $\delta(G) \ge k \ge \max\{|s|, 1\}$ and $|E(G)| > \varepsilon_0(s)$, then $\mathscr{B}_{n+s}(G)$ is isomorphic to a member in $\{K_{n,n}, F_{n,k,s}\}$.*

Proof We assume that $H \ne K_{n,n}$ to show that $H = F_{n,k,s}$. Let t be the largest integer such that $K_{n,t} \subseteq H$. By Lemma 4.1, $n+s-k-1 \le t < n$. Let $V' \subset V$ be the vertex sets of H such that $H[U \cup V'] = K_{n,t}$. If $t \ge n+s-k$, since every vertex in U has degree at least $t \ge n+s-k$ in H and $\delta(H) \ge k$, we have $H = K_{n,n}$, contrary to the assumption. Hence we must have $t = n+s-k-1$.

Define $U_0 = \{u \in U : d_H(u) \ge n+s-k\}$. Since $\delta(H) \ge k$ and since every vertex in U has degree at least $n+s-k-1$ in H, it follows from the definition of the $(n+s)$-closure of G that every vertex in $V \backslash V'$ has degree exactly k in H, and is adjacent to every vertex in U_0. This implies that $|U_0| = k$, and so $H = F_{n,k,s}$. □

We need the following two lemmas to complete the proof of Theorem 1.18.

Lemma 4.3 (*Li and Ning* [12]) *If G is a balanced bipartite graph with $|V(G)| = 2n$, then $\mu(G) \le \frac{|E(G)|}{n} + n$.*

When $|V(G)| \ge 2$, let $\rho_1(G)$ and $\rho_2(G)$ denote the largest and the second largest eigenvalues of $A(G)$, respectively. Thus, $\rho_1(G) = \rho(G)$.

Lemma 4.4 (*Lai et al.* [11]) *If G is a bipartite graph with $|V(G)| \ge 2$, then $(\rho_1(G))^2 + (\rho_2(G))^2 \le |E(G)|$.*

When $0 \le \alpha \le 1$, since $A(G) + \alpha D(G) = \alpha Q(G) + (1-\alpha)A(G)$, from the properties of Rayleigh quotients we have $\Theta(G,\alpha) \le \alpha\mu(G) + (1-\alpha)\rho(G)$. Thus, the corollary below follows immediately from Lemmas 4.3 and 4.4.

Corollary 4.5 *Let α be a real number with $0 \le \alpha \le 1$. If $|V(G)| = 2n \ge 2$, then*

$$\Theta(G,\alpha) \le \alpha\mu(G) + (1-\alpha)\rho(G) \le \alpha\left(\frac{|E(G)|}{n} + n\right) + (1-\alpha)\sqrt{|E(G)|}. \quad (4.6)$$

Recall that $\Theta_0(s)$ and $\varepsilon_0(s)$ have been defined in (1.2). If $|E(G)| \le \varepsilon_0(s)$, then Corollary 4.5 implies that $\Theta(G,\alpha) \le \Theta_0(s)$. This deduces the following result.

Corollary 4.6 *Let α be a real number with $0 \le \alpha \le 1$. If $|V(G)| = 2n \ge 2$ and $\Theta(G,\alpha) > \Theta_0(s)$, then $|E(G)| > \varepsilon_0(s)$.*

Proof of Theorem 1.18 In our hypotheses, $\Theta(G,\alpha) > \Theta_0(s)$, hence, Theorem 4.2 and Corollary 4.6 imply that $\mathscr{B}_{n+s}(G)$ is isomorphic to a member in $\{F_{n,k,s}, K_{n,n}\}$. □

5 The Proof of Theorem 1.14

Given two distinct vertices u, v in a graph G, if $N_G(v)\backslash\big(N_G(u)\cup\{u\}\big) \neq \emptyset \neq N_G(u)\backslash\big(N_G(v)\cup\{v\}\big)$, then we construct a new graph $G' = G'(u,v)$ by replacing all edges vw by uw for each $w \in N_G(v)\backslash\big(N_G(u)\cup\{u\}\big)$. This operation is called the *Kelmans transformation* from v to u (see [6]).

Lemma 5.1 (*Liu et al.* [15]) *Let G be a connected graph. If G' is a graph obtained from G by some Kelmans transformation and $\alpha \geq 0$, then $\Theta(G',\alpha) > \Theta(G,\alpha)$.*

In the discussion of Lemma 5.2 below, the notation in Definition 1.2 (vi) will be adopted.

Lemma 5.2 *Let G be a graph obtained from $Z_{p,q}$ by deleting one edge. If $p \geq k+1$, $q \geq 1$, $\alpha \geq 0$ and $\delta(G) \geq k \geq 1$, then $\Theta(G,\alpha) \leq \Theta\left(Z^0_{p,q},\alpha\right)$, with equality if and only if $G = Z^0_{p,q}$.*

Proof Let $G' = Z_{p,q}$ and $G_0 = Z^0_{p,q}$. Let $e = w_0z_0 \in E(G')$, and $G = G' - e$. It suffices to show that if $G \neq G_0$, then

$$\Theta(G,\alpha) < \Theta(G_0,\alpha). \tag{5.1}$$

Let U and V be the bipartition of G' such that V contains q vertices of degree k and U contains k vertices of degree $p+q$ in G'. Let U' and V' be the vertices of degrees $p+q$ and n, respectively, in U and V of G'. Since every vertex of $V\backslash V'$ has degree k and since $G \neq G_0$, by symmetry, we may assume that $w_0 \in U'$ and $z_0 \in V'$.

Choose $v \in U\backslash U'$. Then, $N_G(v)\backslash\big(N_G(w_0)\cup\{w_0\}\big) = \{z_0\}$ and $N_G(w_0)\backslash\big(N_G(v)\cup\{v\}\big) \neq \emptyset$. It is routine to verify that G_0 is isomorphic to the graph obtained from G by a Kelmans transformation from v to w_0. By Lemma 5.1, $\Theta(G,\alpha) < \Theta(G_0,\alpha)$, and so (5.1) holds. □

Let G be a connected graph. For any real number $\alpha \geq 0$, it is well known that $A(G)$ is nonnegative and irreducible if and only if G is connected, and thus $A(G) + \alpha D(G)$ is a nonnegative irreducible matrix. This implies the existence of a unique positive unit eigenvector $f = \big(f(v_1), f(v_2), \ldots, f(v_n)\big)^T$ corresponding to $\Theta(G,\alpha)$. This vector f is often called the *Perron vector* of G.

Lemma 5.3 *For any integers n, q and a real number α, define a polynomial in θ as follows:*

$$\begin{aligned}\Psi(\theta) =&\theta^4 - 2(n+q-1)\alpha\theta^3 + \Big(\alpha^2\big(n^2+4nq-3n+q^2-3q+1\big) - nq + 1\Big)\theta^2\\ &- \alpha\Big(\alpha^2(2nq-q-n)(n+q-1) - nq(n+q-2)\Big)\theta\\ &+ \big(\alpha^2-1\big)(n-1)(q-1)\big(nq\alpha^2-1\big).\end{aligned}$$

If $2 \le q \le n$ and $\alpha \ge 0$, then $\Theta(K_{n,q} - e, \alpha)$ is the maximum root of $\Psi(\theta)$.

Proof Denote $G = K_{n,q} - e$ and $\Theta = \Theta(K_{n,q} - e, \alpha)$. Let f be the Perron vector of G, and let U and V be the two partite sets of G such that $|U| = n$ and $|V| = q$. For convenience, we suppose that $e = w_0z_0$ with $w_0 \in U$ and $z_0 \in V$.

Let $x_1 = f(w)$ for $w \in U\backslash\{w_0\}$, let $x_2 = f(w)$ for $w \in V\backslash\{z_0\}$, let $x_3 = f(w_0)$ and $x_4 = f(z_0)$. it follows from $\big(A(G) + \alpha D(G)\big)f = \Theta f$ that

$$\begin{cases}\big(\Theta - q\alpha\big)\,x_1 = (q-1)x_2 + x_4,\\ \big(\Theta - n\alpha\big)\,x_2 = (n-1)x_1 + x_3,\\ \big(\Theta - (q-1)\alpha\big)\,x_3 = (q-1)x_2,\\ \big(\Theta - (n-1)\alpha\big)\,x_4 = (n-1)x_1.\end{cases} \tag{5.2}$$

By multiplying $\Theta - (n-1)\alpha$ in both side of the first equation of (5.2), and then multiplying $\Theta - (q-1)\alpha$ in both side of the second equation of (5.2), it follows that

$$\begin{cases}\big(\Theta - q\alpha\big)\big(\Theta - (n-1)\alpha\big)\,x_1 = (q-1)\big(\Theta - (n-1)\alpha\big)x_2 + \big(\Theta - (n-1)\alpha\big)x_4,\\ \big(\Theta - n\alpha\big)\big(\Theta - (q-1)\alpha\big)\,x_2 = \big(\Theta - (q-1)\alpha\big)(n-1)x_1 + \big(\Theta - (q-1)\alpha\big)x_3.\end{cases} \tag{5.3}$$

By substituting the last two equation of (5.2) into (5.3), we have

$$\begin{cases}\big((\Theta - q\alpha)(\Theta - (n-1)\alpha) - (n-1)\big)\,x_1 = (q-1)(\Theta - (n-1)\alpha)x_2,\\ \big((\Theta - n\alpha)(\Theta - (q-1)\alpha) - (q-1)\big)\,x_2 = (\Theta - (q-1)\alpha)(n-1)x_1.\end{cases} \tag{5.4}$$

Now, by (5.4), Θ is equal to the maximum root of $\Psi(\theta)$, as required. □

Corollary 5.4 *Let k and s be two nonnegative integers such that $k \ge \max\{s, 1\}$. Each of the following holds.*

(i) If $n \ge (k+1)(k-s+2)+2$, then $\rho\big(K_{n,n+s-k-1} - e\big) > \sqrt{\varepsilon_0(s)}$.

(ii) If $n \ge 4k(k+1)$, then $\mu\big(K_{n,n+s-k-1} - e\big) > n + \frac{\varepsilon_0(s)}{n}$.

Proof In proofs below, denote $G = K_{n,n+s-k-1} - e$ and use ρ and μ for $\rho(G)$ and $\mu(G)$, respectively. Define

$$\Psi_1(\theta) = \theta^4 - \big(n(n+s-k-1)-1\big)\theta^2 + (n+s-k-2)(n-1), \text{ and}$$
$$\Psi_2(\theta) = \theta^3 - 2(2n+s-k-2)\theta^2 + \big((k-s)^2 + (n-1)(5n+5s-5k-6)\big)\theta - (n-1)(n+s-k-2)(2n+s-k-1).$$

By setting $q = n+s-k-1$ and $\alpha \in \{0,1\}$ in Lemma 5.3, ρ and μ are equal to the maximum roots of $\Psi_1(\theta)$ and $\Psi_2(\theta)$, respectively. As $n \geq (k+1)(k-s+2) + 2 > k-s+4$ and by $\Psi_1(\rho) = 0$ it follows that

$$\begin{aligned}\rho^2 &= \frac{1}{2}\Big(n(n+s-k-1)-1 \\ &\quad + \sqrt{\big(n(n+s-k-1)-1\big)^2 - 4(n+s-k-2)(n-1)}\Big) \\ &> n(n+s-k-1) - 2 \geq \varepsilon_0(s).\end{aligned}$$

This completes the proof of (i).

To prove (ii), we first prove the following claim.

Claim 1. $\Psi_2\Big(2n+s-k-2+\frac{(k+1)(k+2)}{n}\Big) < 0$.

By algebraic manipulations, we have

$$\Psi_2\left(2n+s-k-2+\frac{(k+1)(k+2)}{n}\right) = -\frac{1}{n^3}\Psi_3(n),$$

where $\Psi_3(n) = n^5 - \Big(k(k+4)-s+5\Big)n^4 - \Big((k+2)(k+1)s - (k+2)^3 + s\Big)n^3 - (k+2)(k+1)\big(2k^2+7k-s+6\big)n^2 + (k+2)^2(k+1)^2(k-s+2)n - (k+2)^3(k+1)^3$.

Recall that $n \geq 4k(k+1)$. Thus, $\Psi_3'''(n) = 6\Big(10n^2 - 4\big(k(k+4)-s+5\big)n - (k+2)(k+1)s + (k+2)^3 - s\Big) \geq \Psi_3'''(4k(k+1)) = 6\Big(s\big(15k^2+13k-3\big) + k\big(144k^3+241k^2+22k-68\big)+8\Big) > 0$, and so $\Psi_3''(n) \geq \Psi_3''(4k(k+1)) = 2(k+1)\Big(s\big(84k^3+60k^2-35k+2\big) + k^2\big(544k^3+812k^2-154k-347\big) + 76k - 12\Big) > 0$.

This leads to $\Psi_3'(n) \geq \Psi_3'(4k(k+1)) = (k+1)^2\Big(s\big(208k^4+112k^3-137k^2+12k-4\big) + k\big(1024k^5+1328k^4-752k^3-791k^2+230k-84\big)+8\Big) > 0$, and so $\Psi_3(n) \geq \Psi_3(4k(k+1)) = (k+1)^3\Big(4ks\big(48k^4+16k^3-45k^2+4k-4\big) + k^2\big(768k^5+832k^4-928k^3-684k^2+215k-150\big) + 4(5k-2)\Big) > 0$. This completes the proof of Claim 1.

Direct computation yields that $\Psi_2(0) = -(n-1)(n+s-k-2)(2n+s-k-1) < 0$ and $\Psi_2(n+s-k-2) = n+s-k-2 > 0$. It is observed that $\Psi_2(\theta)$ tends

to infinity when θ tends to infinity. Combining this with $\Psi_2\Big(2n+s-k-2+\frac{(k+1)(k+2)}{n}\Big)<0$ by Claim 1, we conclude that

$$\mu > 2n+s-k-2+\frac{(k+1)(k+2)}{n} \geq n+\frac{\varepsilon_0(s)}{n},$$

and so (ii) follows. □

Proof of Theorem 1.14 Since $K_{n,n+s-k-1}-e \subset F^0_{n,k,s}$, by Corollary 5.4, $\rho\big(F^0_{n,k,s}\big) > \sqrt{\varepsilon_0(s)}$ and $\mu\big(F^0_{n,k,s}\big) > n+\frac{\varepsilon_0(s)}{n}$. Thus Theorem 1.14 follows from Lemma 5.2 and Theorem 1.18. □

6 The proofs of Theorem 1.16 and Proposition 1.17

By Definition 1.2 (vi) and (1.1), for an edge $w_0z_0 \in E(F_{n,k,s})$ with $d_{F_{n,k,s}}(w_0) = n+s-k-1$ and $d_{F_{n,k,s}}(z_0)=n$, $F^0_{n,k,s} = F_{n,k,s}-w_0z_0$. Throughout this section, we let $J = F^0_{n,k,s}$ and $J_0 = F^0_{n,k,0}$. Unless specially indicated, we assume that k and s are two nonnegative integers such that $k \geq \max\{s,1\}$.

Lemma 6.1 *If $n \geq (k+1)(k-s+2)+2$, then $\rho_2(F^0_{n,k,s}) < \sqrt{n(n+s-k-1)}$.*

Proof By Corollary 5.4 and as $K_{n,n+s-k-1}-e \subset F^0_{n,k,s} = J$, we have $\rho(J) > \sqrt{\varepsilon_0(s)}$. By Lemma 4.4, it follows that

$$\begin{aligned}\rho_2(J) &< \sqrt{|E(J)|-\varepsilon_0(s)}\\ &= \sqrt{n^2-(k+1-s)(n-k)-1-n(n+s-k-2)-(k+1)(k+2-s)}\\ &= \sqrt{n-(2k-s+3)}.\end{aligned}$$

Since $n > 2(k+1)$, $n(n+s-k-1)-\big(n-(2k-s+3)\big) = n^2-(k+2-s)n+2k-s+3 \geq 2k(k+s)+4k+s+3 > 0$. This completes the proof of the lemma. □

Lemma 6.2 *If $n \geq 2(k+1)-s$, then $\rho(F^0_{n,k,s})$ is equal to the maximum root of $\Psi_4(x)$, where $\Psi_4(x) = x^2\Big(x^2-(n+s-k-2)\Big)\Big(x^2-k(k+1-s)\Big)-\Big(x^2+(n+s-k-2)(x^2-1)\Big)\Big(kx^2+(n-k-1)(x^2-k(k+1-s))\Big)$.*

Proof By Definition 1.2 (vi) and (1.1), $J=[U,V]$ is a bipartite graph and we may assume that V contains $k+1-s$ vertices of degree k and U contains k vertices of degree n in J. Define

$$\begin{aligned}U_1 &= \big\{u \in U : d_J(u) = n\big\} \text{ and } U_2 = U\backslash U_1,\\ V_1 &= \big\{v \in V : n-1 \leq d_J(v) \leq n\big\} \text{ and } V_2 = V\backslash V_1.\end{aligned} \tag{6.1}$$

By symmetry, we may assume that $w_0 \in U_2$ and $z_0 \in V_1$.

Let f be the Perron vector of J, and let $\rho = \rho(J)$. We shall adopt the following notation in the rest of the arguments:

$$\begin{cases} x_1 = f(w) \quad \text{if} \quad w \in U_1, \\ x_2 = f(w) \quad \text{if} \quad w \in V_2, \\ x_3 = f(w) \quad \text{if} \quad w \in V_1 \backslash \{z_0\}, \\ x_4 = f(w) \quad \text{if} \quad w \in U_2 \backslash \{w_0\}, \\ x_5 = f(w_0), \text{ and } x_6 = f(z_0). \end{cases} \tag{6.2}$$

As $\big(A(J)\big)f = \rho f$, it follows that

$$\begin{cases} \rho x_1 = (k+1-s)x_2 + (n+s-k-2)x_3 + x_6, \\ \rho x_2 = kx_1, \\ \rho x_3 = kx_1 + (n-k-1)x_4 + x_5, \\ \rho x_4 = (n+s-k-2)x_3 + x_6, \\ \rho x_5 = (n+s-k-2)x_3, \\ \rho x_6 = kx_1 + (n-k-1)x_4. \end{cases} \tag{6.3}$$

The first four equations of (6.3) imply that

$$x_4 = \left(1 - \frac{k(k+1-s)}{\rho^2}\right)x_1. \tag{6.4}$$

The equations on x_3, x_5 and x_6 of (6.3) lead to

$$x_3 = \frac{\rho^2}{\rho^2 - (n+s-k-2)}x_6. \tag{6.5}$$

It follows from (6.5) and the first two equations of (6.3) that

$$x_6 = \frac{\big(\rho^2 - (n+s-k-2)\big)\big(\rho^2 - k(k+1-s)\big)}{\rho\big(\rho^2 + (n+s-k-2)(\rho^2-1)\big)}x_1. \tag{6.6}$$

With algebraic manipulations and utilizing (6.4), (6.6) and the sixth equation of (6.3), ρ is equal to the maximum root of $\Psi_4(x)$, as desired. □

Proof of Proposition 1.17 Let $\Psi_4(x)$ as defined in Lemma 6.2.

To complete the proof, by Lemma 6.1, it suffices to show that

$$\Psi_4\Big(\sqrt{n(n+s-k-1)}\Big) > 0. \tag{6.7}$$

Let $\Phi_2(n) = \Psi_4\Big(\sqrt{n(n+s-k-1)}\Big)$. Algebraic manipulation yields $\Phi_2(n) = 2n^4 - \Big((k^2+4)(k+1-s)+2\Big)n^3 + \Big(2k^3(k-2s+2)+ \quad 2k^2(s-1)^2 - (2s-5)(k-s) - 2(s-3)\Big)n^2 - (k-s+1)(k-s+2)$
$\Big(k^2(k-s) - 2k + 1\Big)n - k(k+1)(k-s+1)(k-s+2)$.

Case 1. $s \geq 1$.

Let $\Phi_3(n) = \Big(2k^3(k-2s+2) + 2k^2(s-1)^2 - (2s-5)(k-s) - 2(s-3)\Big)n^2 - (k-s+1)(k-s+2)\Big(k^2(k-s) - 2k + 1\Big)n - k(k+1)(k-s+1)(k-s+2)$ and $\Phi_4(n) = 2n^4 - \big((k^2+4)(k+1-s)+2\big)n^3$.

When $2n \geq (k^2+4)(k+1)$, we have $\Phi_3'(n) \geq \Phi_3'\Big(\frac{1}{2}(k^2+4)(k+1)\Big) = 2k^5(k-s)^2 + 2k^4(k-s)(3k-s) + k^3(k-s)(13k-6s+28) + k^3(s^2-7s+13) + 7k^2(s-1)s + 22k^2(k-s) + k^2(s^3-4s+4) + 5k(2s^2-8s+7k) + 45k - 25s + 7s^2 + 22 > 0$. This implies that $\Phi_3(n) \geq \Phi_3\Big(\frac{1}{2}(k^2+4)(k+1)\Big) = \frac{1}{4}(k+1)\Big(2k^7(k-s)^2 + 2k^6(k-s)(3k-s) + 4k^5(k-s)(5k-3s) + k^4(k-s)(49k-12s) + k^3(k-s)(83k-16s) + 12k^3\big(s(s-1) + 12(k-s)\big) + 2k^2s\big(k^2s^2 - 2k + 4s^2\big) + 2k^2(11s^2 - 77s + 91k) + 4(46k^2 - 41ks + 6s^2) + 44(ks^2 - 2s + 4k) + 80\Big) > 0$.

When $2n \geq (k^2+4)(k+1)$, we have $2n - \big((k^2+4)(k+1-s)+2\big) \geq s(k^2+4) - 2 \geq k^2 + 2 > 0$, and so $\Phi_4(n) > 0$. As $\Phi_2(n) = \Phi_3(n) + \Phi_4(n) > 0$, it follows that (6.7) must hold.

Case 2. $s = 0$.

Define $\Phi_5(n) = 2n^3 - \Big(k^2(k+1) + 2k + 4\Big)n^2 + (k+2)\big(k^3 - k + 1\big)n + k(k+2)(k+1)$. As $s = 0$, $\Phi_2(n) = (n-k-1)\Phi_5(n)$. Since $2n \geq (k^2+4)(k+1) > k^2(k+1) + 2k + 4$, we have $\Phi_5(n) > (k+2)\big(k^3 - k + 1\big)n + k(k+2)(k+1) > k(k+2)(k+1) > 0$. Thus, $\Phi_2(n) > 0$ and so (6.7) holds. □

Lemma 6.3 *If* $n \geq 3k(k+1)$ *and* $k \geq 2$, *then* $\rho(F^0_{n,k,0}) > \sqrt{n(n-k-2) + (k+2)^2}$.

Proof Throughout this proof, we let $\rho = \rho(J_0)$ to simplify the notation.

By Lemma 6.2, ρ is equal to the maximum root of $\Psi_5(x)$, where $\Psi_5(x) = x^2\Big(x^2 - (n-k-2)\Big)\Big(x^2 - k(k+1)\Big) - \Big(x^2 + (n-k-2)(x^2-1)\Big)\Big(kx^2 + (n-k-1)(x^2 - k(k+1))\Big)$. To show that $\rho > \sqrt{n(n-k-2) + (k+2)^2}$, it suffices to prove $\Psi_5\big(\sqrt{n(n-k-2) + (k+2)^2}\big) < 0$.

Denote by $\Phi_6(n) = \Phi\big(\sqrt{n(n-k-2) + (k+2)^2}\big) = -n^5 + (k^2 + 6k + 10)n^4 - \big(3k(k^2+5k+13) + 37\big)n^3 + (k+2)(4k^3 + 17k^2 + 45k + 44)n^2 - (k^3(3k^2 + 22k + 78) + 174k^2 + 219k + 112)n + (k+2)(k^5 + 7k^4 + 26k^3 + 64k^2 + 85k + 44)$.

When $n \geq 3k(k+1)$ and $k \geq 2$, we have $\Phi''''_6(n) = 24\big(-5n + k^2 + 6k +$

$10\big) \le -24(14k^2+9k-10) < 0$ and thus $\Phi'''_6(n) \le \Phi'''_6(3k(k+1)) = -6\big(k^2(78k^2-87)+9k(11k^2-9)+37\big) < 0$. Once again, since $n \ge 3k(k+1)$ and $k \ge 2$, we have $\Phi''_6(n) \le \Phi''_6(3k(k+1)) = -2\big(k^4(216k^2-274)+k^3(405k^2-673)+65k^2+199k-88\big) < 0$ and so $\Phi'_6(n) \le \Phi'_6(3k(k+1)) = -\big(k^3(297k^5+729k^4-375k^3-1899k^2-575k+303)+159k^2(k-1)+309k(k^2-1)+112\big) < 0$.

This implies that $\Phi_6(n) \le \Phi_6(3k(k+1)) = -\big(162k^{10}+486k^9-198k^8-1827k^7-$-. Denote by $\Phi_7(k) = 162k^4+486k^3-198k^2-1827k-1339$. Since $\Phi_7(2) = 695 > 0$ and $\Phi_7(k) = 175k^3-1339+k^2(311k-198)+k(162k^3-1827) > 0$ for $k \ge 3$, we have $\Phi_6(n) < 0$, as desired. □

Lemma 6.4 *If $n \ge 2(k+2)^2$ and $k \ge 1$, then $\mu(F^0_{n,k,0}) > 2n-k-1.5$.*

Proof Throughout this proof, we let $\mu = \mu(J_0)$ to simplify the notation. Define U_1, U_2, V_1 and V_2 as in (6.1) with $s=0$ and let $w_0 \in U_2$ and $z_0 \in V_1$. Moreover, we let f be the Perron vector of J_0 and we also adopt the same notation from (6.2). As $\big(Q(J_0)\big)f = \mu f$, it follows that

$$\begin{cases} (\mu-n)\,x_1 = (k+1)x_2 + (n-k-2)x_3 + x_6, \\ (\mu-k)\,x_2 = kx_1, \\ (\mu-n)\,x_3 = kx_1 + (n-k-1)x_4 + x_5, \\ (\mu-n+k+1)\,x_4 = (n-k-2)x_3 + x_6, \\ (\mu-n+k+2)\,x_5 = (n-k-2)x_3, \\ (\mu-n+1)x_6 = kx_1 + (n-k-1)x_4. \end{cases} \tag{6.8}$$

The first four equations of (6.8) imply that

$$x_4 = \frac{(\mu-n)(\mu-k)-k(k+1)}{(\mu-k)(\mu-n+k+1)}x_1. \tag{6.9}$$

The equations on x_3, x_5 and x_6 of (6.8) lead to

$$x_3 = \frac{(\mu-n+1)(\mu-n+k+2)}{(\mu-n)(\mu-n+k+2)-(n-k-2)}x_6. \tag{6.10}$$

It follows from (6.10) and the first two equations of (6.8) that

$$x_6 = \frac{(\mu^2-(k+n)\mu+k(n-k-1))(\mu^2-(2n-k-2)\mu+(n-1)(n-k-2))}{(\mu-k)((n-k-1)\mu^2-(2n^2-(3k+5)n+(k+2)^2)x+(n-1)(n-k-1)(n-k-2))}x_1. \tag{6.11}$$

With algebraic manipulations and utilizing (6.9), (6.11) and the sixth equation of (6.8), μ is equal to the maximum root of $\Psi_6(x)$, where $\Psi_6(x) = x^4-\big(4n-4-k\big)x^3+\big(5n^2-(k+11)n-2k^2+6\big)x^2-\big(2n^3+(2k-7)n^2-(6k^2+7k-7)n+2k^3+8k^2+6k-2\big)x+2k(n-1)(n-k-1)(n-k-2)$.

Since $\Psi_6(2n-k-1.5)=\frac{-1}{16}\Phi_8(n)$, where $\Phi_8(n)=16n^3+4(4k^2-4k-19)n^2-4(4k^3-25k-23)n-8k^3-36k^2-66k-33=4n(4n^2-19n-4k^3+25k+23)+16k(k-1)n^2-8k^3-36k^2-66k-33$. Note that $n\geq 2(k+2)^2$. Thus, $\Phi_8''(n)=8(12n+4k^2-4k-19)\geq\Phi_8''(2(k+2)^2)=8(28k^2+92k+77)>0$ and so $\Phi_8'(n)\geq\Phi_8'(2(k+2)^2)=4(64k^4+428k^3+1076k^2+1193k+487)>0$. This implies that $\Phi_8(n)\geq\Phi_8(2(k+2)^2)=192k^6+1952k^5+8272k^4+18624k^3+23348k^2+15294k+4031$. Now, we can conclude that $\Psi_6(2n-k-1.5)<0$, completing the proof of this result. □

Lemma 6.5 (*Li and Ning* [13]) *Let G be a balanced bipartite graph on $2n$ vertices. If $\delta(G)\geq k\geq 1$, $n\geq 2k+3$ and $|E(G)|>n(n-k-2)+(k+2)^2$, then G is traceable unless $G\subseteq F_{n,k,0}$ or $k=1$ and $G\subseteq K_{n-1,n-1}\cup K_2$.*

Proof of Theorem 1.16 Let G denote the balanced bipartite graph satisfying the hypotheses of Theorem 1.16. By (4.6) and Lemmas 6.3–6.4, we have

$$n+\frac{n(n-k-2)+(k+2)^2}{n}\leq 2n-k-1.5<\mu(J_0)\leq\frac{|E(J_0)|}{n}+n, \tag{6.12}$$

$$\sqrt{n(n-k-2)+(k+2)^2}<\rho(J_0)\leq\sqrt{|E(J_0)|}. \tag{6.13}$$

Each of (6.12) and (6.13) implies that $|E(J_0)|>n(n-k-2)+(k+2)^2$. By Lemma 6.5, by the assumption that either $\rho(G)\geq\rho\big(F^0_{n,k,s}\big)$ or $\mu(G)\geq\mu\big(F^0_{n,k,s}\big)$, and as $\delta(G)\geq 2$, we conclude that either G is traceable or $G\subseteq F_{n,k,0}$. It follows by Lemma 5.2 that $G\in\left\{F_{n,k,0},\,F^0_{n,k,0}\right\}$. □

7 The proof of Theorem 1.21

Throughout this section, we assume that $G=[U,V]$ is an almost balanced bipartite graph with $|U|=|V|+1=n$. Let v_0 be a vertex not in $V(G)$ and define a balanced bipartite graph G^{v_0} from G by adding v_0 and n edges joining v_0 to all vertices of U.

Lemma 7.1 *If G^{v_0} is (q,q)-Hamiltonian, then G is (q,q)-traceable.*

Proof As the case when $q=0$ follows from definition immediately, we assume that $q\geq 1$. Let S be an arbitrary set of $2q$ vertices of G such that $|S\cap U|=q=|S\cap V|$. Choose a vertex $v\in S\cap V$. Let $S_1=\big(S\backslash\{v\}\big)\cup\{v_0\}$ and $V_1=V\cup\{v_0\}$. Then $|S_1\cap U|=q=|S_1\cap V_1|$. Since G^{v_0} is (q,q)-Hamiltonian, $G^{v_0}\big[V(G^{v_0})\backslash S_1\big]$ contains a Hamiltonian cycle, and hence $G\big[V(G)\backslash S\big]$ is traceable, as $G^{v_0}\big[(V(G^{v_0})\backslash S_1)\backslash\{v\}\big]=G\big[V(G)\backslash S\big]$. By the arbitrariness of S, G is (q,q)-traceable. □

Proof of Theorem 1.21 (i): We first show that, under the assumption of Theorem 1.21, we have

$$|E(G)| > n(n+q-k-2)+(k+1)(k+1-q). \tag{7.1}$$

Assume that $|E(G)| \le n(n+q-k-2)+(k+1)(k+1-q)$. By (1.3) and Corollary 4.5, we have $\Omega(\alpha) \ge \alpha\left(\frac{|E(G)|}{n}+n\right)+(1-\alpha)\sqrt{|E(G)|} \ge \Theta(G,\alpha)$, contrary to the assumption that $\Omega(\alpha) < \Theta(G,\alpha)$. Hence (7.1) follows.

From (7.1), it follows that $|E(G^{v_0})| > n(n+q-k-1)+(k+1)(k+1-q) = \varepsilon_0(q+1)$. By Theorem 4.2 and Proposition 1.13, either G^{v_0} is (q, q)-Hamiltonian or $G^{v_0} \subseteq F_{n,k,q+1}$. It follows by Lemma 7.1 that either G is (q, q)-traceable or $G \subseteq Z_{n+q-k-1,k-q}$. □

Proof of Theorem 1.21 (ii): By Corollary 5.4, we have $\rho\left(K_{n,n+q-k-1}-e\right) > \sqrt{\varepsilon_0(q)} > \Omega(0)$ and $\mu\left(K_{n,n+q-k-1}-e\right) > n+\frac{\varepsilon_0(q)}{n} > \Omega(1)$. Note that $K_{n,n+q-k-1}-e \subset Z^0_{n+q-k-1,k-q}$. Thus, Theorem 1.21 (i) implies that G is (q, q)-traceable unless $G \subseteq Z_{n+q-k-1,k-q}$. Now, the result follows from Lemma 5.2. □

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Spectral results on Hamiltonian problem

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ABSTRACT

Let α be a non-negative real number, and let $\Theta(G,\alpha)$ be the largest eigenvalue of $A(G)+\alpha D(G)$. Specially, $\Theta(G,0)$ and $\Theta(G,1)$ are called the spectral radius and signless Laplacian spectral radius of G, respectively. A graph G is said to be Hamiltonian (traceable) if it contains a Hamiltonian cycle (path), and a graph G is called Hamilton-connected if any two vertices are connected by a Hamiltonian path in G. The number of edges of G is denoted by $e(G)$. Recently, the (signless Laplacian) spectral property of Hamiltonian (traceable, Hamilton-connected) graphs received much attention. In this paper, we shall give a general result for all these existed results. To do this, we first generalize the concept of Hamiltonian, traceable, and Hamilton-connected to s-suitable, and we secondly present a lower bound for $e(G)$ to confirm the existence of s-suitable graphs. Thirdly, when $0 \le \alpha \le 1$, we obtain a lower bound for $\Theta(G,\alpha)$ to confirm the existence of s-suitable graphs. Consequently, our results generalize and improve all these existed results in this field, including the main results of Chen et al. (2018), Feng et al. (2017), Füredi et al. (2017), Ge et al. (2016), Li et al. (2016), Nikiforov et al. (2016), Wei et al. (2019) and Yu et al. (2013, 2014).

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1. Introduction

In this paper, we only consider simple connected undirected graph, and $G=(V,E)$ is a connected graph with n vertices and $e(G)$ edges. Let $N_G(u)$ and $d_G(u)$ be the neighbor set and the degree of vertex u, respectively. Let $\delta(G)$ and $\Delta(G)$ be the minimum degree and maximum degree of G, respectively. If there is no rise of confusion, we always simplify $N_G(u)$ and $d_G(u)$ as $N(u)$ and $d(u)$, respectively. As usual, K_n, C_n, P_n and $K_{1,n-1}$ denote the complete graph, cycle, path and star graph with n vertices, respectively, and $G_1 \vee G_2$ denotes the *join graph* of two vertex disjoint graphs G_1 and G_2. In other words, $G_1 \vee G_2$ is the graph having vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$. When t is a positive integer, then tK_1 denotes the set of t isolated vertices.

When n, s and k are three integers such that $\max\{0,s\} \le k \le \frac{1}{2}(n+s-2)$, we define the graphs $M_n^{k,s}$ and $N_n^{k,s}$ with n vertices and minimum degree k as follows:

$$N_n^{k,s} \cong K_k \vee \left(K_{n+s-2k-1} \cup (k+1-s)K_1\right), \quad \text{and}$$

$$M_n^{k,s} \cong \begin{cases} K_s \vee \left(K_{n-k-1} \cup K_{k+1-s}\right) & \text{for } s>0, \\ K_{n-k-1} \cup K_{k+1} & \text{for } s=0. \end{cases}$$

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If $A(G)$ and $D(G)$, respectively, define the adjacency matrix and the diagonal matrix of G, then the *signless Laplacian matrix* of G is defined as $Q(G) = D(G) + A(G)$. Hereafter, let $\rho(G)$ and $\mu(G)$ be the largest eigenvalues of $A(G)$ and $Q(G)$, respectively, and we call $\rho(G)$ and $\mu(G)$ the spectral radius and signless Laplacian spectral radius of G, respectively. Throughout this paper, α defines a non-negative real number and let $\Theta(G, \alpha)$ be the largest eigenvalue of $A(G) + \alpha D(G)$. From the definition, it is easy to see that $\Theta(G, 0) = \rho(G)$, and $\Theta(G, 1) = \mu(G)$.

A cycle (path) of a graph G that contains every vertex of G is called a *Hamiltonian cycle* (*path*) of G. A graph G is said to be *Hamiltonian* (*traceable*) if it contains a Hamiltonian cycle (path), and a graph G is called *Hamilton-connected* if any two vertices are connected by a Hamiltonian path in G.

Recently, the (signless Laplacian) spectral properties of traceable graph, Hamiltonian graph and Hamilton-connected received more and more attention. For the spectral properties of traceable graph, Fiedler et al. [7] firstly proved that: For a graph G with n vertices, if $\rho(G) \geq n - 2$, then G is traceable unless $G \cong M^{0,0}$. In 2016, Li et al. [11] generalized Fiedler's result to: For a graph G with $n \geq \max\left\{6k + 10,\ \frac{1}{2}(k^2 + 7k + 8)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 0$, if $\rho(G) \geq \rho\left(N_n^{k,0}\right)$, then G is traceable unless $G \cong N_n^{k,0}$. Soon later, Nikiforov [14] improved Li's result to:

Theorem 1.1 ([14]). *Let G be a graph with $n \geq k^3+k^2+2k+5$ vertices and minimum degree $\delta(G) \geq k \geq 1$. If $\rho(G) \geq n-k-2$, then G is traceable unless $G \in \left\{N_n^{k,0},\ M_n^{k,0}\right\}$.*

For the spectral properties of Hamiltonian graphs, Fiedler et al. [7] firstly proved that: For a graph G with n vertices, if $\rho(G) > n - 2$, then G is Hamiltonian unless $G \cong M_n^{1,1}$. In 2016, Li et al. [11] generalized Fiedler's result to: For a graph G with $n \geq \max\left\{6k + 5,\ \frac{1}{2}\left(k^2 + 6k + 4\right)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 1$, if $\rho(G) \geq \rho\left(N_n^{k,1}\right)$, then G is Hamiltonian unless $G \cong N_n^{k,1}$. Soon later, Nikiforov [14] improved Li's result to:

Theorem 1.2 ([14]). *Let G be a graph with $n \geq k^3 + k + 4$ vertices and minimum degree $\delta(G) \geq k \geq 1$. If $\rho(G) \geq n - k - 1$, then G is Hamiltonian unless $G \in \left\{N_n^{k,1},\ M_n^{k,1}\right\}$.*

Very recently, Ge et al. [9] improved Nikiforov's result to $n \geq \max\left\{\frac{1}{2}\left(k^3 + 2k + 5\right),\ 6k + 5\right\}$. Researchers also concerned with the (signless Laplacian) spectral properties of Hamilton-connected graphs. In this line, Yu et al. [17] proved that: For a graph G with n vertices, if either $\rho(G) > \frac{1}{2}\left(\sqrt{4n^2 - 12n + 17} - 1\right)$ or $\mu(G) > 2n-4+\frac{2}{n-1}$, then G is Hamilton-connected unless $G \cong M_n^{2,2}$. In 2017, Zhou et al. [20] proved that: For a graph G with minimum degree $\delta(G) \geq 3$ and $n \geq 9$ vertices, if either $\rho(G) \geq \sqrt{n^2 - 6n + 19}$ or $\mu(G) \geq 2n-6+\frac{14}{n-1}$, then G is Hamilton-connected. Later, Yu et al. [18] generalized the spectral radius version of Zhou's results to: For a graph G with $n \geq 2k^2 + 1$ vertices and minimum degree $\delta(G) \geq k \geq 2$, if $\rho(G) \geq n - k$, then G is Hamilton-connected unless $G \cong M_n^{k,2}$. Recently, Chen et al. [3] and Yu et al. [19], independently, improved Yu's result of [18] by showing that: For a graph G with $n \geq \max\left\{6k^2-8k+5,\ \frac{1}{2}\left(k^3-k^2+4k-1\right)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 2$, if $\rho(G) \geq n - k$, then G is Hamilton-connected unless $G \in \left\{N_n^{k,2},\ M_n^{k,2}\right\}$. Soon later, Wei et al. [16] improved Chen's result to $n \geq \max\left\{\frac{1}{2}\left(k^3 - k^2 + 2k + 8\right),\ 6k\right\}$, that is,

Theorem 1.3 ([16]). *Let G be a graph with $n \geq \max\left\{\frac{1}{2}\left(k^3 - k^2 + 2k + 8\right),\ 6k\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 3$. If $\rho(G) \geq n - k$, then G is Hamilton-connected unless $G \in \left\{N_n^{k,2},\ M_n^{k,2}\right\}$.*

For the signless Laplacian spectral properties of traceable graphs, Yu et al. [17] firstly proved that: For a graph G with n vertices, if $\mu(G) \geq 2(n - 2)$, then G is traceable unless $G \cong N_n^{0,0}$. In 2016, Li et al. [11] generalized Yu's result to:

Theorem 1.4 ([11]). *Let G be a graph with $n \geq \max\left\{6k + 10,\ \frac{1}{2}\left(3k^2 + 9k + 8\right)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 0$. If $\mu(G) \geq \mu\left(N_n^{k,0}\right)$, then G is traceable unless $G \cong N_n^{k,0}$.*

For the signless Laplacian spectral properties of Hamiltonian graphs, Yu et al. [17] proved that: For a graph G with n vertices, if $\mu(G) > 2(n - 2)$, then G is Hamiltonian unless $G \cong N_n^{1,1}$. In 2016, Li et al. [11] generalized Yu's result to:

Theorem 1.5 ([11]). *Let G be a graph with $n \geq \max\left\{6k + 5,\ \frac{1}{2}\left(3k^2 + 5k + 4\right)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq 1$. If $\mu(G) \geq \mu\left(N_n^{k,1}\right)$, then G is Hamiltonian unless $G \cong N_n^{k,1}$.*

By comparing these results of Theorems 1.1–1.5, it is rather interesting for us to consider the following problem:

Problem 1.1. How can we generalize these results of Theorems 1.1–1.5?

To this aim, we need to introduce the concepts of *q-traceable* and *q-Hamiltonian*. For any non-negative integer q, a graph G with $n \geq 3$ vertices is called *q-traceable* if any removal of at most q vertices to G results in a traceable graph, while a graph G with $n \geq 3$ vertices is called *q-Hamiltonian* if any removal of at most q vertices to G results in a Hamiltonian

graph. From the definitions, a q-Hamiltonian graph must be a $(q+1)$-traceable graph. However, a $(q+1)$-traceable graph is not necessarily a q-Hamiltonian graph. For instance, the Petersen graph is 1-traceable, but it is not 0-Hamiltonian.

Hereafter, we use $G[X]$ to denote the subgraph of G induced by X. It is easy to see that a traceable graph is also a 0-traceable graph, and a Hamiltonian graph is both a 0-Hamiltonian and a 1-traceable graph. If G is Hamilton-connected, then for any two vertices $\{u, v\}$ of G, there is a Hamiltonian path connecting u and v. Thus, $G\big[V(G)\backslash\{u, v\}\big]$ contains a Hamiltonian path and $G\big[V(G)\backslash\{u\}\big]$ also contains a Hamiltonian path, and hence G is 2-traceable.

A graph G is *q-edge-Hamiltonian* if any collection of vertex-disjoint paths with at most q edges altogether belongs to a Hamiltonian cycle in G. A connected graph G is said to be *q-connected* if it has more than q vertices and remains connected whenever fewer than q vertices are deleted. Similarly, G is *q-edge-connected* if it has at least two vertices and remains connected whenever fewer than q edges are deleted. A graph G is *q-path-coverable* if $V(G)$ can be covered by q or fewer vertex-disjoint paths.

Recently, Feng et al. [6] obtained the generalized result for spectral property of q-Hamiltonian (respectively, q-edge-Hamiltonian) graphs, that is

Theorem 1.6 ([6]). *For a graph G with $n \geq q+6 \geq 7$ vertices and minimum degree at least one, if $\rho(G) \geq \sqrt{(n-2)^2+2q+1}$, then G is q-edge-Hamiltonian and q-Hamiltonian.*

Except for this, Feng et al. [6] also obtained the generalized result for spectral property of q-connected (respectively, q-edge-connected, q-path-coverable) graphs, that is

Theorem 1.7 ([6]). *(i) For a graph G with $n \geq q+1 \geq 2$ vertices and minimum degree at least one, if $\rho(G) \geq \sqrt{n(n-4)+2q+1}$, then G is q-connected. (ii) For a graph G with $n \geq q+1 \geq 3$ vertices and minimum degree at least one, if $\rho(G) \geq \sqrt{n(n-q-5)+2q(q+1)+5}$, then G is q-edge-connected. (iii) For a graph G with $n \geq 5q+6 \geq 16$ vertices and minimum degree at least one, if $\rho(G) \geq \sqrt{(n-q-2)^2+q+1}$, then G is q-path-coverable.*

For a non-negative integer q, the *q-closure*, denoted by $C_q(G)$, of a graph G is the graph obtained from G by successively joining pairs of nonadjacent vertices whose degree sum is at least q until no such pair remains. It is easy to see that $G \subseteq C_q(G)$.

Let $\mathbb{G}_n$ be the class of graphs with n vertices and q be a non-negative integer. If G has the property P if and only if $C_q(G)$ has property P for each $G \in \mathbb{G}_n$, then the property P is said to be *q-stable* (here, the definition of *q-stable* is a little different from that in [1]).

By an observation to Theorem 1.6, one can easily find that Feng et al. cannot solve Problem 1.1 completely, as Theorems 1.1–1.3 are not a special case of Theorem 1.6. Therefore, positive answer to Problem 1.1 is also valuable, and our main goal of this paper is to solve it. To do this, via analyzing all these referred former results, we find that the key tool to prove them relies on the following k-stable property:

Proposition 1.1 ([1]). *The following stability results hold for graphs with n vertices:*
(i) The property that "G is q-connected" is $(n+q-2)$-stable.
(ii) The property that "G is q-edge-connected" is $(n+q-2)$-stable.
(iii) The property that "G is q-Hamiltonian" is $(n+q)$-stable.
(iv) The property that "G is q-edge-Hamiltonian" is $(n+q)$-stable.
(v) The property that "G is q-path-coverable" is $(n-q)$-stable.

In what follows, we shall give the spectral property to $(n+s-1)$-stable property for graphs with n vertices, which will improve and generalize all these results in Theorems 1.1–1.7. To do this, we need more notations in the following:

Definition 1.1. Let n, s, p and k be four integers such that $\max\{0, s\} \leq p \leq k \leq \frac{1}{2}(n+s-2)$. If $p \geq \max\big\{s, 0\big\}+1$, then $\mathbb{G}_n(p, s, k) = \Big\{G : G \cong K_p \vee \big(K_{n+s-k-1-p} \cup H_0\big)$, where H_0 is a $(k-p)$-regular graph with $k+1-s$ vertices$\Big\}$. If $p = s \geq 0$, then $\mathbb{G}_n(p, s, k) = \big\{M_n^{k,s}\big\}$. If $p = 0 > s$, then $\mathbb{G}_n(p, s, k) = \Big\{K_{n+s-k-1} \cup H_0,$ where H_0 is a k-regular graph with $k+1-s$ vertices$\Big\}$.

Here, we need to point out the fact that s being negative is also permitted in Definition 1.1 (see Remark 1.2). From Definition 1.1, it is easy to see that $\mathbb{G}_n(k, s, k) = \big\{N_n^{k,s}\big\}$ and $\mathbb{G}_n(p, s, k)$ are graphs with n vertices and minimum degree $k \geq 0$. Hereafter, if $G \in \mathbb{G}_n(p, s, k)$ and $\max\{s, 1\} \leq p \leq k$, we let $V_1(G)$, $V_2(G)$ and $V_3(G)$ be the vertex sets corresponding to K_p, $K_{n+s-k-1-p}$ and H_0 of G, respectively. Especially, when $k \geq 1$ and $n+s-2k \geq 3$, we define $N_{n,0}^{k,s}$ as the graph obtained from $N_n^{k,s}$ by deleting one edge with two end vertices in $V_2\left(N_n^{k,s}\right)$, namely, in $K_{n+s-k-1-p}$. In what follows, let

$$\Theta_0 = \alpha\left(\frac{2\varepsilon_0}{n-1}+n-2\right)+\frac{1}{2}(1-\alpha)\left(k-1+\sqrt{(k+1)^2+8\varepsilon_0-4nk}\right),$$

where

$$\varepsilon_0 = \binom{n-k-2+s}{2}+(k+1)(k+2-s).$$

Now, we are ready to give the main results of this paper:

Theorem 1.8. *Let s and k be two integers and let G be a graph with $n \geq 6k+10-5s$ vertices and minimum degree $\delta(G) \geq k \geq \max\{1,s\}$. If $\Theta(G,\alpha) > \Theta_0$ and $0 \leq \alpha \leq 1$, then either $C_{n+s-1}(G) \cong K_n$ or $C_{n+s-1}(G) \in \mathbb{G}_n(p,s,k)$ holds for some integer p, where $\max\{0,s\} \leq p \leq k$.*

Theorem 1.9. *Let s and k be two integers and let G be a graph with $n \geq \max\left\{6k+10-5s,\ \frac{1}{4}(4(k-s)(k+3)+10k+25),\ \frac{1}{3}(2(k-s)(3k-s+5)+8k+15)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq \max\{1,s\}$. If $\Theta(G,\alpha) \geq \Theta\left(N^{k,s}_{n,0},\alpha\right)$ and $0 \leq \alpha \leq 1$, then unless $G \cong N^{k,s}_{n,0}$, either $C_{n+s-1}(G) \cong K_n$ or $G \in \mathbb{G}_n(p,s,k)$ holds for some integer p, where $\max\{0,s\} \leq p \leq k$.*

Now, one can easily see that our Theorems 1.8 and 1.9 give the spectral property to $(n+s-1)$-stable property for graphs with n vertices. In [1,2], many q-stable properties had been given. Thus, we can apply Theorem 1.8 or Theorem 1.9 to give a new spectral property to these q-stable properties.

By comparing Theorems 1.8 and 1.9, it is an interesting question that: How large is $\Theta\left(N^{k,s}_{n,0},\alpha\right)$ or Θ_0. Actually, it is easy to see that $\Theta\left(N^{k,s}_{n,0},\alpha\right) > \Theta_0$ (see (4.8) in the proof of Theorem 1.9). Furthermore, for $\Theta\left(N^{k,s}_{n,0},\alpha\right)$, we have

Proposition 1.2. *Let k, s and n be three integers such that $\max\{1,s\} \leq k \leq \frac{1}{6}(n+5s-10)$. If $n \geq \max\left\{\frac{1}{2}((k^2+4)(k+1-s)+2),\ \frac{1}{2}(k^2(k+1)+6)\right\}$, then $\rho\left(N^{k,s}_{n,0}\right) < n+s-k-2$ and*

$$\mu\left(N^{k,s}_{n,0}\right) < \frac{2n^2-2(k+3-s)n+(k-s+1)(3k-s+2)}{n-1}. \tag{1.1}$$

Remark 1.1. Note that K_n is both q-connected and q-edge-connected, $\sqrt{n(n-4)+2q+1} \geq n+q-\delta(G)-3$ and $\sqrt{n(n-q-5)+2q(q+1)+5} \geq n+q-\delta(G)-3$ hold for large n and $3q \leq 2\delta(G)$. Thus, by Propositions 1.2 and 1.1 (i) and (ii), it is easy to see that Theorem 1.9 improves Theorem 1.7 (i) and (ii) for large n and $3q \leq 2\delta(G)$ by setting $s = q-1$.

Remark 1.2. Note that K_n is q-path-coverable. Thus, by Propositions 1.2 and 1.1 (v), it is easy to see that Theorem 1.9 improves Theorem 1.7 (iii) for large n and $\delta(G) \geq 2$ by setting $s = 1-q$ (here, $s = 1-q$ may be negative).

Remark 1.3. Note that K_n is both q-edge-Hamiltonian and q-Hamiltonian, and $\delta(G) \geq q+2$ holds for any q-Hamiltonian graph G. Thus, by Proposition 1.2 and Proposition 1.1 (iii) and (iv), it is easy to see that Theorem 1.9 improves Theorem 1.6 for large n and $\delta(G) \geq q+2$ by setting $s = q+1$.

As referred before, a traceable graph is also a 0-traceable graph, a Hamiltonian graph is both a 0-Hamiltonian graph and a 1-traceable graph, and a Hamilton-connected graph is also a 2-traceable graph. For any graph G with n vertices, it is well-known that [15]: G is traceable if and only if $C_{n-1}(G)$ is traceable. For the general case of q-traceable, we have

Proposition 1.3. *If $q \geq 0$ and G is a graph with n vertices, then G is q-traceable if and only if $C_{n+q-1}(G)$ is q-traceable.*

Note that K_n is traceable, Hamiltonian and Hamilton-connected. By setting $s = 0, 1, 2$ in Theorem 1.9 and Proposition 1.2, we have: If n is large enough and $\rho(G) \geq n+s-k-2$, then G is traceable (respectively, Hamiltonian Hamilton-connected) unless $G \in \mathbb{G}_n(p,s,k)$ for some integer p, where $s \leq p \leq k$. However, this is somewhat different from that in Theorems 1.1–1.3. Actually, in [3,11,16], the authors had shown that:

Proposition 1.4 (*[3,11,16]*)**.** *For $s = 0$ (respectively, $s = 1, 2$), if $G \in \mathbb{G}_n(p,s,k)$ for some integer p, where $s \leq p \leq k \leq \frac{n+s-2}{2}$, then G is traceable (respectively, Hamiltonian, Hamilton-connected) if and only if $p \in \{s+1, s+2, \ldots, k-1\}$.*

Therefore, to generalize the corresponding results of Theorems 1.1–1.5, we need to generalize Proposition 1.4 to

Proposition 1.5. *Suppose that $q \geq 0$. (i) If $q \leq p \leq k \leq \frac{1}{2}(n+q-2)$ and $G \in \mathbb{G}_n(p,q,k)$, then G is q-traceable if and only if $p \in \{q+1, q+2, \ldots, k-1\}$. (ii) If $q+1 \leq p \leq k \leq \frac{1}{2}(n+q-1)$ and $G \in \mathbb{G}_n(p,q+1,k)$, then G is q-Hamiltonian if and only if $p \in \{q+2, q+3, \ldots, k-1\}$.*

By combining Propositions 1.1 (iii) and 1.3, the property that "G is q-Hamiltonian (respectively, q-traceable)" is $(n+q)$-stable (respectively, $(n+q-1)$-stable). However, Proposition 1.5 and Theorem 1.9 show that: for q-Hamiltonian (respectively, q-traceable) graphs, except for $(n+q)$-stable (respectively, $(n+q-1)$-stable) property, they require more conditions. Now, motivated from Propositions 1.3–1.5, we put forward the concept of *s-suitable graph* as follows:

Definition 1.2. A graph G with n vertices and minimum degree $\delta(G) \geq k$ is called an *s-suitable graph* if G satisfies the following conditions: (i) K_n is s-suitable, (ii) G is s-suitable if and only if $C_{n+s-1}(G)$ is s-suitable, and (iii) If $s_0 \leq p \leq k \leq \frac{1}{2}(n+s-2)$ and $G \in \mathbb{G}(p,s,k)$, then G is s-suitable if and only if $p \in \{s_0+1, s_0+2, \ldots, k-1\}$, where $s_0 = \max\{0,s\}$.

For any non-negative integer q, since K_n is both q-traceable and q-Hamiltonian, by Propositions 1.1 (*iii*), 1.3, 1.5 and Definition 1.2, a q-traceable graph is q-suitable, and a q-Hamiltonian graph is $(q+1)$-suitable. Consequently, a traceable, Hamiltonian, and Hamilton-connected graph is a 0-suitable, 1-suitable and 2-suitable graph, respectively.

Since K_n is s-suitable, by Theorem 1.8, it easily follows that

Corollary 1.1. *Let s and k be two non-negative integers and let G be a graph with $n \geq 6k+10-5s$ vertices and minimum degree $\delta(G) \geq k \geq \max\{1, s\}$. If $\Theta(G, \alpha) > \Theta_0$ and $0 \leq \alpha \leq 1$, then G is s-suitable unless $C_{n+s-1}(G) \in \left\{N_n^{k,s}, M_n^{k,s}\right\}$.*

Note that a Hamilton-connected graph is a 2-suitable graph. Thus, by Corollary 1.1, we have the following remark.

Remark 1.4. In [3], it is shown that: For any graph with $n \geq 6k^2-8k+5$ vertices and minimum degree $\delta(G) \geq k \geq 2$, if either $\rho(G) > \frac{1}{2}(k-1)+\frac{1}{2}\sqrt{4n^2-4(3k-1)n+k^2+10k-15}$ or $\mu(G) > 2n-2k-\frac{2}{n-1}$, then G is Hamilton-connected unless $C_{n+1}(G) \in \left\{N_n^{k,2}, M_n^{k,2}\right\}$. It is easy to see that Corollary 1.1 improves this result for large n by setting $s=2$.

From the definition of s-suitable and Theorem 1.9, we have

Corollary 1.2. *Let s and k be two non-negative integers and let G be a graph with $n \geq \max\left\{6k+10-5s,\ \frac{1}{4}\left(4(k-s)(k+3)+10k+25\right),\ \frac{1}{3}\left(2(k-s)(3k-s+5)+8k+15\right)\right\}$ vertices and minimum degree $\delta(G) \geq k \geq \max\{1, s\}$. If $\Theta(G, \alpha) \geq \Theta\left(N_{n,0}^{k,s}, \alpha\right)$ and $0 \leq \alpha \leq 1$, then G is s-suitable unless $G \in \left\{N_n^{k,s},\ M_n^{k,s},\ N_{n,0}^{k,s}\right\}$.*

Remark 1.5. *Recall that a traceable, Hamiltonian, and Hamilton-connected graph is a 0-suitable, 1-suitable and 2-suitable graph, respectively. By Proposition 1.2, it is easy to see that Corollary 1.2 improves and generalizes these results of Theorems 1.1–1.5 for large n by setting $s=0$, 1 and 2, respectively.*

As the definition of s-suitable is an extension to the concepts of traceable, Hamiltonian and Hamilton-connected, it is easy to see that the graph with more edges has higher chance to be s-suitable. For a graph with n vertices and minimum degree $\delta(G) \geq k \geq 1$, it is natural and interesting for us to consider the following problem:

Problem 1.2. How large for $e(G)$ can confirm that the s-suitability of a graph G?

The corresponding Problem 1.2 of traceable, Hamiltonian, and Hamilton-connected graph had been, respectively, studied in [3,8,11,16]. Now, we will give partial answer to Problem 1.2, which generalizes the above referred results:

Theorem 1.10. *Let s and k be two integers and let G be a graph with $n \geq 6k+10-5s$ vertices, minimum degree $\delta(G) \geq k \geq \max\{1, s\}$ and $e(G) > \varepsilon_0$ edges. If $C_{n+s-1}(G) \ncong K_n$, then $C_{n+s-1}(G) \in \mathbb{G}_n(p, s, k)$ holds for some integer p, where $\max\{s, 0\} \leq p \leq k$.*

2. The Proofs of Propositions 1.3 and 1.5

The following result generalizes the corresponding result of traceable graph due to Ore [15].

Lemma 2.1. *Let G be a graph with n vertices and q be a non-negative integer. If $d_G(w_1)+d_G(w_2) \geq n+q-1$ whenever $w_1w_2 \notin E(G)$, then G is q-traceable if and only if $G' = G+w_1w_2$ is q-traceable.*

Proof. It suffices to show the necessity. Let S be any set of at most q vertices such that $S \subseteq V(G)$ and $|S| = t$. Since G' is q-traceable, $G'\left[V(G)\setminus S\right]$ contains a Hamiltonian path, say P, where $V(P) = V(G)\setminus S$.

If $w_1w_2 \notin E(P)$, then P is also a path of $G\left[V(G)\setminus S\right]$ and hence we are done. Otherwise, $w_1w_2 \in E(P)$ and $w_1w_2 \notin E(G)$. Let $G_1 = G\left[V(G)\setminus S\right]$ and let $P = u_1u_2\cdots u_{n-t}$ be the corresponding Hamiltonian path of $G'\left[V(G)\setminus S\right]$, where $w_1 = u_i$ and $w_2 = u_{i+1}$. Recall that $d_G(u_i)+d_G(u_{i+1}) \geq n+q-1$. Thus, $d_{G_1}(u_i)+d_{G_1}(u_{i+1}) \geq n+q-2t-1 \geq n-t-1$ as $t \leq q$. Furthermore, $u_1u_{i+1} \notin E(G_1)$ and $u_iu_{n-t} \notin E(G_1)$ (otherwise, $G\left[V(G)\setminus S\right]$ also contains a Hamiltonian path, and the result already holds).

We firstly prove the following claim:

Claim 1: There is an index j with either $i+2 \leq j \leq n-t-1$ or $1 \leq j \leq i-2$ such that $u_iu_j \in E(G_1)$ and $u_{i+1}u_{j+1} \in E(G_1)$.

Proof of Claim 1: We suppose that $N_{G_1}(u_{i+1}) = \left\{u_{p_1}, u_{p_2}, \ldots, u_{p_q}, u_{i+2}\right\}$, where $\{1, i\} \cap \{p_1, p_2, \ldots, p_q\} = \emptyset$. If Claim 1 does not hold, then $N_{G_1}(u_i) \subseteq \left\{u_1, u_2, \ldots, u_{i-1}, u_{i+2}, u_{i+3}, \ldots, u_{n-t-1}\right\} \setminus \left\{u_{p_1-1}, u_{p_2-1}, \ldots, u_{p_q-1}\right\}$. Thus, $d_{G_1}(u_i) \leq n-t-3-q$ and hence $d_{G_1}(u_i)+d_{G_1}(u_{i+1}) \leq (n-t-3-q)+(q+1) = n-t-2$, a contradiction. This completes the proof of Claim 1.

By Claim 1, either for some j with $i+2 \leq j \leq n-t-1$, both $u_iu_j \in E(G_1)$ and $u_{i+1}u_{j+1} \in E(G_1)$, whence $u_1u_2\ldots u_iu_ju_{j-1}\ldots u_{i+1}u_{j+1}u_{j+2}\cdots u_{n-t}$ is a Hamiltonian path of $G[V(G)\setminus S]$; or for some j with $1 \leq j \leq i-2$, both

$u_iu_j \in E(G_1)$ and $u_{i+1}u_{j+1} \in E(G_1)$, whence $u_1u_2\dots u_ju_iu_{i-1}\dots u_{j+1}u_{i+1}u_{i+2}\dots u_{n-t}$ is a Hamiltonian path of $G[V(G)\setminus S]$. This proves the lemma. ■

The Proof of Proposition 1.3. By Lemma 2.1, it is easy to see that Proposition 1.3 holds. ■

Lemma 2.2. *Let q be a non-negative integer. Then G is q-traceable if and only if $K_1 \vee G$ is $(q+1)$-traceable, and G is q-Hamiltonian if and only if $K_1 \vee G$ is $(q+1)$-Hamiltonian.*

Proof. Let $V(K_1) = \{u\}$ and also let $G' = K_1 \vee G$. We firstly suppose that $K_1 \vee G$ is $(q+1)$-traceable (respectively, $(q+1)$-Hamiltonian). Let S be any vertex set of G with t vertices, where $0 \le t \le q$. Then, $S_1 = S \cup \{u\}$ is a vertex set of $K_1 \vee G$ with $t+1$ vertices. In this case, since $t \le q$ and since $K_1 \vee G$ is $(q+1)$-traceable (respectively, $(q+1)$-Hamiltonian), $G'\big[V(G')\setminus S_1\big]$ contains a Hamiltonian path (respectively, Hamiltonian cycle). Note that $G\big[V(G)\setminus S\big] \cong G'\big[V(G')\setminus S_1\big]$. Thus, G is q-traceable (respectively, q-Hamiltonian).

Now, we suppose that G is q-traceable (respectively, q-Hamiltonian) and suppose that S_2 is any vertex set of G' with $t+1$ vertices, where $0 \le t \le q$ (Actually, since G is traceable, it is easy to see that G' is Hamiltonian, and hence we may suppose that $|S_2| \ge 1$). If $u \in S_2$, then let $S_3 = S_2 \setminus \{u\}$. In this case, $G\big[V(G)\setminus S_3\big]$ contains a Hamiltonian path (respectively, Hamiltonian cycle). Since $G'\big[V(G')\setminus S_2\big] \cong G\big[V(G)\setminus S_3\big]$, $G'\big[V(G')\setminus S_2\big]$ also contains a Hamiltonian path (respectively, Hamiltonian cycle). Thus, we assume that $u \notin S_2$.

Since $|S_2| \ge 1$, we choose $v \in S_2$ and let $S_4 = S_2 \setminus \{v\}$. It is easy to see that $G'\big[V(G')\setminus S_4\big] \cong K_1 \vee G\big[V(G)\setminus S_4\big]$. Combining this with $G\big[V(G)\setminus S_4\big]$ containing a Hamiltonian path (respectively, Hamiltonian cycle), we can conclude that $G'\big[V(G')\setminus S_2\big]$ contains a Hamiltonian path (respectively, Hamiltonian cycle). ■

The Proof of Proposition 1.5. We prove Proposition 1.5 by induction on q. By Proposition 1.4, the results hold for $q = 0$. Thus, we assume that $q \ge 1$ and Proposition 1.5 holds for smaller values of q.

(*i*) $G \in \mathbb{G}_n(p, q, k)$ with $1 \le q \le p \le k \le \frac{1}{2}(n+q-2)$.

As $p \ge q \ge 1$, by Definition 1.1, there exists a graph G_1 such that $G = K_1 \vee G_1$. By Lemma 2.2, G is q-traceable if and only if G_1 is $(q-1)$-traceable. In this case, $G \cong K_p \vee \big(K_{n+q-k-1-p} \cup H_0\big)$ and $G_1 \cong K_{p-1} \vee \big(K_{n+q-k-1-p} \cup H_0\big)$, where H_0 is a $(k-p)$-regular graph with $k+1-q$ vertices.

Recall that $1 \le q \le p \le k \le \frac{1}{2}(n+q-2)$. Thus, $0 \le q-1 \le p-1 \le k-1 \le \frac{1}{2}(n+q-4)$ and hence $\delta(G_1) = k-1$. Therefore, $G_1 \in \mathbb{G}_{n-1}(p-1, q-1, k-1)$. By the induction hypothesis, G_1 is $(q-1)$-traceable if and only if $p-1 \in \big\{q, q+1, \dots, k-2\big\}$. Thus, G is q-traceable if and only if $p \in \big\{q+1, q+2, \dots, k-1\big\}$.

(*ii*) $G \in \mathbb{G}_n(p, q+1, k)$ with $2 \le q+1 \le p \le k \le \frac{1}{2}(n+q-1)$.

As $p \ge q+1 \ge 2$, we may suppose that $G = K_1 \vee G_1$ by Definition 1.1. By Lemma 2.2, G is q-Hamiltonian if and only if G_1 is $(q-1)$-Hamiltonian. In this case, $G \cong K_p \vee \big(K_{n+q-k-p} \cup H_0\big)$ and $G_1 \cong K_{p-1} \vee \big(K_{n+q-k-p} \cup H_0\big)$, where H_0 is a $(k-p)$-regular graph with $k-q$ vertices.

Recall that $2 \le q+1 \le p \le k \le \frac{1}{2}(n+q-1)$. Thus, $1 \le q \le p-1 \le k-1 \le \frac{1}{2}(n+q-3)$ and hence $\delta(G_1) = k-1$. Therefore, $G_1 \in \mathbb{G}_{n-1}(p-1, q, k-1)$. By the induction hypothesis, G_1 is $(q-1)$-Hamiltonian if and only if $p-1 \in \big\{q+1, q+2, \dots, k-2\big\}$. Thus, G is q-Hamiltonian if and only if $p \in \big\{q+2,\ q+3, \dots, k-1\big\}$. ■

3. The Proofs of Theorems 1.8 and 1.10

For $A, B \subseteq V(G)$ and $A \cap B = \emptyset$, let $e(A, B)$ be the number of edges connecting A and B. Especially, $e(v, B)$ is the number of edges that connect v and B.

Lemma 3.1. *Let s and k be two integers and let G be a graph with $n \ge 6k+10-5s$ vertices, minimum degree $\delta(G) \ge k \ge \max\{1, s\}$ and $e(G) > \varepsilon_0$ edges. If $C_{n+s-1}(G) \ncong K_n$, then $\omega(C_{n+s-1}(G)) \ge n+s-k-1$, where $\omega(C_{n+s-1}(G))$ is the clique number of $C_{n+s-1}(G)$.*

Proof. In the proof of this result, we rewrite $C_{n+s-1}(G)$ as G'. From the definition, it follows that $\delta(G') \ge \delta(G) \ge k$, $e(G') \ge e(G)$ and $d_{G'}(u) + d_{G'}(v) \le n+s-2$ holds for any pair of nonadjacent vertices $\{u, v\} \subseteq V(G')$. Let K be the subset of $V(G')$ containing all vertices which have degree at least $\frac{1}{2}(n+s-1)$. By the definition of G', any two vertices in K are adjacent in G'. Let C be a maximum clique of G' containing all vertices in K and suppose that $|C| = t$. Let $H = G' - C$. Since $G' \ncong K_n$, we can conclude that $H \ne \emptyset$ and $k \le d_{G'}(v) \le \frac{1}{2}(n+s-2)$ holds for each $v \in V(H)$. We consider the following two cases:

Case 1. $0 \le t < \frac{1}{2}(n+s)$.

For every $v \in V(H)$, we have $e(v, C) \le t-1$ and $k \le d_{G'}(v) \le \frac{1}{2}(n+s-2)$, and hence

$$e(H) + e\left(V(H), V(C)\right) = \frac{1}{2}\left(\sum_{v\in V(H)} d_{G'}(v) + \sum_{v\in V(H)} e(v, C)\right) \le \frac{1}{4}(n-t)\,(2t+n+s-4)\,.$$

Combining this with $e(G') = e(C) + e(H) + e\big(V(H), V(C)\big)$, it follows that

$$\begin{aligned}\varepsilon_0 < e(G') &= e(C) + e(H) + e\big(V(H), V(C)\big)\\ &\le \binom{t}{2} + \frac{1}{4}(2t+n+s-4)(n-t) = \frac{1}{4}\Big((n-s+2)t + n(n+s-4)\Big)\\ &< \frac{1}{8}(3n-s)(n+s-2). \end{aligned} \tag{3.1}$$

Since $n \ge 6k+10-5s > 2k-s+4$, $8\varepsilon_0 - (3n-s)(n+s-2) = (n-6k+5s-10)(n+s-4-2k) \ge 0$, contrary to (3.1).

Case 2. $\frac{1}{2}(n+s) \le t \le n+s-k-2$.

Since C is a maximum clique of G' and hence every vertex of C has degree at least $t-1$, and since each pair of vertices with sum of degrees at least $n+s-1$ must be adjacent in G' (Recall that $C_{n+s-1}(G) = G'$), we conclude that $d_{G'}(v) \le n+s-t-1$ holds for every $v \in V(H)$. Thus,

$$e(H) + e\,(V(H), V(C)) = \sum_{v\in V(H)} d_{G'}(v) - e(H) \le (n-t)(n+s-t-1),$$

and hence

$$\begin{aligned} e(G') &= e(C) + e(H) + e\big(V(H), V(C)\big)\\ &\le \binom{t}{2} + (n-t)(n+s-t-1)\\ &= \frac{1}{2}\Big(3t^2 - (4n+2s-1)t + 2n(n+s-1)\Big). \end{aligned} \tag{3.2}$$

Since $\frac{1}{2}(n+s) \le t \le n+s-k-2$, by (3.2) and $n \ge 6k+10-5s$, we have

$$\begin{aligned} e(G') &\le \frac{1}{2}\Big(3t^2 - (4n+2s-1)t + 2n(n+s-1)\Big)\\ &\le \max\left\{\frac{1}{2}\Big(n^2 - (2k+5-2s)n + (k-s+2)(3k-s+5)\Big), \frac{1}{8}(3n-s)(n+s-2)\right\}\\ &\le \varepsilon_0 < e(G'), \end{aligned}$$

which is a contradiction. ■

The Proof of Theorem 1.10. In the proof of this result, we rewrite $C_{n+s-1}(G)$ as G'. From the definition, it follows that $\delta(G') \ge \delta(G) \ge k$, $e(G') \ge e(G)$ and $d_{G'}(u)+d_{G'}(v) \le n+s-2$ holds for any pair of nonadjacent vertices $\{u, v\} \subseteq V\big(G'\big)$. Let C be a maximum clique of G', and let $H = G' - C$. Note that $G' \ncong K_n$. Thus, $H \ne \emptyset$. By Lemma 3.1, we have $|C| \ge n+s-k-1$.

If $|C| \ge n+s-k$ and $v \in V(H)$, then since $d_{G'}(v) \ge k$ and since $d_{G'}(u) + d_{G'}(v) \le n+s-2$ holds for any pair of nonadjacent vertices $\{u, v\} \subseteq V\big(G'\big)$, we can conclude that v will be adjacent with every vertex of C, contrary to the maximality of C. Otherwise, $|C| = n+s-k-1$ and hence $|V(H)| = k+1-s$.

Since $|C| = n+s-k-1$, each vertex of C has degree at least $n+s-k-2$. We call a vertex in C as a frontier vertex if it has degree at least $n+s-k-1$ in G', i.e., it has at least one neighbor in H. By the maximality of C, we can see that every vertex in H has degree exactly k in G'. Let $F = \big\{u_1, u_2, \ldots, u_p\big\}$ be the set of frontier vertices.

If $p \ge 1$, then every vertex in H is adjacent to every frontier vertex in G', as $C_{n+s-1}(G) = G'$. Thus, $G\big[V(H)\big] \cong H_0$ is a $(k-p)$-regular graph. Since $0 \le k-p \le k-s = |V(H)|-1$, we have $s \le p \le k$. Now, we can conclude that $G' \in \mathbb{G}_n(p, s, k)$, where $\max\{s,\ 1\} \le p \le k$.

Otherwise, $p = 0$. In this case, since $C_{n+s-1}(G) = G'$ and $\delta(G') \ge k$, $G\big[V(H)\big] \cong H_0$ is a k-regular graph, and hence $G \cong H_0 \cup K_{n+s-k-1} \in \mathbb{G}_n(0, s, k)$ (here, since $|V(H_0)| = k+1-s$ and H_0 is k-regular, we have $s \le 0$). ■

Lemma 3.2 ([5]). *If G is a graph with n vertices and $e(G)$ edges, then*

$$\mu(G) \le \frac{2e(G)}{n-1} + n - 2,$$

where the equality holds if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Lemma 3.3 ([10,13]). *Let G be a graph with n vertices, $e(G)$ edges and minimum degree $\delta(G)$. If $\delta(G) \ge k \ge 1$, then*

$$\rho(G) \le \frac{1}{2}\left(k - 1 + \sqrt{(k+1)^2 + 8e(G) - 4nk}\right).$$

Theorem 3.1. *Let α be a real number such that $0 \le \alpha \le 1$ and let s and k be two integers. For any graph G with n vertices and minimum degree $\delta(G) \ge k \ge \max\{1, s\}$, if $\Theta(G, \alpha) > \Theta_0$, then $e(G) > \varepsilon_0$.*

Proof. By contradiction, we assume that $e(G) \leq \varepsilon_0$. Since $0 \leq \alpha \leq 1$, we have $A(G) + \alpha D(G) = \alpha Q(G) + (1-\alpha)A(G)$. Combining this with Lemmas 3.2–3.3, it follows that

$$\begin{aligned}\Theta_0 &< \Theta(G,\alpha) \leq \alpha\mu(G) + (1-\alpha)\rho(G)\\ &\leq \alpha\left(\frac{2e(G)}{n-1} + n - 2\right) + \frac{1}{2}(1-\alpha)\left(k - 1 + \sqrt{(k+1)^2 + 8e(G) - 4nk}\right) \leq \Theta_0,\end{aligned}$$

a contradiction. ■

The Proof of Theorem 1.8. We may suppose that $C_{n+s-1}(G) \ncong K_n$. In this case, since $\Theta(G,\alpha) > \Theta_0$, Theorems 1.10 and 3.1 imply that $C_{n+s-1}(G) \in \mathbb{G}_n(p,s,k)$ holds for some integer p, where $\max\{s,\ 0\} \leq p \leq k$. ■

4. The Proof of Theorem 1.9

In what follows, we always suppose that $\alpha \geq 0$. By Rayleigh's theorem, we have

Lemma 4.1 (*see [12]*). *Let G be a connected graph with n vertices and let $\psi = \left(\psi(v_1), \psi(v_2), \ldots, \psi(v_n)\right)^T$ be any non-zero vector defined on $V(G)$. If $H \subset G$, then $\Theta(H,\alpha) < \Theta(G,\alpha) \leq \left(1+\alpha\right)\Delta(G)$. Furthermore,*

$$\Theta(G,\alpha)\psi^T\psi \geq \psi^T\left(A(G) + \alpha D(G)\right)\psi = 2\sum_{uv\in E(G)} f(u)f(v) + \alpha\sum_{i=1}^{n} d_G(v_i)f^2(v_i), \tag{4.1}$$

where the equality holds if and only if ψ is an eigenvector of $\Theta(G,\alpha)$.

If G is connected, since $A(G) + \alpha D(G)$ is non-negative irreducible matrix, there is a unique positive unit eigenvector $f = \left(f(v_1), f(v_2), \ldots, f(v_n)\right)^T$ corresponding to $\Theta(G,\alpha)$. In the sequel, we call f a *Perron vector* of G.

Lemma 4.2 (*[12]*). *Let u, v be two vertices of the connected graph G, and $w_1, w_2, \ldots, w_k$ $\left(1 \leq k \leq d_G(v)\right)$ be some vertices of $N(v) \setminus \left(N(u) \cup \{u\}\right)$. Let $G' = G + w_1u + w_2u + \cdots + w_ku - w_1v - w_2v - \cdots - w_kv$. If f is the Perron vector of G with $f(u) \geq f(v)$, then $\Theta(G',\alpha) > \Theta(G,\alpha)$.*

Given two distinct vertices u, v in a graph G such that $N_G(v) \setminus \left(N_G(u) \cup \{u\}\right) \neq \emptyset \neq N_G(u) \setminus \left(N_G(v) \cup \{v\}\right)$, we construct a new graph $G' = G'(u,v)$ via replacing all edges vw by uw for each $w \in N_G(v) \setminus \left(N_G(u) \cup \{u\}\right)$. This operation is called the *Kelmans transformation* from v to u (see [4]).

Corollary 4.1. *Let G be a connected graph. If G' is a graph obtained from G by some Kelmans transformation, then $\Theta(G',\alpha) > \Theta(G,\alpha)$.*

Proof. We use the idea as that in [4] and we suppose that G' is obtained from G by a Kelmans transformation from the vertex v to vertex u. Let f be the Perron vector of G. The key observation is that up to isomorphism G' is independent of u or v being the beneficiary if we apply the transformation from v to u. Indeed, in G' one of u or v will be adjacent to $N_G(u) \cup N_G(v)$, the other will be adjacent to $N_G(u) \cap N_G(v)$ (and if the two vertices are adjacent in G then they will remain adjacent also). Now, we may assume that $f(u) \geq f(v)$. Then, the result follows from Lemma 4.2. ■

Corollary 4.2. *Let $G \in \mathbb{G}_n(p,s,k)$ and let G_0 be the graph obtained from G by deleting one edge with two end vertices in $V_2(G)$ such that $\delta(G_0) \geq k \geq p \geq \max\{s,1\}$ and $n \geq p + k + 3 - s$. If G' is a graph obtained from G by deleting one edge and $\delta(G') \geq k$, then $\Theta(G',\alpha) \leq \Theta(G_0,\alpha)$, where the equality holds if and only if $G' \cong G_0$.*

Proof. Suppose that G' is a graph obtained from G by deleting one edge (say $e = w_0z_0$). Since $\delta(G) \geq k$ and $d_G(w) = k$ holds for each vertex $w \in V_3(G)$, we only need to consider the following three cases by symmetry:

(1) $\{w_0, z_0\} \subseteq V_1(G)$, (2) $z_0 \in V_1(G)$ and $w_0 \in V_2(G)$, (3) $\{w_0, z_0\} \subseteq V_2(G)$.

Let $G_1 = G - w_0z_0$ for $\{w_0, z_0\} \subseteq V_1(G)$, let $G_2 = G - w_0z_0$ for $z_0 \in V_1(G)$ and $w_0 \in V_2(G)$, and let $G_0 = G - w_0z_0$ for $\{w_0, z_0\} \subseteq V_2(G)$. To complete the proof of this result, it suffices to show that $\Theta(G_1,\alpha) < \Theta(G_2,\alpha) < \Theta(G_0,\alpha)$. Since $k \geq \max\{s,1\}$, we get $|V_3(G)| = k + 1 - s \geq 1$. We choose $w \in V_3(G)$.

For G_1, we choose $v \in V_2(G_1)$ and $w \in V_3(H)$, and we rewrite z_0 as u. In this case, $\{w_0\} = N_{G_1}(v) \setminus (N_{G_1}(u) \cup \{u\})$ and $w \in N_{G_1}(u) \setminus (N_{G_1}(v) \cup \{v\})$. It is easy to see that G_2 is isomorphic to the graph obtained from G_1 by a Kelmans transformation from v to u. By Corollary 4.1, $\Theta(G_1,\alpha) < \Theta(G_2,\alpha)$.

For G_2, we choose $v \in V_2(G_2) \setminus \{w_0\}$, and we rewrite z_0 as u. In this case, $\{w_0\} = N_{G_2}(v) \setminus (N_{G_2}(u) \cup \{u\})$ and $w \in N_{G_1}(u) \setminus (N_{G_1}(v) \cup \{v\})$. It is easy to see that G_0 is isomorphic to the graph obtained from G_2 by a Kelmans transformation from v to u. By Corollary 4.1, $\Theta(G_2,\alpha) < \Theta(G_0,\alpha)$. ■

Lemma 4.3. *Let s and k be two integers and let G be a proper subgraph of $\mathbb{G}_n(p,s,k)$ such that G contains $n \geq 6k+10-5s$ vertices and minimum degree $\delta(G) \geq k \geq \max\{1,s\}$. If $\max\{0,s\} \leq p \leq k$, then $\Theta(G,\alpha) \leq \Theta\left(N_{n,0}^{k,s},\alpha\right)$, with equality holding if and only if $G \cong N_{n,0}^{k,s}$.*

Proof. By Corollary 4.2 and Lemma 4.1, the result already holds for $p=k$. Thus, we may suppose that $0 \leq p \leq k-1$ in what follows. We consider the following two cases:

Case 1. $p=0$.

In this case, $s \leq 0$ and hence $G \subset K_{n+s-k-1} \cup H_0$, where H_0 is a k-regular graph with $k+1-s$ vertices. Recall that $\delta(G) \geq k$. Thus, G is obtained from $K_{n+s-k-1} \cup H_0$ by deleting some edges from $K_{n+s-k-1}$. Since $n \geq 6k+10-5s$, and $K_{n+s-k-2} \subset K_{n+s-k-1}-e \subset N_{n,0}^{k,s}$, Lemma 4.1 implies that

$$\Theta(H_0,\alpha) \leq (1+\alpha)k < (1+\alpha)(n+s-k-3) = \Theta\left(K_{n+s-k-2},\alpha\right) < \Theta(K_{n+s-k-1}-e,\alpha) < \Theta\left(N_{n,0}^{k,s},\alpha\right).$$

Thus,

$$\Theta(G,\alpha) \leq \Theta(K_{n+s-k-1}-e,\alpha) < \Theta\left(N_{n,0}^{k,s},\alpha\right),$$

and hence this result holds.

Case 2. $1 \leq p \leq k-1$.

In this case, since $p \geq \max\{0,s\} \geq s$ and since $n \geq 6k+10-5s$, we have $\max\{1,s\} \leq p \leq k-1$ and $n > p+k+9-s$. Suppose that $G_1 \in \mathbb{G}_n(p,s,k)$ and $G_2 \in \mathbb{G}_n(p+1,s,k)$. Let G and G' be the graphs obtained from G_1 and G_2 by deleting one edge from $V_2(G_1)$ and $V_2(G_2)$, respectively. By Corollary 4.2 and Lemma 4.1, it suffices to show that

$$\Theta(G,\alpha) < \Theta(G',\alpha). \tag{4.2}$$

For convenience, we may suppose that G is obtained from G_1 by deleting the edge w_0z_0 with $\{w_0,z_0\} \subseteq V_2(G_1)$, and we rewrite $\Theta(G,\alpha)$ as Θ. Let f be the Perron vector of G. We firstly prove the following claim:

Claim 1. For any pairs of vertices $\{u,v\} \subseteq V_3(G)$, we have $f(u)=f(v)$.

Proof of Claim 1. By contradiction, we assume that Claim 1 does not hold. Let $\{w_1,w_2\} \subseteq V_3(G)$ such that $f(w_1) = \max\{f(w): w \in V_3(G)\}$ and $f(w_2) = \min\{f(w): w \in V_3(G)\}$. Then, $f(w_1) > f(w_2)$. Note that $H_0 \cong G[V_3(G)]$. Thus,

$$\begin{aligned}\Theta(f(w_1)-f(w_2)) &= \alpha k(f(w_1)-f(w_2)) + \sum_{w\in N_{H_0}(w_1)} f(w) - \sum_{z\in N_{H_0}(w_2)} f(z)\\ &\leq \alpha k(f(w_1)-f(w_2)) + (k-p)(f(w_1)-f(w_2)).\end{aligned}$$

Recall that $f(w_1)-f(w_2)>0$. Thus, $\Theta-\alpha k-(k-p) \leq 0$.

On the other hand, Lemma 4.1 implies that $\Theta > \Theta(K_{n+s-k-2},\alpha) = (1+\alpha)(n+s-k-3)$. Combining this with $n \geq 6k-5s+10$, we have $\Theta-\alpha k-(k-p) \geq (1+\alpha)(n+s-k-3)-\alpha k-(k-p) = \alpha(n+s-3-2k)+n+s+p-3-2k \geq \alpha(4k-4s+7)+4k-4s+7+p > 0$, a contradiction.

Now, we can conclude that $f(w_1)=f(w_2)$. This completes the proof of Claim 1.

With the similar reason with Claim 1, we can set $x_1=f(w)$ for $w \in V_1(G)$, set $x_2=f(w)$ for $w \in V_2(G)\backslash\{w_0,z_0\}$, set $x_3=f(w_0)=f(z_0)$, and set $x_4=f(w)$ for $w \in V_3(G)$. Now, from $(A(G)+\alpha D(G))f = \Theta f$, it follows that

$$\begin{cases}\Theta x_1 = \alpha(n-1)x_1 + (k+1-s)x_4 + (p-1)x_1 + (n+s-k-3-p)x_2 + 2x_3,\\ \Theta x_2 = \alpha(n+s-k-2)x_2 + px_1 + (n+s-k-p-4)x_2 + 2x_3,\\ \Theta x_3 = \alpha(n+s-k-3)x_3 + px_1 + (n+s-k-p-3)x_2,\\ \Theta x_4 = \alpha k x_4 + (k-p)x_4 + px_1.\end{cases} \tag{4.3}$$

By the second to fourth equations of (4.3), we have

$$\begin{cases} x_2 = \dfrac{p\left(\Theta+2-\alpha(n+s-k-3)\right)}{\left(\Theta+2+p-(\alpha+1)(n+s-k-2)\right)\left(\Theta+2-\alpha(n+s-k-3)\right)-2\left(\Theta+1-\alpha(n+s-k-2)\right)}x_1,\\ x_3 = \dfrac{p\left(\Theta+1-\alpha(n+s-k-2)\right)}{\left(\Theta+2+p-(\alpha+1)(n+s-k-2)\right)\left(\Theta+2-\alpha(n+s-k-3)\right)-2\left(\Theta+1-\alpha(n+s-k-2)\right)}x_1,\\ x_4 = \dfrac{px_1}{\Theta-(\alpha+1)k+p}.\end{cases} \tag{4.4}$$

Now, from Lemma 4.1 we can deduce that

$$\begin{aligned}\Theta(G',\alpha) - \Theta(G,\alpha) &\geq f^T(A(G')+\alpha D(G'))f - f^T(A(G)+\alpha D(G))f\\ &= (k+1-s)(2x_2-x_4)x_4 + \alpha(k+1-s)x_2^2.\end{aligned} \tag{4.5}$$

By (4.5), to prove (4.2), it suffices to show that $2x_2 > x_4$, that is equivalent to

$$\Phi(\Theta) > 0, \tag{4.6}$$

where $\Phi(\Theta) = \Theta^2 + \Big(n+p+s+\alpha(1-2k)-3k\Big)\Theta - \alpha(\alpha+1)n^2 + \Big(\alpha\Big((\alpha+1)(4k-2s+5)+2-p\Big)+2\Big)n - \Big((k-s)(3k-s+5)+6k+6\Big)\alpha^2 - \Big((k-s)(3k-s+7-p)-3p+10k+12\Big)\alpha - 2(3k-p-s+3)$.

Combining this with $n \geq 6k-5s+10$ and $\Theta > (1+\alpha)(n+s-k-3)$, we have $\Phi'(\Theta) = 2\Theta+n+p+s+\alpha(1-2k)-3k > 2(1+\alpha)(n+s-k-3)+n+p+s+\alpha(1-2k)-3k = (2n+2s-4k-5)\alpha+3n+3s+p-5k-6 \geq 3n+3s+p-5k-6 \geq 13k+p-12s+24 > 0$.

Let $\Phi_1(n) = 2n^2-(6k+7-4s)n+2(2k-s)(k-s)+9k-7s+3$. Since $\Phi_1'(n) = 4n-(6k+7-4s) \geq 18k-16s+33 > 0$ by $n \geq 6k+10-5s$, $\Phi_1(n) \geq \Phi_1(6k+10-5s) = 8(k-s)(5k-4s)+(147k-132s)+133 > 0$. Combining with $\Phi'(\Theta) > 0$, $\Phi_1(n) > 0$ and $n \geq 6k-5s+10$, it follows that

$$\begin{aligned}\Phi(\Theta) &> \Phi((1+\alpha)(n+s-k-3))\\ &= \Big(2n^2-(6k+7-4s)n+2(2k-s)(k-s)+9k-7s+3\Big)\alpha\\ &\quad +(2n-4k+p+2s-3)(n+s-k-3)+2(n+p+s-3k-3)\\ &\geq (2n-4k+p+2s-3)(n+s-k-3)+2(n+p+s-3k-3)\\ &= 4k^2-(6n+6s+p-9)k+(n+s)(2n+2s+p-7)+3-p = \Phi_2(k).\end{aligned}$$

Since $n \geq 6k+10-5s$, we have

$$\Phi_2'(k) = 8k-(6n+6s+p-9) \leq \frac{4}{3}(n+5s-10)-(6n+6s+p-9) = -\frac{1}{3}(14n+3p-2s+13) < 0,$$

which implies that

$$\begin{aligned}\Phi(\Theta) &> \Phi_2(k) \geq \Phi_2\left(\frac{1}{6}(n+5s-10)\right)\\ &= \frac{1}{18}\Big(20n^2+(15p-16s+41)n+4(3p-4)-s(11+4s-3p)\Big) = \Phi_3(n).\end{aligned}$$

If $s \geq 1$, since $n \geq 6k+10-5s \geq 10+s$, it follows that $18\Phi_3'(n) = 40n+15p-16s+41 \geq 24s+15p+441 > 0$, and hence

$$\Phi(\Theta) > \Phi_2(k) \geq \Phi_3(n) \geq \Phi_3(s+10) = 9p+15s+ps+133 > 0.$$

If $s \leq 0$, since $n \geq 6k+10-5s \geq 10-5s$, it follows that $18\Phi_3'(n) = 40n+15p-16s+41 > 0$, and hence

$$\Phi(\Theta) > \Phi_2(k) \geq \Phi_3(n) \geq \Phi_3(10-5s) = 32s^2-(4p+132)s+9p+133 > 0.$$

Now, (4.6) holds and this completes the proof of this result. ■

Lemma 4.4. *Let α and q be two real numbers such that $0 \leq \alpha \leq 1$ and $0 \leq q < 1$. If $n \geq \max\Big\{\frac{1}{2}\big(3k+3+2q-2s\big),\ \frac{1}{2(1-q)}\big((k-q)(k+q-s)+(q-4)(s-3)-k(3q-7)-4\big),\ \frac{1}{2-q}\big((k-s)(3k-s+5)+4(k+2)-q\big)\Big\}$, then $(1+\alpha)(n+s-k-2)-q \geq \Theta_0$.*

Proof. Let $\Phi(\alpha) = (1+\alpha)(n+s-k-2)-q-\Theta_0$. Note that

$$\Phi'(\alpha) = s-k-\frac{2\varepsilon_0}{n-1}+\frac{1}{2}\left(k-1+\sqrt{(k+1)^2+8\varepsilon_0-4nk}\right).$$

Thus, $\Phi(\alpha) \geq \min\big\{\Phi(0),\ \Phi(1)\big\}$. To complete the proof of this result, it suffices to show that

$$\min\big\{\Phi(0),\ \Phi(1)\big\} \geq 0. \tag{4.7}$$

Since $2(1-q)n \geq (k-q)(k+q-s)+(q-4)(s-3)-k(3q-7)-4$, we have

$$\Phi(0) = n+s-\frac{3}{2}k-\frac{3}{2}-q-\sqrt{n^2-(3k-2s+5)n+\frac{(13k-3s)(k-s)+s(s-28)+46k+41}{4}} \geq 0.$$

Furthermore, since $(2-q)n \geq (k-s)(3k-s+5)+4(k+2)-q$, we have

$$\begin{aligned}\Phi(1) &= n+2s-2k-2-q-\frac{1}{n-1}\Big((n-k-2+s)(n-k-3+s)+2(k+1)(k+2-s)\Big)\\ &= \frac{1}{n-1}\Big((2-q)n-(k-s)(3k-s+5)-4(k+2)+q\Big) \geq 0.\end{aligned}$$

Now, we can conclude that (4.7) holds. ■

Lemma 4.5. *Let $\alpha \geq 0$ and $q > 0$ be two real numbers. If $n \geq \frac{1}{q}\Big((1-q)(\alpha-q)+\alpha+2\Big)$, then $\Theta\Big(K_n-e, \alpha\Big) \geq (1+\alpha)(n-1)-q$.*

Proof. Throughout the proof of this result, we rewrite $K_n - e$ as G and simplify $\Theta(G, \alpha)$ as Θ, where $e = w_0z_0$. Let f be the Perron vector of Θ. For convenience, let $x_1 = f(w)$ for $w \in V(G) \setminus \{w_0, z_0\}$ and let $x_2 = f(w)$ for $w \in \{w_0, z_0\}$. Now, from $\big(A(G) + \alpha D(G)\big)f = \Theta(G, \alpha)f$, it follows that

$$\begin{cases} \Theta x_1 = \alpha(n-1)x_1 + (n-3)x_1 + 2x_2, \\ \Theta x_2 = \alpha(n-2)x_2 + (n-2)x_1. \end{cases}$$

Thus, Θ satisfies

$$\Phi(\Theta) = \Theta^2 - \Big(\alpha(2n-3)+n-3\Big)\Theta + (\alpha+1)(n-2)\Big(\alpha(n-1)-2\Big),$$

which implies

$$\Theta = \frac{1}{2}\left(\alpha(2n-3)+n-3+\sqrt{n^2+2(\alpha+1)n+(\alpha+1)(\alpha-7)}\right).$$

Note that $qn \geq (1-q)(\alpha-q)+\alpha+2$. Thus, $\Theta \geq (1+\alpha)(n-1)-q$. ■

The Proof of Theorem 1.9. When $q = \frac{1}{2}$, since $n \geq 6k-5s+10 > \frac{1}{2}\big(3k+4-2s\big) = \frac{1}{2}\big(3k+3+2q-2s\big)$ and $0 \leq \alpha \leq 1$, we have

$$n+s-k-1 \geq 6k-5s+10+s-k-1 > \frac{13}{2} \geq 3\alpha+\frac{7}{2} = \frac{1}{q}\Big((1-q)(\alpha-q)+\alpha+2\Big).$$

Combining this with $K_{n+s-k-1} - e \subset N^{k,s}_{n,0}$ and $\alpha \geq 0$, by setting $q = \frac{1}{2}$ in Lemmas 4.4 and 4.5 it follows that

$$\Theta\left(N^{k,s}_{n,0}, \alpha\right) > \Theta\big(K_{n+s-k-1} - e, \alpha\big) \geq \Theta_0. \tag{4.8}$$

If $C_{n+s-1}(G) \ncong K_n$, then $k \leq \frac{1}{2}\big(n+s-2\big)$ and Theorem 1.8 implies that $C_{n+s-1}(G) \in \mathbb{G}_n(p, s, k)$ for some integer p, where $\max\{0, s\} \leq p \leq k$. Hence, Theorem 1.9 follows from Lemma 4.3. ■

Remark 4.1. By an observation to the proof of Theorem 1.9, we can improve the lower bound for n of Theorem 1.9 by setting suitable q in Lemmas 4.4 and 4.5, where $0 < q < 1$.

5. The proof of Proposition 1.2

This section dedicates to the proof of Proposition 1.2.

The Proof of Proposition 1.2. In the proof of this result, we rewrite $N^{k,s}_{n,0}$ as G and we suppose that $N^{k,s}_{n,0} = N^{k,s}_n - w_0z_0$. Note that $e(G) = \frac{1}{2}(n+s-k-1)(n+s-k-2)+k(k+1-s)-1$. Thus, (1.1) follows from Lemma 3.2. To complete the proof of this result, it suffices to show that $\rho(G) < n+s-k-2$.

Let f be the Perron vector of G, and let $\rho = \rho(G)$. For convenience, let $x_1 = f(w)$ for $w \in V_1(G)$, let $x_2 = f(w)$ for $w \in V_2(G)\backslash\{w_0, z_0\}$, let $x_3 = f(w_0) = f(z_0)$, and let $x_4 = f(w)$ for $w \in V_3(G)$. Now, from $(A(G))f = \rho f$, it follows that

$$\begin{cases} \rho x_1 = (k-1)x_1 + (n-2k-3+s)x_2 + 2x_3 + (k+1-s)x_4, \\ \rho x_2 = kx_1 + (n+s-2k-4)x_2 + 2x_3, \\ \rho x_3 = kx_1 + (n+s-2k-3)x_2, \\ \rho x_4 = kx_1. \end{cases} \tag{5.1}$$

From the second and third equations of (5.1), we have $(\rho+1)x_2 = (\rho+2)x_3$. Now, from the second equation of (5.1), we have

$$x_2 = \frac{k(\rho+2)}{(\rho+4+2k-n-s)(\rho+2)-2(\rho+1)}x_1. \tag{5.2}$$

Furthermore, combining with $(\rho+1)x_2 = (\rho+2)x_3$, by the first and fourth equations of (5.1), we have

$$x_2 = \frac{(\rho+2)\big((\rho-k)(\rho+1)-k(k-s)\big)}{\rho\big((n-2k-3+s)(\rho+2)+2(\rho+1)\big)}x_1. \tag{5.3}$$

By (5.2) and (5.3), ρ satisfies $0 = \Phi(\rho) = \rho^4 - (n-k+s-5)\rho^3 - \Big((k-2)(k-s)+3n+s-10\Big)\rho^2 - \Big(k(k-s)(2k-n-s+5) - (n-k-2)k + 2(n+s-3)\Big)\rho + 2k(k-s+1)(n+s-2k-3)$.

Let $\Phi\big(n+s-k-2\big) = 2n^2 - \Big(\big(k^2+4\big)(k-s)+k^2+6\Big)n + (k-s+1)(k^3-sk^2-2s+4) = \Phi_1(n)$.

Claim 1. $\Phi\big(n+s-k-2\big) = \Phi_1(n) > 0$.

Proof of Claim 1. We consider the following two cases:

Case 1. $k \geq s+1$.

In this case, since $n \geq \frac{1}{2}\big((k^2+4)(k+1-s)+2\big)$, we have

$$\Phi_1'(n) \geq \Phi_1'\left(\frac{1}{2}\big((k^2+4)(k+1-s)+2\big)\right) = 4(k-s)+k^2(k-s+1)+6 > 0.$$

Combining this with $k \geq s+1$, we can conclude that

$$\begin{aligned}\Phi_1(n) &\geq \Phi_1\left(\frac{1}{2}\big((k^2+4)(k+1-s)+2\big)\right)\\ &= (k-s+1)\big(k^2(k-s)-2s+4\big) \geq 2\big(k^2-2s+4\big) > 0,\end{aligned}$$

and hence Claim 1 holds.

Case 2. $k = s$.

In this case, $k = s \geq 1$. Since $n \geq \frac{1}{2}\big(k^2(k+1)+6\big)$ and $k = s$, we have

$$\Phi_1'(n) \geq \Phi_1'\left(\frac{1}{2}\big(k^2(k+1)+6\big)\right) = 2s^3+s^2+6 > 0.$$

Now, we can conclude that

$$\Phi_1(n) \geq \Phi_1\left(\frac{1}{2}\big(k^2(k+1)+6\big)\right) = \frac{1}{2}(s+2)\left(s^4(s-1)+2s^3+2(s-1)^2+2\right) > 0,$$

and hence Claim 1 holds. This completes the proof of Claim 1.

In what follows, let $\rho_1 \geq \rho_2 \geq \rho_3 \geq \rho_4$ be the four roots of $\Phi(\rho) = 0$. Then, $\rho_1+\rho_2+\rho_3+\rho_4 = n-k+s-5$. Now, $\Phi(\rho) \to +\infty$ as $\rho \to +\infty$ and $\Phi\big(n+s-k-2\big) > 0$ by Claim 1. Since the sum of four roots of $\Phi(\rho) = 0$ is equal to $n+s-k-5$, either no roots are in $\big(n+s-k-2, +\infty\big)$ or exactly two roots are in $\big(n+s-k-2, +\infty\big)$.

If no roots are in $\big(n+s-k-2, +\infty\big)$, then $\rho(G) = \rho_1 < n+s-k-2$ and we are done. Otherwise, we must have exactly two roots are in $\big(n+s-k-2, +\infty\big)$, that is, $\rho_1 \geq \rho_2 > n+s-k-2$ in what follows.

When $k(k+1-s) \geq 2$, then $\Phi(-2) = 4-2k(k+1-s) \leq 0$. Combining this with $\Phi(n+s-k-2) > 0$ by Claim 1, there is at least one root in $[-2, n+s-k-2)$, and hence $\rho_3 \geq -2$. Since the absolute value of any eigenvalue of $A(G)$ is not greater than the spectral radius of G, namely, ρ_1, we have $\rho_1+\rho_4 \geq 0$. Thus,

$$n+s-k-5 = \sum_{i=1}^{4}\rho_i \geq \rho_2+\rho_3 > n+s-k-2-2 > n+s-k-5, \quad \text{a contradiction.}$$

When $k(k+1-s) \leq 1$, then $k = s = 1$. In this case, we have

$$\Phi(\rho) = \rho^4-(n-5)\rho^3-(3n-9)\rho^2-(n-1)\rho+2n-8.$$

Recall that $n \geq 6k-5s+10 = 11$. Thus, it is easy to see that $\Phi(0) = 2(n-4) > 0$ and $\Phi(n-3) = -n^3+8n^2-21n+16 = -n^2(n-8)-21n+16 < 0$. Combining this with $\Phi(n-2) > 0$ by Claim 1, we have $0 < \rho_4 < n-3 < \rho_3$. Since $\rho_1+\rho_2+\rho_3+\rho_4 = n+s-k-5$ and $\rho_1 > n+s-k-2$, we must have $\rho_4 < 0$, a contradiction. ■

6. Further discussion

Recently, Zhou et al. [21] showed that: If $\delta(G) \geq k \geq 2$ and $\mu(G) \geq 2(n-k)$, where $n \geq k^4+5k^3+2k^2+8k+12$, then G is Hamilton-connected unless G is either obtained from $N_n^{k,2}$ deleting at most $\frac{1}{4}k(k-1)$ edges or G is obtained from $M_n^{k,2}$ by deleting at most $\frac{1}{2}(k-1)$ edges. This result strengthens that of Theorem 1.9 for $s = 2$ and $\alpha = 1$.

In Lemma 4.4, we have showed that $\Theta_0 \leq (1+\alpha)(n+s-k-2)-q$ for $0 \leq \alpha \leq 1$, $0 \leq q < 1$, and $n \geq \max\Big\{\frac{1}{2}\big(3k+3+2q-2s\big), \frac{1}{2(1-q)}\big((k-q)(k+q-s)+(q-4)(s-3)-k(3q-7)-4\big), \frac{1}{2-q}\big((k-s)(3k-s+5)+4(k+2)-q\big)\Big\}$. Note that $\Theta_0 \leq 2(n-k)-q \leq 2n-2k$ for $s = 2$, $0 \leq q < 1$ and $\alpha = 1$. By Theorem 1.8 and Proposition 1.4, to improve Zhou's result, it suffices to give the characterization of those proper subgraphs G of $N_n^{k,2}$ and $M_n^{k,2}$ such that $\Theta(G,\alpha) > \Theta_0$.

As in Remark 4.1, we can improve the lower bounds for n in Theorem 1.9 such that

$$\Theta_0 \leq (1+\alpha)(n+s-k-2)-q \leq \Theta\left(K_{n+s-k-1}-e, \alpha\right)$$

by setting suitable positive real number q.

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Extremal graphs for vertex-degree-based invariants with given degree sequences☆

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ABSTRACT

For a symmetric bivariable function $f(x, y)$, let the *connectivity function* of a connected graph G be $M_f(G) = \sum_{uv\in E(G)} f(d(u), d(v))$, where $d(u)$ is the degree of a vertex u. In this paper, we prove that for an escalating (de-escalating) function $f(x, y)$, there exists a BFS-graph with the maximum (minimum) connectivity function $M_f(G)$ among all graphs with a c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ and $d_n = 1$, and obtain the majorization theorem for connectivity function for unicyclic and bicyclic degree sequences. Moreover, some applications of graph invariants based on degree are included.

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1. Introduction

Throughout this paper, G denotes a simple connected graph with n vertices and m edges, unless specified otherwise. If $m = n + c - 1$, then G is called a *c-cyclic graph*. In particular, when $c = 0$, 1 or 2, then G is called a *tree*, *unicyclic graph* or *bicyclic graph*, respectively. As usual, denote $N_G(v)$ by the neighbor set of vertex v in G, $d_G(v)$ by the degree of v, and $N_G[v] = N_G(v) \cup \{v\}$, respectively. When there is no confusion, we simplify $N_G(v)$, $N_G[v]$ and $d_G(v)$ as $N(v)$, $N[v]$ and $d(v)$, respectively. If $d(v) = 1$, then v is called a *pendant vertex*. The nonnegative integer sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v_i)$ holds for $1 \le i \le n$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$. Moreover, we use d_i to denote the ith largest degree of G and $d(v_i) = d_i$, for $1 \le i \le n$. Let $\Gamma(\pi)$ be the set of all connected graphs with a given degree sequence π.

Among those vertex-degree-based graph invariants, the *Randić index* $R(G)$ [13] and *second Zagreb index* $M_2(G)$ [5] are two famous topological indices, where

$$R(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-\frac{1}{2}}, \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} (d(u)d(v)).$$

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Bollobás and Erdős [1] generalized the concepts of Randić index and second Zagreb index to the *general Randić index* $W_\alpha(G)$, where

$$W_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^\alpha.$$

Similarly with the general Randić index of G, the *general sum-connectivity index* [24] $\chi_\alpha(G)$ of G is defined to be

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u)+d(v))^\alpha,$$

where $\chi_{-\frac{1}{2}}(G)$ is known as the *sum-connectivity index* of G [23], $\chi_2(G)$ is also called the *third Zagreb index* of G [14], while $2\chi_{-1}(G)$ is equal to the *harmonic index* of G [3]. The *reformulated Zagreb index* $Z_2(G)$ of G [12] is a slight modification of $\chi_2(G)$, where

$$Z_2(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^2.$$

Another famous vertex-degree-based graph invariants, called the *Atom-Bond connectivity index* of G [2], is defined as follows:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

For more results on vertex-degree-based graph invariants, one can refer to [4,8,17,18]. In order to study on such graph invariants based on adjacency vertex degree, Wang [16] recently proposed a new symmetric function.

A symmetric bivariate function $f(x,y)$ defined on positive real numbers is called *escalating* (de-escalating) (see [16]) if

$$f(x_1,x_2)+f(y_1,y_2) \geq (resp.\ \leq) f(y_1,x_2)+f(x_1,y_2) \tag{1.1}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (1.1) is strict if $x_1 > y_1$ and $x_2 > y_2$. Furthermore, an escalating (de-escalating) function $f(x,y)$ is called a *good escalating (de-escalating) function,* if $f(x,y)$ satisfies

$$\frac{\partial f(x,y)}{\partial x} > 0, \quad \frac{\partial^2 f(x,y)}{\partial x^2} \geq 0,$$

and

$$f(x_1+1,x_2)+f(x_1+1,y_1-1) \geq f(x_2,y_1)+f(x_1,y_1)$$

holds for any $x_1 \geq y_1$ and $x_2 \geq 1$.

Further, Wang [16] defined the *connectivity function* of a connected graph G associated with a symmetric bivariate function $f(x,y)$ to be

$$M_f(G) = \sum_{uv\in E(G)} f\left(d(u),d(v)\right). \tag{1.2}$$

For a connected graph G with root v_0, denote $h_G(v)$ by the distance between v and v_0, and $\mathcal{A}_i(G) = \left\{v : h_G(v) = i \text{ and } v \in V(G)\right\}$. Then $\mathcal{A}_0(G) = \{v_0\}$. If there is no confusion, we simply write $h(v)$ and $\mathcal{A}_i$ in place of $h_G(v)$ and $\mathcal{A}_i(G)$, respectively.

Definition 1.1. Let G be a connected graph. If there exists an ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ satisfying the following (i) and (ii), then G is called a *BFS-graph* (see [20]):

(i) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$.

(ii) let $v \in N(u)\setminus N(w), z \in N(w)\setminus N(u)$ such that $h(u) = h(w) = h(v)-1 = h(z)-1$. If $u \prec w$, then $v \prec z$.

In some literatures, a *BFS*-tree is also called a *greedy tree* (see [16,22]). It is well-known that the *BFS*-tree is unique for any given tree degree sequence π [20]. Recently, Wang in [16] proved the following important result.

Theorem 1.1 ([16]). *For an escalating function $f(x,y)$, the connectivity function $W_f(T)$ is maximized by the greedy tree among trees with a given degree sequence.*

Later, Zhang et al. [22] studied relations between the extremal trees of two different degree sequences. In order to state their results, we need the following notation. Let $\pi = (x_1,x_2,\ldots,x_n)$ and $\pi' = (x_1',x_2',\ldots,x_n')$ be two different non-increasing sequences of nonnegative real numbers, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^n x_i = \sum_{i=1}^n x_i'$, and $\sum_{i=1}^j x_i \leq \sum_{i=1}^j x_i'$ for all $j = 1,2,\ldots,n$. Such an ordering is sometimes called *majorization* (for example, see [11]). Zhang et al. in [22] proved the following majorization theorem:

Theorem 1.2 ([22]). *Given two tree degree sequences π and π' and an escalating function with $\frac{\partial f(x,y)}{\partial x} > 0$, and $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$, let T_π^* and $T_{\pi'}^*$ be the two trees with the maximum connectivity function $M_f(T)$ with degree sequences π and π', respectively. If $\pi \lhd \pi'$, then $M_f(T_\pi^*) \leq M_f(T_{\pi'}^*)$.*

Motivated by the above results, we continue to study on the properties of connectivity function for (good) escalating or de-escalating functions for c-cyclic graphs. The rest of this paper is organized as follows. In Section 2, we prove that for an escalating (de-escalating) function $f(x, y)$, there exists a BFS-graph G with the maximum (minimum) connectivity function $M_f(G)$ among all graphs with a c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ and $d_n = 1$. In Section 3, the majorization theorem for connectivity function is obtained for a good escalating function for tree, unicyclic and bicyclic degree sequences. In Section 4, the properties of some graph invariants based on degree are obtained.

2. The extremal graphs of $\Gamma(\pi)$

Hereafter, we call G an extremal graph of some graph category $\mathcal{G}$ if either $M_f(G)$ is maximized in $\mathcal{G}$ when $f(x, y)$ is escalating or $M_f(G)$ is minimized in $\mathcal{G}$ when $f(x, y)$ is de-escalating.

Let $G - uv$ (respectively, $G - u$) denote the graph obtained from G by deleting the edge $uv \in E(G)$ (respectively, vertex u and the edges incident with it). Similarly, $G + uv$ is a graph obtained from G by adding an edge $uv \notin E(G)$.

Lemma 2.1. *Let $G = (V, E)$ be a connected graph with $u_1w_1 \in E$, $u_2w_2 \in E$, $w_1w_2 \notin E$ and $u_1u_2 \notin E$, $d(w_1) \geq d(u_2)$ and $d(w_2) \geq d(u_1)$. Let $G' = G - u_1w_1 - u_2w_2 + w_1w_2 + u_1u_2$.*

(i) If $f(x, y)$ is escalating, then $M_f(G') \geq M_f(G)$. Moreover $M_f(G') > M_f(G)$ if and only if $d(w_1) > d(u_2)$ and $d(w_2) > d(u_1)$.

(ii) If $f(x, y)$ is de-escalating, then $M_f(G') \leq M_f(G)$. Moreover $M_f(G') < M_f(G)$ if and only if $d(w_1) > d(u_2)$ and $d(w_2) > d(u_1)$.

Proof. By (1.2) and $f(d(u_1), d(u_2)) = f(d(u_2), d(u_1))$, we have

$$M_f(G') - M_f(G) = f(d(w_1), d(w_2)) + f(d(u_2), d(u_1)) - f(d(u_2), d(w_2)) - f(d(u_1), d(w_1)).$$

Hence the results follow from the definitions of escalating and de-escalating functions. ■

Hereafter, let P_{uv} be a shortest path connecting u and v in G, and let C_q be a cycle with q vertices.

Lemma 2.2. *Let $G \in \Gamma(\pi)$. If there exist three vertices u, v, w of G such that $uv \in E(G)$, $uw \notin E(G)$, $d(v) < d(w) \leq d(u)$, and $d(u) > d(x)$ for all $x \in N(w)$, then G is not an extremal graph of $\Gamma(\pi)$.*

Proof. We firstly suppose that $uv \notin P_{uw}$, and we may suppose that $z \in N(w) \cap V(P_{uw})$. If $vz \notin E(G)$, let $G_1 = G+vz+uw-wz-uv$. Clearly, $G_1 \in \Gamma(\pi)$. Since $d(u) > d(z)$ and $d(w) > d(v)$, the result follows from Lemma 2.1. If $vz \in E(G)$, then there exists a vertex $w' \in N(w)$ such that $w' \notin N[v]$ and $w' \notin V(P_{uw})$ by $d(w) > d(v)$. Let $G_2 = G+vw'+uw-ww'-uv$. Then $G_2 \in \Gamma(\pi)$. Note that $d(u) > d(w')$ and $d(w) > d(v)$. Thus the result follows from Lemma 2.1.

We secondly consider the case of $uv \in P_{uw}$. In this case, since $d(w) > d(v)$, there exists a vertex $w'' \in N(w) \setminus V(P_{uw})$ such that $w'' \notin N[v]$. Let $G_3 = G + vw'' + uw - ww'' - uv$. Clearly, $G_3 \in \Gamma(\pi)$ and hence the result follows from Lemma 2.1. ■

Lemma 2.3. *If π is a c-cyclic degree sequence with $c \geq 0$, then there exists an extremal graph $G \in \Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$.*

Proof. Let G be an extremal graph of $\Gamma(\pi)$. If $v_1v_2 \notin E(G)$, then there is some vertex v such that $v_1v \in E(G)$ and $d(v_1) \geq d(v_2) > d(v)$ and $d(v_1) > d(x)$ holds for all $x \in N(v_2)$, which contradicts Lemma 2.2. Thus, $v_1v_2 \in E(G)$. Now, we assume that $v_1v_3 \notin E(G)$. Then, $d(v_3) > d(v)$ holds for every $v \in N(v_1) \setminus \{v_2\}$. By Lemma 2.2, we may assume that there exists some vertex $u \in N(v_3)$ such that $d(u) = d_1$. If $u = v_2$, the result already holds. Otherwise, $u \neq v_2$, and hence $d(u) = d_1 = d_2 = d_3$.

If $v_2 \notin V(P_{v_1v_3})$, choose $u_0 \in N(v_1) \cap V(P_{v_1v_3})$. Since $v_1 \in N(u_0) \setminus N(v_3)$, there must exist some vertex $v_0 \in N(v_3) \setminus V(P_{v_1v_3})$ such that $v_0 \notin N[u_0]$. Let $G_1 = G+v_1v_3+u_0v_0-v_1u_0-v_3v_0$. By Lemma 2.1 and $G_1 \in \Gamma(\pi)$, the result already holds. Otherwise, $v_2 \in V(P_{v_1v_3})$. In this case, $v_1 \notin P_{v_2v_3}$ and $d_1 = d_2 = d_3$. Now, it can be proved similarly with the case $v_2 \notin V(P_{v_1v_3})$. ■

Let $N_G(v, p)$ be the neighbor set of vertices of v in G with degree at least p.

Lemma 2.4. *Let C_q be a cycle of an extremal graph G of $\Gamma(\pi)$ with $w_1w_2 \in E(C_q)$ and $P = u_1 \cdots u_{s-1}u_s$ be a path connecting u_1 and u_s such that $u_1 \in V(C_q)$ and $d(w_1) \geq d(w_2) > d(u_s)$. If $d(u_k) \geq d(w_2)$ holds for some vertex $u_k \in V(P) \setminus \{u_1\}$, $N(w_1) \cap \{u_k, u_{k+1}, \ldots, u_s\} = \emptyset$ and $N(w_2) \cap \{u_{k+1}, u_{k+2}, \ldots, u_s\} = \emptyset$, then there exists an extremal graph G' of $\Gamma(\pi)$ such that $P' = u_1u_2 \cdots u_k$ is a part of one cycle in G' with $N_G(u_k, d(w_2)) \subseteq N_{G'}(u_k, d(w_2))$ and $N_G(u_i) = N_{G'}(u_i)$, where $2 \leq i \leq k-1$. Furthermore, every cycle of G, which do not contain the edge w_1w_2, is also a cycle of G'.*

Proof. By the hypothesis, we may suppose that u_k is the last vertex of P such that $d(u_k) \geq d(w_2)$, namely, $\max\{d(u_j) : k+1 \leq j \leq s\} < d(w_2)$. Since $d(u_s) < d(w_2)$, we have $2 \leq k \leq s-1$. If $P' = u_1u_2 \cdots u_k$ is a part of some cycle of G, then the result already holds by setting $G' = G$. Thus, we may suppose that $P' = u_1u_2 \cdots u_k$ is not a part of any cycle of G.

Let $G_1 = G + w_1u_k + w_2u_{k+1} - w_1w_2 - u_ku_{k+1}$. Since $d(w_2) \leq d(u_k)$ and $d(w_1) \geq d(w_2) > d(u_{k+1})$, G_1 is also an extremal graph of $\Gamma(\pi)$ by Lemma 2.1. In this case, $P' = u_1u_2 \cdots u_k$ is a part of one cycle of G_1 such that $N_G(u_k, d(w_2)) \subseteq N_{G_1}(u_k, d(w_2))$ and $N_G(u_i) = N_{G_1}(u_i)$, where $2 \leq i \leq k-1$. Furthermore, every cycle of G, which does not contain the edge w_1w_2, is also a cycle of G_1. Thus, the result holds. ■

Remark 2.1. By an observation to the proof of Lemma 2.4, $u_1 \in \{w_1, w_2\}$ is also permitted and $u_1 \notin \{w_1, w_2\}$ guarantees the existence of an extremal graph G' of $\Gamma(\pi)$ such that $P' = u_1u_2\cdots u_k$ is a part of one cycle in G' with $N_G(u_k, d(w_2)) \subseteq N_{G'}(u_k, d(w_2))$ and $N_G(u_i) = N_{G'}(u_i)$, where $1 \le i \le k-1$.

Let G be a connected graph with $X \subseteq V(G)$. Denote by $G[X]$ the subgraph induced by X, and denote by $\mathcal{R}(G)$ the *base graph* obtained from G by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. If G is a c-cyclic graph, it is easy to see that $\mathcal{R}(G)$ is also a c-cyclic graph for $c \ge 1$ and $\mathcal{R}(G) = \emptyset$ holds for $c = 0$.

Lemma 2.5. *Let π be a c-cyclic degree sequence. If $c \ge 1$ and $d_n = 1$, then there exists an extremal graph G of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle.*

Proof. It suffices to prove the following four claims:

Claim 1. *There exists an extremal graph G of $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$ and v_1 lies on a cycle of G.*

By Lemma 2.3, there is an extremal graph $G \in \Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$. We assume that Claim 1 does not hold.

If $v_1 \notin V(\mathcal{R}(G))$, then there must exist one edge w_1w_2 in a cycle and one vertex u in $N(v_1)$ such that $u \notin V(\mathcal{R}(G))$ and $d(u) \ge d(w_1) \ge d(w_2)$ (since $\{v_2, v_3\} \subseteq N(v_1)$). By Lemma 2.4 and Remark 2.1, there exists an extremal graph G_1 of $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N_{G_1}(v_1)$ and v_1 lies on a cycle of G_1, a contradiction.

Otherwise, $v_1 \in V(\mathcal{R}(G))$. Now, since v_1 does not lie on any cycle of G, v_1 is a cut vertex and $G - v_1$ contains d_1 components, say $D_1, D_2, \ldots, D_{d_1}$. Since $d_n = 1$, we may suppose that v_n lies on D_1 and D_2 is a component containing a cycle (recall that $v_1 \in V(\mathcal{R}(G))$, $G - v_1$ contains at least two components containing cycles). In this case, by Lemma 2.4 and Remark 2.1, there exists an extremal graph G_2 of $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N_{G_2}(v_1)$ and v_1 lies on a cycle of G_2, a contradiction. This completes the proof of Claim 1.

Claim 2. *There exists an extremal graph G of $\Gamma(\pi)$ such that v_1v_2 lies on a cycle of G and $\{v_2, v_3\} \subseteq N(v_1)$.*

By Claim 1, we may directly suppose that G is an extremal graph of $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$ and v_1 lies on some cycle C_q of G. We assume that Claim 2 does not hold. Let $d(w_0) = \max\{d(v) : v \in V(C_q) \setminus \{v_1\}\}$. If $d(w_0) \ge d(v)$ for some vertex $v \in N(v_2) \setminus \{v_1\}$, then $vw \notin E(G)$ and $v_2w_0 \notin E(G)$, where $w \in (N(w_0) \cap V(C_q)) \setminus \{v_1\}$ (otherwise, Claim 2 already holds). Let $G_3 = G + v_2w_0 + vw - w_0w - v_2v$. Since $d(w_0) \ge d(v)$ and $d(v_2) \ge d(w)$, G_3 is an extremal graph of $\Gamma(\pi)$ such that Claim 2 holds, a contradiction. Otherwise, $2 \le d(w_0) < d(v)$ holds for each $v \in N(v_2)$. Let $v' \in N(v) \setminus \{v_2\}$ and let $w' \in (N(v_1) \cap V(C_q)) \setminus \{v_3\}$, where $v \in N(v_2) \setminus \{v_1\}$. Since Claim 2 does not hold, $v_1v \notin E(G)$ and $v'w' \notin E(G)$. Let $G_4 = G + v_1v + v'w' - v_1w' - vv'$. Since $d(v_1) \ge d(v')$ and $d(v) > d(w_0) \ge d(w')$, G_4 is an extremal graph of $\Gamma(\pi)$ such that Claim 2 holds. This completes the proof of Claim 2.

Claim 3. *There is an extremal graph G of $\Gamma(\pi)$ such that v_1v_2 and v_1v_3 lie on a cycle of G.*

By Claim 2, we may directly suppose that G is an extremal graph of $\Gamma(\pi)$ such that v_1v_2 lies on a cycle of G and $\{v_2, v_3\} \subseteq N(v_1)$. Choose $u_0 \in (V(C_q) \cap N(v_2)) \setminus \{v_1\}$.

If Claim 3 does not hold, then $v_2v_3 \notin E(G)$, $u_0v_3 \notin E(G)$ and there exists $v_0 \in N(v_3) \setminus \{v_1\}$ such that $v_0 \notin N[u_0]$ (as $d(v_3) \ge d(u_0) \ge 2$), let $G_5 = G + v_2v_3 + u_0v_0 - v_0v_3 - u_0v_2$. By Lemma 2.1, G_5 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle of G_5, a contradiction. Thus, Claim 3 holds.

Claim 4. *There is an extremal graph G of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle of G.*

By Claim 3, we may directly suppose that G is an extremal graph of $\Gamma(\pi)$ such that $\{v_1v_2, v_1v_3\}$ are two edges of some cycle of G, while $v_2v_3 \notin E(G)$. Furthermore, we may suppose that

$$q = \min\{p, \text{ where } v_1v_2 \in E(C_p) \text{ and } v_1v_3 \in E(C_p)\},$$

and hence $|N(v_2) \cap V(C_q)| = |N(v_3) \cap V(C_q)| = 2$. We assume that Claim 4 does not hold. Two cases occur as follows:

Case 1. $d_2 \ge 3$.

Choose $w_1 \in (N(v_3) \cap V(C_q)) \setminus \{v_1\}$. If there exists some vertex $w_2 \in N(v_2) \setminus V(C_q)$ such that $w_1w_2 \notin E(G)$, then let $G_6 = G + v_2v_3 + w_1w_2 - w_2v_2 - w_1v_3$. By Lemma 2.1, G_6 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle in G_6, and hence Claim 4 holds, a contradiction. Otherwise, $w \in N(w_1)$ holds for each $w \in N(v_2) \setminus V(C_q)$, which implies that $d(v_2) = d(v_3) = d(w_1) \ge 3$.

Note that $v_1w_1 \notin E(G)$. Otherwise, $\{v_1, v_3, w_1\}$ forms a triangle of G, and hence Claim 4 holds (since $d(v_2) = d(v_3) = d(w_1)$), a contradiction. If there exists some vertex $z \in N(v_1) \setminus \{v_2, v_3\}$ such that $zw \notin E(G)$, then let $G_7 = G + v_1w_1 + wz - w_1w - v_1z$. By Lemma 2.1, G_7 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_3, w_1\}$ forms a triangle in G_7, a contradiction. Thus, $z \in N(w)$ holds for each $z \in N(v_1) \setminus \{v_2, v_3\}$. Since $w_1 \in N(w) \setminus N(v_1)$, we have $d(v_1) = d(v_2) = d(v_3) = d(w_1) = d(w) \ge 3$.

In this case, $wv_3 \notin E(G)$ (otherwise, Claim 4 already holds). Since $w \in N(v_2) \setminus N(v_3)$ and $d(v_2) = d(v_3)$, there exists some vertex $z' \in N(v_3) \setminus V(C_q)$ such that $v_2z' \notin E(G)$. Let $G_8 = G + v_3w + v_2z' - v_2w - v_3z'$. Since $d(v_1) = d(v_2) = d(v_3) =$

$d(w_1) = d(w)$, by Lemma 2.1, G_8 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_3, w_1, w\}$ forms a triangle of G_8, contrary with $d(v_1) = d(v_2) = d(v_3) = d(w_1) = d(w)$.

Case 2. $d_2 = 2$.

Suppose $P = v_1u_1\cdots u_s$ is a longest path among these paths connecting v_1 and a pendant vertex in G. Let $G_9 = G + v_2v_3 + u_sv_0 - v_0v_3 - u_0v_2$, where $v_0 \in (N(v_3) \cap V(C_q)) \setminus \{v_1\}$ and $u_0 \in (N(v_2) \cap V(C_q)) \setminus \{v_1\}$ (here, $u_0 = v_0$ is also permitted).

If $s \geq 2$, then $M_f(G_9) = M_f(G)$ and hence G_9 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle in G_9, and hence Claim 4 holds. Otherwise, $s = 1$. In this case, $M_f(G_9) - M_f(G) = f(d(v_1), 2) + f(2, 1) - f(d(v_1), 1) - f(2, 2)$. By the definition of $f(x, y)$, G_9 is also an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle in G_9. ■

Lemma 2.6. *Let G be an extremal c-cyclic graph of $\Gamma(\pi)$ with $d_n = 1$ and $c \geq 1$. If $\{v_2, v_3, \ldots, v_k\} \subseteq N_{\mathcal{R}(G)}(v_1)$ and $G[\{v_1, v_2, v_3, \ldots, v_k\}] \subseteq \mathcal{R}(G)$, then there exists an extremal graph $G' \in \Gamma(\pi)$ such that G' is a BFS-graph with $\{v_2, v_3, \ldots, v_k\} \subseteq N_{\mathcal{R}(G')}(v_1)$ and $G[\{v_1, v_2, v_3, \ldots, v_k\}] \subseteq \mathcal{R}(G')$.*

Proof. We create an ordering $\prec$ of $V(G)$ by the breadth-first-search method as follows: Firstly, let $v_1 \prec v_2 \prec \cdots \prec v_k$; secondly, append all neighbors $u_{k+1}, u_{k+2}, \ldots, u_{d_1+1}$ of $N(v_1) \setminus \{v_2, v_3, \ldots, v_k\}$ to the ordered list, these neighbors are ordered such that $u \prec v$ whenever $d(u) > d(v)$ (in the remaining case the ordering can be arbitrary); thirdly append all neighbors of $N(v_2) \setminus N[v_1]$ to the ordered list, these neighbors are ordered such that $u \prec v$ whenever $d(u) > d(v)$ (in the remaining case the ordering can be arbitrary). Then, with the same method we can append the vertices $N(v_i) \setminus (N[v_1] \cup N(v_2) \cup \cdots \cup N(v_{i-1}))$ in the ordered list, where $3 \leq i \leq k$, and then to the vertices $N(w) \setminus (N[v_1] \cup N(v_2) \cup \cdots \cup N(v_k))$, where $d(w) = \max\{d(z)$: $z \in N(v_1) \setminus \{v_2, v_3, \ldots, v_k\}\}$. Continue recursively with all vertices $v_1, v_2, \ldots, v_n$ until all vertices of G are processed. It suffices to show the following two claims.

Claim 1. *If $i < j$, then $d(u) \geq d(v)$ holds for any $u \in \mathcal{A}_i$ and $v \in \mathcal{A}_j$.*

Suppose that there exist vertices u and v with $h(u) < h(v)$, while $d(u) < d(v)$. Furthermore, for convenience, we may choose u as the first vertex in the ordering $\prec$ with such property and let $d(v) = \max\{d(w)$: where $h(w) > h(u)\}$. Then, $1 \leq i < j$ and $u \notin \{v_1, v_2, \ldots, v_k\}$.

If $u \in V(P_{vv_1})$, then we choose $u' \in \mathcal{A}_{i-1} \cap V(P_{vv_1})$ such that $u'u \in E(G)$. Since $d(v) > d(u)$, there exists vertex $v' \in N(v) \setminus V(P_{vv_1})$ such that $v' \notin N(u)$. By the choice of u and v', we have $d(u') \geq d(v')$ and $d(v) > d(u)$. Let $G_1 = G + uv' + u'v - u'u - vv'$. By Lemma 2.1 and the choice of G, we can conclude that G_1 is also an extremal graph of $\Gamma(\pi)$. Now, we construct a new ordering $\prec'$ of $V(G_1)$ with the similar method as $\prec$. We suppose that $v_1 \prec v_2 \prec \cdots \prec v_k \prec u_1 \prec u_2 \prec \cdots \prec u_t \prec u$ are the first $t + k + 1$ elements in the ordering $\prec$ of $V(G)$. By the choice of u and v, we have $v_1 \prec' v_2 \prec' \cdots \prec' v_k \prec' u_1 \prec' u_2 \prec' \cdots \prec' u_t \prec' v$ are the first $t + k + 1$ elements in the ordering $\prec'$ of $V(G_1)$. By the choice of u and v, for every $w \in \{v_1, v_2, \ldots, v_k, u_1, u_2, \ldots, u_t, v\}$, if $w \in \mathcal{A}_t(G_1)$, then $d_{G_1}(w) \geq d_{G_1}(w')$ holds for every $w' \in \mathcal{A}_s(G_1)$, where $t < s$.

In what follows, we suppose that $u \notin V(P_{vv_1})$.

Choose $w \in V(P_{vv_1}) \cap \mathcal{A}_{j-1}$ and choose $u' \in \mathcal{A}_{i-1}$ such that $wv \in E(G)$ and $u'u \in E(G)$. By the former argument, we may suppose that $u \neq w$.

If $uw \notin E(G)$, by the choice of u and $j - 1 > i - 1$, $d(u') \geq d(w)$. Recall that $d(v) > d(u)$. Let $G_2 = G + uw + u'v - uu' - vw$. By Lemma 2.1, G_2 is also an extremal graph of $\Gamma(\pi)$.

Otherwise, $uw \in E(G)$. Recall that $d(v) > d(u)$. There exists vertex $w' \in N(v)$ such that $w' \notin V(P') \cup N[u]$, where P' is a path connected v and u with $\{u', v_1, w\} \subseteq V(P')$. Let $G_2 = G + uw' + u'v - uu' - vw'$. By the choice of u and $j - 1 > i - 1$, $d(u') \geq d(w')$. In this case, Lemma 2.1 implies that G_2 is also an extremal graph of $\Gamma(\pi)$.

Now, we construct a new ordering $\prec'$ of $V(G_2)$ with the similar method as $\prec$. We suppose that $v_1 \prec v_2 \prec \cdots \prec v_k \prec u_1 \prec u_2 \prec \cdots \prec u_t \prec u$ are the first $t + k + 1$ elements in the ordering $\prec$ of $V(G)$. By the choice of u and v, we have $v_1 \prec' v_2 \prec' \cdots \prec' v_k \prec' u_1 \prec' u_2 \prec' \cdots \prec' u_t \prec' v$ are the first $t + k + 1$ elements in the ordering $\prec'$ of $V(G_2)$. By the choice of u and v, for every $w \in \{v_1, v_2, \ldots, v_k, u_1, u_2, \ldots, u_t, v\}$, if $w \in \mathcal{A}_t(G_2)$, then $d_{G_2}(w) \geq d_{G_2}(w')$ holds for every $w' \in \mathcal{A}_s(G_2)$, where $t < s$.

Repeating the above process finitely many times, we can achieve a graph G^* and an ordering $\prec^*$ such that Claim 1 holds for G^*. Thus, we may directly suppose that Claim 1 holds for G.

Claim 2. *If $h(u') = h(v') = i$ and $u' \prec v'$, then $d(u) \geq d(v)$ holds for every $u \in (N(u') \cap \mathcal{A}_{i+1}) \setminus N(v')$ and every $v \in (N(v') \cap \mathcal{A}_{i+1}) \setminus N(u')$.*

If Claim 2 does not hold, we may suppose that u' is the first vertex in the ordering $\prec$ with the property that there exist vertices $v' \in \mathcal{A}_i$ (suppose that $u' \in \mathcal{A}_i$), $u \in (N(u') \cap \mathcal{A}_{i+1}) \setminus N(v')$ and $v \in (N(v') \cap \mathcal{A}_{i+1}) \setminus N(u')$ such that $u' \prec v'$, but $d(u) < d(v)$. Furthermore, according to this, we may suppose that u is the first vertex in the ordering $\prec$ and suppose that $d(v) = \max\{d(z) : z \in \mathcal{A}_{i+1} \setminus N(u')$, where $u \prec z\}$. It is easy to see that $u \notin \{v_1, v_2, \ldots, v_k\}$. Let $G_3 = G + u'v + v'u - u'u - v'v$. Then, $G_3 \in \Gamma(\pi)$. By the choice of u, we have $d(u') \geq d(v')$. Thus, Lemma 2.1 implies that G_3 is also an extremal graph of $\Gamma(\pi)$. Now, we construct a new ordering $\prec'$ of $V(G_3)$ with the similar method as $\prec$. We suppose

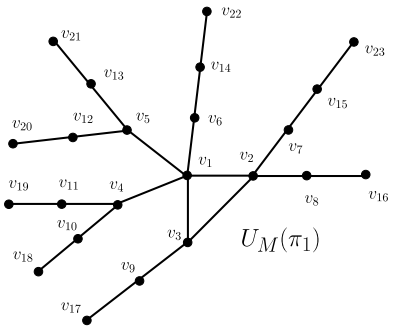


Fig. 2.1. The unicyclic graph $U_M(\pi_1)$.

that $v_1 \prec v_2 \prec \cdots \prec v_k \prec u_1 \prec u_2 \prec \cdots \prec u_t \prec u$ are the first $t+k+1$ elements in the ordering $\prec$ of $V(G)$. By the choice of u and v, $v_1 \prec' v_2 \prec' \cdots \prec' v_k \prec' u_1 \prec' u_2 \prec' \cdots \prec' u_t \prec' v$ are the first $t+k+1$ elements in the ordering $\prec'$ of $V(G_3)$. By the choice of u and v, for every $z \in \{v_1, v_2, \ldots, v_k, u_1, u_2, \ldots, u_t, v\} \cap \mathcal{A}_{i+1}(G_3)$, if $w \in \mathcal{A}_{i+1}(G_3)$ and $z \prec' w$, then $d_{G_3}(z) \geq d_{G_3}(w)$.

Repeating the above process finitely many times, we can obtain a graph G^{**} and an ordering $\prec^{**}$ of $V(G^{**})$ such that $M_f(G^{**}) = M_f(G)$ and Claim 2 holds for G^{**}.

This completes the proof of this result. ■

Theorem 2.1. *If $d_n = 1$, then there exists an extremal graph $G \in \Gamma(\pi)$ such that G is a BFS-graph. Furthermore, $\{v_1, v_2, v_3\}$ forms a triangle of G when $c \geq 1$.*

Proof. We may suppose that $c \geq 1$, as the case of $c = 0$ can be proved easily with the same argument. By Lemma 2.5, we may suppose that G is an extremal graph in $\Gamma(\pi)$ such that G contains a triangle C_3 with $V(C_3) = \{v_1, v_2, v_3\}$. Now, the result follows from Lemma 2.6. ■

Hereafter, we use the symbol $p^{(q)}$ to define q copies of the real number p. Suppose $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$. It has been shown that the *BFS*-tree is unique for any tree degree sequence π [20]. Actually, we can construct a unique unicyclic *BFS*-graph $U_M(\pi)$ by the following breadth-first-search method for any unicyclic degree sequence π: The unique cycle of $U_M(\pi)$ is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Select the vertex v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices $v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}$ as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$. Let $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$ and $N(v_3) = \{v_1, v_2, v_{d_1+d_2}, \ldots, v_{d_1+d_2+d_3-3}\}$. Then, append $d_4 - 1$ vertices to v_4 such that $N(v_4) = \{v_1, v_{d_1+d_2+d_3-2}, \ldots, v_{d_1+d_2+d_3+d_4-4}\}$ .... Informally, for a given unicyclic degree sequence $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, $U_M(\pi_1)$ is the unicyclic graph as shown in Fig. 2.1.

Corollary 2.1. *Let π be a c-cyclic degree sequence with $d_n = 1$.*
(i) [16] *If $c = 0$, then the BFS-tree is an extremal graph of $\Gamma(\pi)$.*
(ii) [21] *If $c = 1$, then $U_M(\pi)$ is an extremal graph of $\Gamma(\pi)$.*

Proof. One can easily check that (i) and (ii) follow from Theorem 2.1. ■

Paths $P_{l_1}, P_{l_2}, \ldots, P_{l_k}$ are said to *have almost equal lengths* if $l_1, l_2, \ldots, l_k$ satisfy $|l_i - l_j| \leq 1$ for $1 \leq i \leq j \leq k$. In what follows, let $B_1, B_2, \ldots, B_7$ be seven bicyclic graphs as shown in Fig. 2.2. If $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence, then $\sum_{i=1}^{n} d_i = 2n + 2$, which implies that π should be one of the following four cases. Moreover, we construct a special bicyclic graph $B_M(\pi)$ of $\Gamma(\pi)$ as follows:

(i) If $d_n = 1$ and $d_1 \geq d_2 \geq 3$, let $B_M(\pi)$ be a *BFS*-graph such that $\mathcal{R}(B_M(\pi)) \cong B_1$ and the remaining vertices appear in a *BFS*-ordering.

(ii) If $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$, let $B_M(\pi)$ be the bicyclic graph with n vertices obtained from B_2 by attaching $d_1 - 4$ paths of almost equal lengths to the maximum degree vertex of B_2.

(iii) If $\pi = (4, 2^{(n-1)})$, let $B_M(\pi) \cong B_3$.

(iv) If $\pi = (3^{(2)}, 2^{(n-2)})$, let $B_M(\pi) \cong B_5$.

Lemma 2.7. *If π is a bicyclic degree sequence with $d_1 \geq d_2 \geq 3$ and $d_n = 1$, then $B_M(\pi)$ is an extremal bicyclic graph of $\Gamma(\pi)$.*

Proof. By Theorem 2.1, we may suppose that G is an extremal bicyclic graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle Δ_1 of G and G is an *BFS*-graph. We firstly prove the following two claims.

Claim 1. *There is an extremal bicyclic graph G of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle Δ_1 of G and G contains a cycle C_q with $\{v_1v_2, v_1v_4\} \subseteq E(C_q)$.*

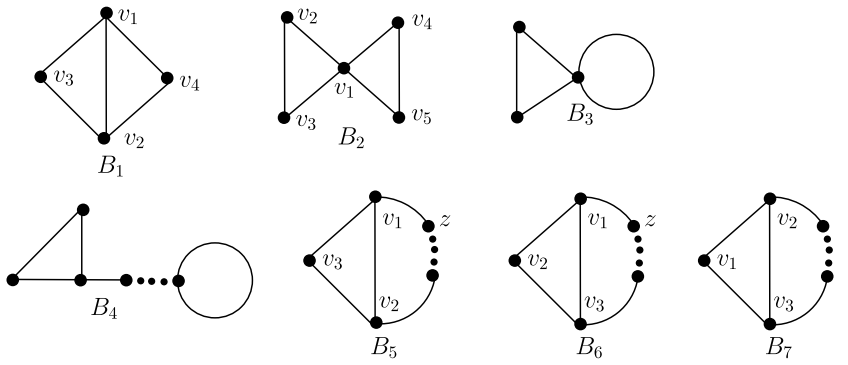


Fig. 2.2. The bicyclic graphs $B_1, B_2, \ldots, B_7$.

Since G is a bicyclic graph, there is another cycle, say C_q such that $C_q \neq \Delta_1$. If v_1v_2 does not lie on C_q, then $\mathcal{R}(G) \cong B_3$ or $\mathcal{R}(G) \cong B_4$. It is easy to see that there exists at least one edge uv on C_q such that $d(u) \geq d(v)$, $\{v_1, v_2, v_3\} \cap \{u, v\} = \emptyset$ and $d_5 \geq d(v)$, by Lemma 2.4 and Remark 2.1, there exists another extremal graph G' such that Δ_1 is also a triangle of G', v_1v_2 also lies on a cycle of G' and $\{v_2, v_3, v_4\} \subseteq N_{G'}(v_1)$. Thus, we may suppose that Δ_1 is a triangle of G, v_1v_2 lies on the cycle C_q of G and $\{v_2, v_3, v_4\} \subseteq N_G(v_1)$. In this case, $\mathcal{R}(G) \in \{B_5, B_6, B_7\}$.

If either $v_4 \in V(C_q)$ or $N(v_4) \cap \{v_1, v_2, v_3\} \neq \{v_1\}$, then Claim 1 already holds. Thus, we may suppose that $v_4 \notin V(C_q)$ and $N(v_4) \cap \{v_1, v_2, v_3\} = \{v_1\}$ (in this case, $v_4 \notin V(\mathcal{R}(G))$). Let $u_0 \in N(v_4) \setminus \{v_1, v_2, v_3\}$ (such vertex exists since G contains a cycle C_q).

If $\mathcal{R}(G) \cong B_5$ or $\mathcal{R}(G) \cong B_7$, we choose $u \in N(v_2) \cap V(B_5)$ such that $u \notin \{v_1, v_3\}$. Let $G_1 = G + uu_0 + v_2v_4 - v_2u - u_0v_4$. Since $d(v_2) \geq d(u_0)$ and $d(v_4) \geq d(u)$, by Lemma 2.1, G_1 is also an extremal graph of $\Gamma(\pi)$ such that Claim 1 holds.

If $\mathcal{R}(G) \cong B_6$, we choose $u \in N(v_3) \cap V(B_6)$ such that $u \notin \{v_1, v_2\}$. Let $G_2 = G + uu_0 + v_3v_4 - v_3u - v_4u_0$. Since $d(v_3) \geq d(u_0)$ and $d(v_4) \geq d(u)$, by Lemma 2.1, G_2 is also an extremal graph of $\Gamma(\pi)$ such that Claim 1 holds. This completes the proof of Claim 1.

Claim 2. *There is an extremal bicyclic graph G of $\Gamma(\pi)$ such that $\{v_1, v_2, v_4\}$ and $\{v_1, v_2, v_3\}$ form two triangles of G.*

By Claim 1, we may suppose that G is an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3\}$ forms a triangle of G and G contains a cycle C_q with $\{v_1v_2, v_1v_4\} \subseteq E(C_q)$. In this case, either $\mathcal{R}(G) \cong B_5$ or $\mathcal{R}(G) \cong B_6$ with $z = v_4$.

If $v_3v_4 \in E(G)$, then $\{v_1, v_2, v_3, v_4\}$ form a C_4 of G (in this case, $\mathcal{R}(G) \cong B_6$). In this case, there exists some vertex $u \in N(v_2) \setminus V(\mathcal{R}(G))$ and $v_2v_4 \notin E(G)$. Let $G_3 = G + v_2v_4 + v_3u - v_3v_4 - v_2u$. By Lemma 2.1, G_3 is also an extremal graph of $\Gamma(\pi)$ such that Claim 2 holds.

Otherwise, $v_3v_4 \notin E(G)$.

If $\mathcal{R}(G) \cong B_6$, then there exists a vertex $w_2 \in N(v_2) \setminus V(\mathcal{R}(G))$. Let $G_4 = G + v_2v_4 + w_2w_0 - v_2w_2 - v_4w_0$, where $w_0 \in (N(v_4) \cap V(B_6)) \setminus \{v_1\}$. By Lemma 2.1, G_4 is an extremal graph of $\Gamma(\pi)$ such that Claim 2 holds.

Therefore, we may suppose that $\mathcal{R}(G) \cong B_5$ in what follows. Furthermore, we may suppose that $v_2v_4 \notin E(G)$. Otherwise, Claim 1 already holds. We choose $u_0 \in (N(v_4) \cap V(B_5)) \setminus \{v_1\}$ and $z_0 \in (N(v_2) \cap V(B_5)) \setminus \{v_1, v_3\}$, where $u_0 = z_0$ is permitted.

If $d_3 \geq 3$, then we choose $w \in N(v_3) \setminus V(B_5)$. Note that $wu_0 \notin E(G)$. Let $G_5 = v_3v_4 + wu_0 - v_3w - v_4u_0$. By Lemma 2.1, G_5 is an extremal graph of $\Gamma(\pi)$ such that $\{v_1, v_2, v_3, v_4\}$ form a C_4 and $\{v_1, v_2, v_3\}$ form a triangle of G_5. From the above argument, Claim 2 holds (see the case of $v_3 \in N(v_4)$ and $\mathcal{R}(G) \cong B_6$).

Otherwise, $d_3 = 2$, and hence $d_1 \geq 4$ (since $d_n = 1$ and $\sum_{i=1}^{n} d_i = 2(n+1)$). Let w_1 be a vertex of $N(v_1) \setminus \{v_2, v_3, v_4\}$, and let $G_6 = G + v_2v_4 + z_0v_1 + w_1u_0 - v_2z_0 - v_4u_0 - v_1w_1$. Now, by (1.2) it follows that $M_f(G_6) - M_f(G) = f(d_1, 2) + f(2, d(w_1)) - f(d_1, d(w_1)) - f(2, 2)$, and hence G_6 is also an extremal graph of $\Gamma(\pi)$ such that Claim 2 holds.

Now, by Claim 2 and Lemma 2.6 we have $G \cong B_M(\pi)$, as desired. ■

Theorem 2.2. *If π is a bicyclic degree sequence, then $B_M(\pi)$ is an extremal graph of $\Gamma(\pi)$.*

Proof. Since $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence, $\sum_{i=1}^{n} d_i = 2n + 2$. Hence it suffices to consider the following four cases.

If $\pi = (4, 2^{(n-1)})$ (respectively, $(3^{(2)}, 2^{(n-2)})$), it is easy to check that B_3 (respectively, B_5) is an extremal graph of $\Gamma(\pi)$. If $d_1 \geq d_2 \geq 3$ and $d_n = 1$, then the result follows from Lemma 2.7. Otherwise, $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$. In this case, by Theorem 2.1, we may suppose that G is an extremal bicyclic graph of $\Gamma(\pi)$ such that G is a *BFS*-graph obtained by attaching $d_1 - 4$ paths of almost equal lengths to the maximum degree vertex of B_3. Now, we assume that $B_3 \ncong B_2$, and hence B_3 contains a cycle C_q, where $q \geq 4$. We suppose that $N(v_1) \cap V(C_q) = \{u_1, w_1\}$, $N(u_1) \cap V(C_q) = \{v_1, u_2\}$ and $N(w_1) \cap V(C_q) = \{v_1, w_2\}$, where $w_2 = u_2$ is permitted. We choose z as a pendant vertex such that the distance between v_1 and z is as small as possible, and suppose that $z_1 \in N(z)$. Let $G_1 = G + u_1w_1 + zw_2 - u_1u_2 - w_1w_2$.

If $z_1 = v_1$, then $M_f(G_1) - M_f(G) = f(d(v_1), 2) + f(2, 1) - f(d(v_1), 1) - f(2, 2)$. If $z_1 \neq v_1$, then $M_f(G_1) = M_f(G)$. In both cases, G_1 is also an extremal bicyclic graph of $\Gamma(\pi)$ such that $\mathcal{R}(G_1) \cong B_2$. Now, the result follows from Lemma 2.6. ■

3. The majorization theorem of connectivity function

If $\pi = (d_1, d_2, \ldots, d_n)$ is a non-increasing integer sequence and $d_i \geq d_j + 2$ holds for some integers $1 \leq i < j \leq n$, then the following operation is called a *unit transformation* from i to j on π: subtract 1 from d_i and add 1 to d_j. The following famous lemma about majorization for integer sequences is due to Muirhead (for instance, see [10,11]).

Lemma 3.1 (*Muirhead Lemma*). *If π and π' are two non-increasing integer sequences and $\pi \lhd \pi'$, then π can be obtained from π' by a finite sequence of unit transformations.*

Lemma 3.2. *Let u, v be two vertices of a connected graph G with $d(u) \geq d(v) \geq 2$ and w be some vertex of $N(v)\setminus(V(P_{uv}) \cup N[u])$. Let $G' = G+wu-wv$. Suppose that $N(v)\setminus\{w, u\} = \{z'_1, z'_2, \ldots, z'_{|N(v)\setminus\{w,u\}|}\}$, and there exist $\{z_1, z_2, \ldots, z_{|N(v)\setminus\{w,u\}|}\} \subseteq N(u)\setminus\{v\}$ such that $d(z_i) \geq d(z'_i)$ for $1 \leq i \leq |N(v) \setminus \{w, u\}|$. If $f(x, y)$ is a good escalating function, then $M_f(G') > M_f(G)$.*

Proof. If $uv \notin E(G)$, by (1.2) it follows that

$$\begin{aligned} &M_f(G') - M_f(G) \\ &= \sum_{z\in N(u)} \left(f\left(d(u)+1, d(z)\right) - f\left(d(u), d(z)\right)\right) - \sum_{z'\in N(v)\setminus\{w\}} \left(f\left(d(v), d(z')\right) - f\left(d(v)-1, d(z')\right)\right) \\ &\quad + f\left(d(u)+1, d(w)\right) - f\left(d(v), d(w)\right). \end{aligned}$$

Let $g(x, y) = \frac{\partial f(x,y)}{\partial x}$. We may suppose that $N(v) \setminus \{u, w\} = \{z'_1, z'_2, \ldots, z'_{d(v)-1}\}$. Then, there exist $\{z_1, z_2, \ldots, z_{d(v)-1}\} \subseteq N(u)\setminus\{v\}$ such that $d(z_i) \geq d(z'_i)$. Recall that $d(u) \geq d(v)$, $d(z_i) \geq d(z'_i)$ and $f(x, y)$ is good escalating. Thus, for $1 \leq i \leq d(v)-1$, there exist $0 \leq a \leq 1$ and $0 \leq b \leq 1$ such that

$$\begin{aligned} &f(d(u)+1, d(z_i)) - f(d(u), d(z_i)) - (f(d(v), d(z'_i)) - f(d(v)-1, d(z'_i))) \\ &= f(d(u)+1, d(z_i)) - f(d(u), d(z_i)) - (f(d(v), d(z_i)) - f(d(v)-1, d(z_i))) \\ &\quad + f(d(v), d(z_i)) + f(d(v)-1, d(z'_i)) - f(d(v)-1, d(z_i)) - f(d(v), d(z'_i)) \\ &\geq f(d(u)+1, d(z_i)) - f(d(u), d(z_i)) - (f(d(v), d(z_i)) - f(d(v)-1, d(z_i))) \\ &= g(d(u)+a, d(z_i)) - g(d(v)-1+b, d(z_i)) \geq 0, \end{aligned}$$

which implies that $M_f(G') - M_f(G) \geq f\left(d(u)+1, d(w)\right) - f\left(d(v), d(w)\right) > 0$, as $g(x, y) > 0$.

Otherwise, $uv \in E(G)$. In this case, by (1.2) it follows that

$$\begin{aligned} &M_f(G') - M_f(G) \\ &= \sum_{z\in N(u)\setminus\{v\}} \left(f\left(d(u)+1, d(z)\right) - f\left(d(u), d(z)\right)\right) - \sum_{z'\in N(v)\setminus\{u,w\}} \left(f\left(d(v), d(z')\right) - f\left(d(v)-1, d(z')\right)\right) \\ &\quad + f\left(d(u)+1, d(w)\right) - f\left(d(v), d(w)\right) + f\left(d(u)+1, d(v)-1\right) - f\left(d(u), d(v)\right). \end{aligned}$$

Since $|N(u) \setminus \{v\}| > |N(v) \setminus \{u, w\}|$, there exists some vertex $z_0 \in N(u) \setminus \{v\}$ such that

$$\begin{aligned} &\sum_{z\in N(u)\setminus\{v\}} \left(f\left(d(u)+1, d(z)\right) - f\left(d(u), d(z)\right)\right) - \sum_{z'\in N(v)\setminus\{u,w\}} \left(f\left(d(v), d(z')\right) - f\left(d(v)-1, d(z')\right)\right) \\ &\geq f\left(d(u)+1, d(z_0)\right) - f\left(d(u), d(z_0)\right) > 0. \end{aligned}$$

Furthermore, since $f(x, y)$ is good escalating, we can conclude that

$$\begin{aligned} M_f(G') - M_f(G) &> f\left(d(u)+1, d(w)\right) + f\left(d(u)+1, d(v)-1\right) - f\left(d(v), d(w)\right) - f\left(d(u), d(v)\right) \\ &\geq 0. \end{aligned}$$

This completes the proof of this result. ■

Suppose that $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two c-cyclic graphic degree sequences. If $\pi \lhd \pi'$, by Lemma 3.1, we may suppose that π and π' differ only in two positions where the difference is 1, that is, $d_i = d'_i$, $i \neq p, q$, $1 \leq p < q \leq n$, and $d'_p = d_p + 1$, $d'_q = d_q - 1$.

Let G and G' be an extremal c-cyclic *BFS*-graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If w is a vertex of G such that $w \in N(v_q) \setminus \left(V(P_{v_p v_q}) \cup N[v_p]\right)$, then we call w a *surprising vertex* of G. If $f(x, y)$ is good escalating and G contains some surprising vertex w, then let $G_1 = G + v_p w - v_q w$. Thus, $G_1 \in \Gamma(\pi')$. Since $p < q$, by Theorem 2.1, we can conclude that $d(v_p) \geq d(v_q)$,

and there exists $\{z_1, z_2, \ldots, z_{|N(v_q)\setminus\{w,v_p\}|}\} \subseteq N(v_p)\setminus\{v_q\}$ such that $d(z_i) \geq d(z_i')$ for $1 \leq i \leq |N(v_q)\setminus\{w, v_p\}|$, where $N(v_q)\setminus\{w, v_p\} = \{z_1', z_2', \ldots, z_{|N(v_q)\setminus\{w,v_p\}|}'\}$. Now, Lemma 3.2 implies that $M_f(G) < M_f(G_1) \leq M_f(G')$. Thus,

$$\text{if } G \text{ contains a surprising vertex, then } M_f(G) < M_f(G'). \tag{3.1}$$

Zhang et al. [22] showed that the size of $M_f(T)$ and $M_f(T')$ can be deduced from the relation $\pi \lhd \pi'$ when $f(x, y)$ is a special symmetric bivariable function for any extremal trees T and T' of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Actually, if $\pi \lhd \pi'$ and $f(x, y)$ is good escalating, by Corollary 2.1 (i) we can conclude that the *BFS*-tree of $\Gamma(\pi)$ contains a surprising vertex. Thus, by (3.1) and Corollary 2.1 (i) it follows that

Theorem 3.1. *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Let T and T' be an extremal tree of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is a good escalating function, then $M_f(T) < M_f(T')$.*

Theorem 3.2. *Let π and π' be two different non-increasing unicyclic degree sequences with $\pi \lhd \pi'$. Let U and U' be an extremal unicyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is a good escalating function, then $M_f(U) < M_f(U')$.*

Proof. Suppose that $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d_1', d_2', \ldots, d_n')$. Since $\pi \lhd \pi'$, by Lemma 3.1 we may suppose that π and π' differ only in two positions, where the differences are 1. Thus, we may assume that $d_i = d_i'$ for $i \neq p, q$, and $d_p + 1 = d_p'$, $d_q - 1 = d_q'$, where $p < q$.

If $d_n = 2$, then $\pi = (2, 2, \ldots, 2)$ and $\pi' = (3, 2, \ldots, 2, 1)$. By Corollary 2.1 (ii), it suffices to show that $M_f(C_n) < M_f(U_M(\pi'))$. Since $U_M(\pi')$ contains at least one pendant vertex, $n \geq 4$. We may suppose that $n \geq 5$, as the case of $n = 4$ can be proved similarly. Let $g(x, y) = \frac{\partial f(x,y)}{\partial x}$. In this case, since $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$ and $g(x, y) > 0$, by Corollary 2.1 (ii) we have

$$\begin{aligned} M_f(U_M(\pi')) - M_f(C_n) &= 3f\,(3, 2) + f(2, 1) - 4f(2, 2) \\ &> f\,(3, 2) + f(2, 1) - 2f(2, 2) \\ &= f\,(3, 2) - f(2, 2) - (f(2, 2) - f(1, 2)) \\ &= g(2 + a, 2) - g(1 + b, 2) \geq 0, \end{aligned}$$

where $0 \leq a \leq 1$ and $0 \leq b \leq 1$.

Otherwise, $d_n = 1$. In this case, it suffices to show that $M_f(U_M(\pi)) < M_f(U_M(\pi'))$ by Corollary 2.1 (ii). If $2 \leq q \leq 3$, then $d_q = d_q' + 1 \geq 3$ since $U_M(\pi') \in \Gamma(\pi')$. If $q \geq 4$, then $d_q \geq 2$. In both cases, $U_M(\pi)$ contains a surprising vertex. Now, the result follows from (3.1). ■

Theorem 3.3. *Let π and π' be two different non-increasing bicyclic degree sequences with $\pi \lhd \pi'$. Let B and B' be an extremal bicyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is a good escalating function, then $M_f(B) < M_f(B')$.*

Proof. Suppose that $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d_1', d_2', \ldots, d_n')$. Since $\pi \lhd \pi'$, by Lemma 3.1 we may suppose that π and π' differ only in two positions, where the differences are 1. Thus, we may assume that $d_i = d_i'$ for $i \neq p, q$, and $d_p + 1 = d_p'$, $d_q - 1 = d_q'$, where $p < q$. It suffices to show that $M_f(B_M(\pi)) < M_f(B_M(\pi'))$ by Theorem 2.2.

We firstly consider the case of $d_n \geq 2$. In this case, either $\pi = (4, 2^{(n-1)})$ or $\pi = (3^{(2)}, 2^{(n-2)})$. If $\pi = (4, 2^{(n-1)})$, then either $\pi' = (5, 2^{(n-2)}, 1)$ or $\pi' = (4, 3, 2^{(n-3)}, 1)$. If $\pi = (3^{(2)}, 2^{(n-2)})$, then $\pi' = (4, 2^{(n-1)})$ or $\pi' = (3^{(3)}, 2^{(n-4)}, 1)$ or $\pi' = (4, 3, 2^{(n-3)}, 1)$. Whenever which case happens, according to Theorem 2.2, $B_M(\pi)$ contains a surprising vertex, and hence the result follows from (3.1). We secondly consider the case of $d_n = 1$.

Case 1. $d_n = 1$ and $d_2 = 2$.

In this case, $\pi = (k + 4, 2^{(n-k-1)}, 1^{(k)})$, where $k \geq 1$. Then, either $\pi' = (k + 5, 2^{(n-k-2)}, 1^{(k+1)})$ or $\pi' = (k + 4, 3, 2^{(n-k-3)}, 1^{(k+1)})$. According to Theorem 2.2, $\mathcal{R}(B_M(\pi)) \cong B_2$.

If $\pi' = (k+4, 3, 2^{(n-k-3)}, 1^{(k+1)})$, since $v_5 \in N_{B_M(\pi)}(v_4)\setminus N_{B_M(\pi)}[v_2]$ and $v_5 \notin V(P_{v_2v_4})$, it is easy to see that v_5 is a surprising vertex of $B_M(\pi)$.

If $\pi' = (k + 5, 2^{(n-k-2)}, 1^{(k+1)})$, then $p = 1$, $q \geq 6$ and $d_q = 2$. By the structure of $B_M(\pi)$, there exists a vertex v_k $(k > q)$ such that $v_k \in N_{B_M(\pi)}(v_q)\setminus N_{B_M(\pi)}[v_p]$ and $v_k \notin V(P_{v_pv_q})$. In this case, it is easy to see that v_k is a surprising vertex of $B_M(\pi)$.

In both cases, the result follows from (3.1).

Case 2. $d_n = 1$ and $d_1 \geq d_2 \geq 3$.

By Theorem 2.2, $\mathcal{R}(B_M(\pi)) \cong B_1$. If $q \geq 5$, then $d_q = d_q' + 1 \geq 2$. If $3 \leq q \leq 4$, since $B_M(\pi')$ is a bicyclic graph, $d_q = d_q' + 1 \geq 3$. In both cases, by the structure of $B_M(\pi)$, there exists vertex v_k $(k > q)$ such that $v_k \in N_{B_M(\pi)}(v_q)\setminus N_{B_M(\pi)}[v_p]$ and $v_k \notin V(P_{v_pv_q})$. In this case, it is easy to see that v_k is a surprising vertex of $B_M(\pi)$. Now, the result follows from (3.1). Thus, we may suppose that $q = 2$, and hence $p = 1$ in the sequel.

If $q = 2$ and $d_2 \geq 4$, since $\mathcal{R}(B_M(\pi)) \cong B_1$, there exists a vertex $v_k \in N_{B_M(\pi)}(v_2)\setminus N_{B_M(\pi)}[v_1]$ and $v_k \notin V(P_{v_1v_2})$, which implies that v_k is a surprising vertex of $B_M(\pi)$. Now, the result follows from (3.1).

If $q = 2$ and $d_2 = 3$, then $d_2' = 2$. Thus, $\pi = (k + 3, 3, 2^{(n-k-2)}, 1^{(k)})$ and $\pi' = (k + 4, 2^{(n-k-1)}, 1^{(k)})$, where $k \geq 1$. By Theorem 2.2, $\mathcal{R}(B_M(\pi)) \cong B_1$ and $\mathcal{R}(B_M(\pi')) \cong B_2$.

Then, $B_M(\pi)$ is obtained from B_1 by attaching k paths, say $P_{l_1}, P_{l_2}, \ldots, P_{l_k}$, of almost equal lengths to one vertex of degree three of B_1, where $l_1 \geq l_2 \geq \cdots \geq l_k \geq 1$ and $l_1 \geq 2$.

If $l_1 \geq 3$, since $g(x,y) = \frac{\partial f(x,y)}{\partial x} > 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$, we have $M_f(B_M(\pi')) - M_f(B_M(\pi)) = (k+4)f(k+4,2) + f(2,2) - (k+2)f(k+3,2) - f(k+3,3) - 2f(3,2) = (k+2)g(k+3+a,2) - 2f(3,2) + 2f(k+4,2) + f(2,2) - f(k+3,3) = (k+2)g(k+3+a,2) - g(2+b,2) + 2f(k+4,2) - f(k+3,3) - f(3,2) > 2f(k+4,2) - f(k+3,3) - f(3,2) \geq 0$, where $0 \leq a \leq 1$ and $0 \leq b \leq 1$.

Otherwise, $l_1 = 2$. We may suppose that $(l_1, l_2, \ldots, l_k) = (2^{(s)}, 1^{(k-s)})$, where $1 \leq s \leq k$. In this case, $M_f(B_M(\pi')) - M_f(B_M(\pi)) = (s+3)f(k+4,2) + 2f(2,2) + (k+1-s)f(k+4,1) - (s+2)f(k+3,2) - f(k+3,3) - 2f(3,2) - (k-s)f(k+3,1) - f(2,1) \geq (s+2)g(k+3+a,2) - 2g(2+b,2) + f(k+4,2) + f(k+4,1) - f(k+3,3) - f(2,1) > f(k+4,2) + f(k+4,1) - f(k+3,3) - f(2,1) \geq f(k+3,3) + f(3,1) - f(k+3,3) - f(2,1) > 0$, where $0 \leq a \leq 1$ and $0 \leq b \leq 1$. ■

Let $F_n(k)$ (respectively, $F'_n(k)$, $F''_n(k)$) be the tree (respectively, unicyclic graph, bicyclic graph) on n vertices obtained by attaching k paths of almost equal lengths to one isolated vertex (respectively, one vertex of C_3, the vertex of degree four of B_2). From Theorems 2.1–2.2 and 3.1–3.3, we can deduce the following extremal results easily:

Corollary 3.1. *If $k \geq 1$ and $f(x,y)$ is good escalating, then $F''_n(k)$ (respectively, $F'_n(k)$, $F_n(k)$) is an extremal bicyclic graph (respectively, unicyclic graph, tree) among all bicyclic graphs (respectively, unicyclic graphs, trees) with n vertices and k pendant vertices when $n \geq k+5$ (respectively, $n \geq k+3$, $n \geq k+1$).*

Proof. Here, we only prove the case of bicyclic graphs, as the cases of unicyclic graphs and trees can be proved similarly. Let $\pi' = (k+4, 2^{(n-k-1)}, 1^{(k)})$. Suppose that G is a bicyclic graph with $\pi = (d_1, d_2, \ldots, d_n)$ as its degree sequence, where $d_n = d_{n-1} = \cdots = d_{n-k+1} = 1$ and $d_{n-k} \geq 2$. If $\pi \neq \pi'$, then $\pi \lhd \pi'$. Now, the result follows from Theorems 2.2 and 3.3. ■

Let $S_n^{(0)}$ be the star with n vertices, let $S_n^{(1)}$ be the unicyclic graph obtained from the star $S_n^{(0)}$ by adding one edge between two pendant vertices of $S_n^{(0)}$, and let $S_n^{(2)}$ be the bicyclic graph obtained from B_1 by attaching $n-4$ pendant vertices to one vertex of degree three of B_1.

Corollary 3.2. *If $n \geq 4$ and $f(x,y)$ is good escalating, then $S_n^{(c)}$ is the unique extremal c-cyclic graph among all c-cyclic graphs with n vertices for $0 \leq c \leq 2$.*

Proof. Here, we only prove the case of bicyclic graphs, as the cases of unicyclic graphs and trees can be proved similarly. Let $\pi' = (n-1, 3, 2^{(2)}, 1^{(n-4)})$. Then, π' uniquely maximizes those degree sequences of bicyclic graphs with n vertices in the relation $\lhd$. Furthermore, $S_n^{(2)}$ is the unique bicyclic graphs of $\Gamma(\pi')$. Now, the result follows from Theorem 3.3. ■

4. Some applications

As an extension of $Z_2(G)$, we define $Z_\alpha(G)$ as follows:

$$Z_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^\alpha. \tag{4.1}$$

In [22], Zhang et al. have shown that $\chi_\alpha(G)$ is escalating for $\alpha > 1$ and $\chi_\alpha(G)$ is de-escalating for $0 < \alpha < 1$, and $W_\alpha(G)$ is escalating for $\alpha > 0$. In the following, we will extend these results.

Theorem 4.1. *Let G be a connected graph with at least three vertices. Then, (i) $Z_\alpha(G)$ and $\chi_\alpha(G)$ are escalating for $\alpha > 1$ and $\alpha < 0$. Furthermore, $Z_\alpha(G)$ and $\chi_\alpha(G)$ are good escalating for $\alpha > 1$. (ii) $Z_\alpha(G)$ and $\chi_\alpha(G)$ are de-escalating for $0 < \alpha < 1$.*

Proof. Here, we only prove (i) and $Z_\alpha(G)$, as (ii) and $\chi_\alpha(G)$ can be proved similarly. By (4.1), we may define $f(x,y) = (x+y-2)^\alpha$ with $\min\{x,y\} \geq 1$ and $\max\{x,y\} \geq 2$. Suppose that $x_1 \geq y_1$ and $x_2 \geq y_2$. To show that $f(x,y) = (x+y-2)^\alpha$ is escalating, by (1.1) it suffices to show that

$$\int_{y_1+x_2-2}^{x_1+x_2-2} \alpha t^{\alpha-1} dt \geq \int_{y_1+y_2-2}^{x_1+y_2-2} \alpha t^{\alpha-1} dt,$$

which is equivalent to

$$\int_{y_1}^{x_1} \alpha (t + x_2 - 2)^{\alpha-1} dt \geq \int_{y_1}^{x_1} \alpha (t + y_2 - 2)^{\alpha-1} dt. \tag{4.2}$$

When $\alpha > 1$ or $\alpha < 0$, since $t + x_2 - 2 \geq t + y_2 - 2 \geq y_1 + y_2 - 2 \geq 1$, we can conclude that inequality (4.2) holds. Thus, $f(x,y)$ is escalating. When $\alpha > 1$, it is easy to see that $f(x_1+1, x_2) + f(x_1+1, y_1-1) - f(x_2, y_1) - f(x_1, y_1) = (x_1+x_2-1)^\alpha - (y_1+x_2-2)^\alpha \geq 0$ holds for any $x_1 \geq y_1$ and $x_2 \geq 1$ (since $\max\{x_1, y_1\} \geq 2$, $\max\{x_2, y_1\} \geq 2$). Furthermore, since $x + y \geq 3$, $g(x,y) = \frac{\partial f(x,y)}{\partial x} = \alpha(x+y-2)^{\alpha-1} > 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} = \alpha(\alpha-1)(x+y-2)^{\alpha-2} > 0$. Thus, $Z_\alpha(G)$ is a good escalating function for $\alpha > 1$. ■

Theorem 4.2. *Let G be a connected graph with at least three vertices. Then, $W_\alpha(G)$ is escalating for any real number $\alpha \neq 0$. Furthermore, $W_\alpha(G)$ is good escalating for $\alpha = 1$.*

Proof. Let $f(x, y) = (xy)^\alpha$ and $g(x, y) = \frac{\partial f(x,y)}{\partial x}$, where $\alpha \neq 0$, $\min\{x, y\} \geq 1$ and $\max\{x, y\} \geq 2$. For any real number α, it is easy to see that

$$f(x_1, x_2) + f(y_1, y_2) - f(x_1, y_2) - f(x_2, y_1) = \left(x_1^\alpha - y_1^\alpha\right)\left(x_2^\alpha - y_2^\alpha\right) \geq 0$$

holds for any $x_1 \geq y_1 \geq 1$ and $x_2 \geq y_2 \geq 1$, and hence $W_\alpha(G)$ is escalating.

It is easy to check that $W_\alpha(G)$ is good escalating for $\alpha = 1$. ■

Remark 4.1. Note that $W_1(G) = M_2(G)$. By Theorems 3.1–3.3 and 4.2, we can easily deduce the main results of [9,10,19], that is "If $\pi \lhd \pi'$, then $M_2(G') > M_2(G)$ holds for any two extremal graphs $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$ when G is a c-cyclic graph for $0 \leq c \leq 2$".

Remark 4.2. By Theorems 2.1 and 4.2, we can conclude that an extremal graph G of the Randić index or second Zagreb index among these connected graphs with fixed degree sequence is a *BFS*-tree [9,15] (respectively, $U_M(\pi)$, $B_M(\pi)$) when G is a tree (respectively, a unicyclic graph, a bicyclic graph with $d_n = 1$ [10,19]).

Remark 4.3. By Theorems 2.1 and 2.2, we can conclude that an extremal graph G of sum-connectivity index, the third Zagreb index, reformulated Zagreb index or harmonic index among these connected graphs with fixed degree sequence is a *BFS*-tree (respectively, $U_M(\pi)$, $B_M(\pi)$) when G is a tree (respectively, a unicyclic graph, a bicyclic graph with $d_n = 1$). Furthermore, Theorem 4.1 implies that Theorems 3.1–3.3 are also suitable for the third Zagreb index or reformulated Zagreb index.

Remark 4.4. Zhang et al. [22] have shown that $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$ is de-escalating, and hence the results of Theorems 2.1–2.2 are also suitable for the Atom-Bond connectivity index of G [8,17].

Remark 4.5. By Theorem 4.1, $Z_2(G)$ is a good escalating function. Thus, Corollary 3.2 implies that $S_n^{(c)}$ is the unique extremal c-cyclic graph with maximum reformulated Zagreb indices among all c-cyclic graphs with $n \geq 4$ vertices for $0 \leq c \leq 2$. These results had been proved in [6,7].

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On the ordering of distance-based invariants of graphs

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ABSTRACT

Let $d(u,v)$ be the distance between u and v of graph G, and let $W_f(G)$ be the sum of $f(d(u,v))$ over all unordered pairs $\{u,v\}$ of vertices of G, where $f(x)$ is a function of x. In some literatures, $W_f(G)$ is also called the Q-index of G. In this paper, some unified properties to Q-indices are given, and the majorization theorem is illustrated to be a good tool to deal with the ordering problem of Q-index among trees with n vertices. With the application of our new results, we determine the four largest and three smallest (resp. four smallest and three largest) Q-indices of trees with n vertices for strictly decreasing (resp. increasing) nonnegative function $f(x)$, and we also identify the twelve largest (resp. eighteen smallest) Harary indices of trees of order $n \geq 22$ (resp. $n \geq 38$) and the ten smallest hyper-Wiener indices of trees of order $n \geq 18$, which improve the corresponding main results of Xu (2012) and Liu and Liu (2010), respectively. Furthermore, we obtain some new relations involving Wiener index, hyper-Wiener index and Harary index, which gives partial answers to some problems raised in Xu (2012).

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1. Introduction

Throughout this paper, $G = (V, E)$ denotes a connected undirected simple graph with n vertices and m edges. If $m = n + c - 1$, then G is called a c-cyclic graph. When $c = 0, 1, 2$, then G is called a tree, unicyclic and bicyclic graphs, respectively. Let $\mathbb{T}(n)$ be the class of trees on n vertices, and let $\mathbb{T}(n, \Delta)$ be the class of trees with n vertices and maximum degree Δ. Similarly, let $\mathcal{G}(n)$, $\mathcal{B}(n)$, $\mathbb{U}(n)$ and $\mathbb{B}(n)$ be the class of connected graphs, connected bipartite, unicyclic and bicyclic graphs on n vertices, respectively. As usual, let $N_G(v)$ be the neighbor set of vertex v in G, and let $d_G(v)$ be the degree of v. A vertex of degree one is called a *pendent vertex* of G, and a vertex with degree at least three is called a *branching vertex* of G. The distance between u and v, denoted by $d_G(u,v)$, is equal to the number of edges in a shortest path from u to v. When there is no confusion, we simplify $N_G(v)$, $d_G(v)$ and $d_G(u,v)$ as $N(v)$, $d(v)$ and $d(u,v)$, respectively.

Hereafter, r defines a positive integer. Let $P_r(G)$ (resp. $Q_r(G)$) be the number of unordered pairs $\{u,v\}$ of vertices in a graph G such that $d(u,v) \leq r$ (resp. $d(u,v) > r$). For any graph G with n vertices, we have (See [18])

$$P_r(G) + Q_r(G) = \frac{n(n-1)}{2}. \tag{1.1}$$

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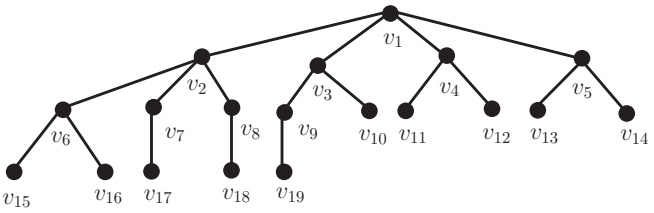


Fig. 1.1. The greedy tree with $(4^{(2)}, 3^{(4)}, 2^{(3)}, 1^{(10)})$ as its degree sequence.

If f is a nonnegative function of x, then let

$$W_f(G) = \sum_{\{u,v\}\subseteq V(G)} f(d(u,v)).$$

In some literature, $W_f(G)$ is called the Q-index of G [1]. It easily follows that

$$\begin{aligned} W_f(G) &= f(1)\binom{n}{2} + \sum_{r\geq 1}(f(r+1)-f(r))|\{\{u,v\}\subseteq V(G),\ d(u,v)>r\}| \\ &= f(1)\binom{n}{2} + \sum_{r\geq 1}(f(r+1)-f(r))Q_r(G). \end{aligned} \tag{1.2}$$

If $d_i = d(v_i)$ for $i = 1, 2, \ldots, n$, then we call the sequence $\pi = (d_1, d_2, \ldots, d_n)$ the *degree sequence* of G. In what follows, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$, and we use $\Gamma(\pi)$ to define the class of connected graphs with a prescribed degree sequence π.

Let T be a tree of order n. A well-ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(T)$ is called a *BFS*-ordering if the following hold for all vertices $u, v \in V(T)$:

(i) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1.
(ii) If $v \in N(u)\backslash N(x)$, $y \in N(x)\backslash N(u)$ such that $h(u) = h(x) = h(v) - 1 = h(y) - 1$, then $u \prec x$ if and only if $v \prec y$.

Furthermore, if $V(T)$ has a *BFS*-ordering, then T is called a *greedy tree* or a *BFS*-tree (See [18,23,24]). It has been shown that the greedy tree is unique in $\Gamma(\pi)$ for any given tree degree sequence π [24]. For instance, the unique greedy tree of $\Gamma(\pi)$ is shown in Fig. 1.1 for $\pi = (4^{(2)}, 3^{(4)}, 2^{(3)}, 1^{(10)})$, where $s^{(t)}$ means t copy of the positive integer s. Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two non-increasing integer sequences, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is sometimes called *majorization* (See [12,24,26]).

The following Theorem 1.1 is known as majorization theorem for distance-based graph invariants of trees. Actually, the majorization theorem is an important tool in the research of extremal theory of graph spectrum and/or topological index theory. For the recent results on this line, the readers can be referred to [12,25,26].

Theorem 1.1. *[26] Let π and π' be two different degree sequences of trees and let T^*_π and $T^*_{\pi'}$ the greedy trees with degree sequences π and π', respectively. If $\pi \lhd \pi'$, then $P_r(T^*_\pi) \leq P_r(T^*_{\pi'})$, and the inequality is strict for at least one $r \geq 1$.*

Among these distance-based graph invariants of a graph G, the Wiener index $W(G)$, hyper-Wiener index $WW(G)$ and Harary index $H(G)$ are three famous topological indices (See [23]), where

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v), \quad H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)}, \quad \text{and}$$

$$WW(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{2}\big(d(u,v) + d^2(u,v)\big).$$

The ordering of topological indices among some graph categories is an important topic of the theory of topological index [2–4,11,15,23]. For instance, the trees with the seven smallest and the fifteen greatest hyper-Wiener indices among trees of order $n \geq 20$ were determined in [8,10], the twelve smallest Wiener indices among trees of order $n \geq 24$ were identified in [6,8,14], the fifteen greatest Wiener indices among trees of order $n \geq 28$ were identified in [5,8,13], the seven smallest and eight greatest Harary indices among trees of order $n \geq 16$ were identified in [19]. Furthermore, the present authors and their cooperators proposed the following problem for further research on the distance-based topological indices (See Remark 5.4 of [23]): Giving a general method to characterize the extremal graphs in some particular sets of graphs and/or giving some unified properties for Q-indices. In this paper, we give some unified properties to Q-indices, and we also illustrate that the majorization theorem is an ideal method to deal with the largest (resp. smallest) Q-indices of trees with n vertices when $f(x)$ is nonnegative nonincreasing (resp. nondecreasing) function on x. From our new results, we determine the four largest and three smallest (resp. four smallest and three largest) Q-indices of trees with n vertices for strictly decreasing (resp.

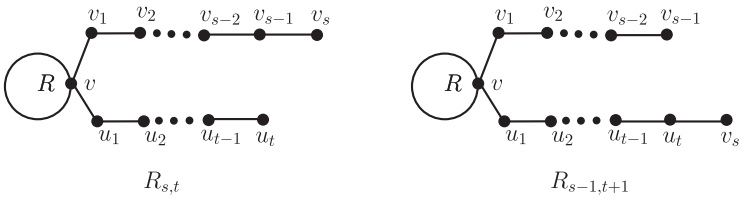


Fig. 2.1. The graphs $R_{s,t}$ and $R_{s-1,t+1}$.

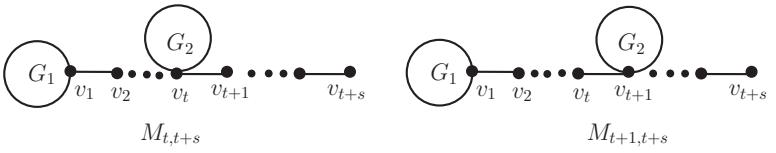


Fig. 2.2. The graphs $M_{t,t+s}$ and $M_{t+1,t+s}$.

increasing) nonnegative function $f(x)$, we extend the ordering of [19] to the twelve largest (resp. eighteen smallest) Harary indices of trees of order $n \geq 22$ (resp. $n \geq 38$), and we also extend the ordering of [10] to the ten smallest hyper-indices of trees of order $n \geq 18$. Furthermore, we obtain some new relations involving Wiener index, hyper-Wiener index and Harary index, which gives partial answers to some problems raised in [7,19].

2. Some unified properties for the Q-indices of graphs

Let G be a graph, and let X a subset of $V(G)$. We use $G[X]$ to denote the subgraph of G induced by X. Let $G - uv$ (resp., $G - v$) denote the graph obtained from G by deleting the edge $uv \in E(G)$ (resp., the vertex $v \in V(G)$). Similarly, $G + uv$ is a graph obtained from G by adding an edge $uv \notin E(G)$.

Hereafter, a path on n vertices is referred as P_n, and a star on n vertices is denoted by S_n. Suppose v is a vertex of graph R. As shown in Fig. 2.1, let $R_{s,t}$ $(t \geq s \geq 1)$ be the graph obtained from R by attaching two new paths P_s: $v_1v_2\cdots v_s$ and P_t: $u_1u_2\cdots u_t$ at v, respectively. Let $R_{s-1,t+1} = R_{s,t} - v_{s-1}v_s + u_tv_s$.

Proposition 2.1. *Let R be a connected graph with at least two vertices, $f(x)$ a nonnegative function of x, and let $t \geq s \geq 1$ be two positive integers. (i) If $f(x)$ is nonincreasing, then $W_f(R_{s,t}) \geq W_f(R_{s-1,t+1})$, where the inequality is strict when $f(x)$ is strictly decreasing. (ii) If $f(x)$ is nondecreasing, then $W_f(R_{s,t}) \leq W_f(R_{s-1,t+1})$, where the inequality is strict when $f(x)$ is strictly increasing.*

Proof. Let $V_1 = V(R) \setminus \{v\}$, then $R_{s,t}[V(R_{s,t}) \setminus V_1] \cong R_{s-1,t+1}[V(R_{s-1,t+1}) \setminus V_1]$. Let $V_2 = V(R_{s,t}) \setminus V_1$. It is easy to see that

$$\begin{aligned} W_f(R_{s-1,t+1}) - W_f(R_{s,t}) &= \sum_{w \in V(R_{s-1,t+1})} f\big(d_{R_{s-1,t+1}}(w, v_s)\big) - \sum_{w \in V(R_{s,t})} f\big(d_{R_{s,t}}(w, v_s)\big) \\ &= \sum_{w \in V_1} f\big(d_{R_{s-1,t+1}}(w, v_s)\big) - \sum_{w \in V_1} f\big(d_{R_{s,t}}(w, v_s)\big) \\ &= \sum_{w \in V_1} \Big(f\big(d_{R_{s-1,t+1}}(w, v_s)\big) - f\big(d_{R_{s,t}}(w, v_s)\big)\Big). \end{aligned} \tag{2.1}$$

Since $|V(R)| \geq 2$ and $t \geq s$, then $d_{R_{s-1,t+1}}(w, v_s) > d_{R_{s,t}}(w, v_s)$ holds for every $w \in V_1$. Now, the result follows from (2.1). □

Suppose that G_1 and G_2 are two connected graphs with $v_1 \in V(G_1)$ and $u_0 \in V(G_2)$. Let G_3 be the graph obtained from G_1 by attaching a new path P_{t+s-1}: $v_2v_3\cdots v_{t+s}$ at v_1 of G_1 (i.e., adding the edge v_1v_2), and then let $M_{t+i,t+s}$ be the graph obtained from G_3 and G_2 by identifying the two vertices v_{t+i} and u_0 (suppose that the new vertex is still v_{t+i}), where $0 \leq i \leq s-1$. For $0 \leq i \leq 1$, the graphs $M_{t+i,t+s}$ are shown in Fig. 2.2.

Proposition 2.2. *Let G_1 and G_2 be two connected graphs with $|V(G_1)| \geq 2$, $|V(G_2)| \geq 2$, $f(x)$ a nonnegative function of x, and let $t \geq s \geq 1$ be two positive integers. (i) If $f(x)$ is nonincreasing, then $W_f(M_{t,t+s}) \geq W_f(M_{t+1,t+s})$, where the inequality is strict when $f(x)$ is strictly decreasing. (ii) If $f(x)$ is nondecreasing, then $W_f(M_{t,t+s}) \leq W_f(M_{t+1,t+s})$, where the inequality is strict when $f(x)$ is strictly increasing.*

Proof. For convenience, we simplify $M_{t,t+s}$ and $M_{t+1,t+s}$ as G and G', respectively, in the proof of this lemma. Let $V_1 = V(G_1) \setminus \{v_1\}$, $V_2 = V(G_2) \setminus \{u_0\}$ and $V_3 = V(G) \setminus (V_1 \cup V_2)$. Then,

$$W_f(G') - W_f(G) = \sum_{v\in V_2}\left(\sum_{w\in V(G')} f(d_{G'}(w,v)) - \sum_{w\in V(G)} f(d_G(w,v))\right)$$

$$= \sum_{v\in V_2}\sum_{w\in V_1}(f(d_{G'}(w,v)) - f(d_G(w,v))) + \sum_{v\in V_2}\left(\sum_{w\in V_3} f(d_{G'}(w,v)) - \sum_{w\in V_3} f(d_G(w,v))\right)$$

$$= \sum_{v\in V_2}\sum_{w\in V_1}(f(d_{G'}(w,v)) - f(d_G(w,v))) + \sum_{v\in V_2}(f(t + d_{G_2}(u_0,v)) - f(s + d_{G_2}(u_0,v))). \tag{2.2}$$

Since $d_{G'}(w,v) > d_G(w,v)$ for any pair $\{w,v\}$ with $w \in V_1$ and $v \in V_2$, and since $t \geq s$, the result follows from (2.2). □

Proposition 2.3. *Let G_1 and G_2 be two connected graphs with $|V(G_1)| \geq 2$, $|V(G_2)| \geq 2$, $f(x)$ a nonnegative function of x, and let $t \geq 2$ and $s \geq 2$ be two positive integers. (i) If $f(x)$ is nonincreasing, then $W_f(M_{t,t+s}) \geq W_f(M_{t+s-1,t+s})$, where the inequality is strict when $f(x)$ is strictly decreasing. (ii) If $f(x)$ is nondecreasing, then $W_f(M_{t,t+s}) \leq W_f(M_{t+s-1,t+s})$, where the inequality is strict when $f(x)$ is strictly increasing.*

Proof. For convenience, we simplify $M_{t,t+s}$ and $M_{t+s-1,t+s}$ as G and G', respectively, in the proof of this lemma. Let $V_1 = V(G_1) \setminus \{v_1\}$, $V_2 = V(G_2) \setminus \{u_0\}$, $V_3 = V(G)\setminus(V_1 \cup V_2)$ and $V_4 = \{v_1, v_2, \ldots, v_{t-2}\}$ (When $t = 2$, $V_4 = \emptyset$). Then,

$$W_f(G') - W_f(G) = \sum_{v\in V_2}\left(\sum_{w\in V(G')} f(d_{G'}(w,v)) - \sum_{w\in V(G)} f(d_G(w,v))\right)$$

$$= \sum_{v\in V_2}\sum_{w\in V_1}(f(d_{G'}(w,v)) - f(d_G(w,v))) + \sum_{v\in V_2}\left(\sum_{w\in V_3} f(d_{G'}(w,v)) - \sum_{w\in V_3} f(d_G(w,v))\right).$$

$$= \sum_{v\in V_2}\sum_{w\in V_1}(f(d_{G'}(w,v)) - f(d_G(w,v))) + \sum_{v\in V_2}\left(\sum_{w\in V_4} f(d_{G'}(w,v)) - \sum_{w\in V_4} f(d_G(w,v))\right)$$

$$= \sum_{v\in V_2}\sum_{w\in V_1}(f(d_{G'}(w,v)) - f(d_G(w,v))) + \sum_{v\in V_2}\sum_{i=1}^{t-2}(f(s + d_{G_2}(v,u_0) + i) - f(1 + d_{G_2}(v,u_0) + i)).$$

Since $d_{G'}(w,v) > d_G(w,v)$ for any pair $\{w,v\}$ with $w \in V_1$ and $v \in V_2$, and since $s \geq 2$, the result holds. □

We denote a tree $T \cong T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$ with n vertices and two branching vertices u_1 and u_2, where $d(u_1) = r$ and $d(u_2) = t$, as follows: The orders of $r-1$ components, which are paths, of $T - u_1$ are $p_1, p_2, \ldots, p_{r-1}$, the order of the component which is not a path of $T - u_1$ is $p_r = n - p_1 - \cdots - p_{r-1} - 1$; The orders of $t-1$ components, which are paths, of $T - u_2$ are $q_1, q_2, \ldots, q_{t-1}$, the order of the component which is not a path of $T - u_2$ is $q_t = n - q_1 - \cdots - q_{t-1} - 1$.

Proposition 2.4. *Let n, $p_1 \geq 1$, $p_2 \geq 1$ and $q_1 \geq 2$ be four positive integers such that $n - p_1 - p_2 - q_1 \geq 3$, and let $f(x)$ be a nonnegative function of x.*

(i) If $f(q_1+1) + f(n-p_1-p_2-q_1) > f(n-p_2-q_1) + f(n-p_1-q_1)$, then $W_f(T_n(p_1,p_2;q_1,1)) > W_f(T_n(p_1,p_2;q_1-1,1))$.

(ii) If $f(q_1+1) + f(n-p_1-p_2-q_1) < f(n-p_2-q_1) + f(n-p_1-q_1)$, then $W_f(T_n(p_1,p_2;q_1,1)) < W_f(T_n(p_1,p_2;q_1-1,1))$.

Proof. In the proof of this result, we simplify $T_n(p_1, p_2; q_1, 1)$ and $T_n(p_1, p_2; q_1 - 1, 1)$ as T and T', respectively. Suppose the pendent vertex which is adjacent to u_2 in T is v_0 (See the definition of $T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$). Let $V_1 = V(T) \setminus \{v_0\}$. Then, $T - v_0 \cong T' - v_0$, and

$$W_f(T) - W_f(T') = \sum_{w\in V_1} f(d_{T'}(w,v_0)) - \sum_{w\in V_1} f(d_T(w,v_0))$$

$$= f(q_1+1) + f(n-p_1-p_2-q_1) - f(n-p_2-q_1) - f(n-p_1-q_1).$$

Thus, the result follows. □

The following result is used frequently in [18,26], and it can be seen as another majorization theorem for distance-based topological indices.

Proposition 2.5. *Let π and π' be two different degree sequences of trees with $\pi \lhd \pi'$ and let T_π^* and $T_{\pi'}^*$ the greedy trees with degree sequences π and π', respectively. Let $f(x)$ be a nonnegative function of x. (i) If $f(x)$ is nonincreasing, then $W_f(T_\pi^*) \leq$*

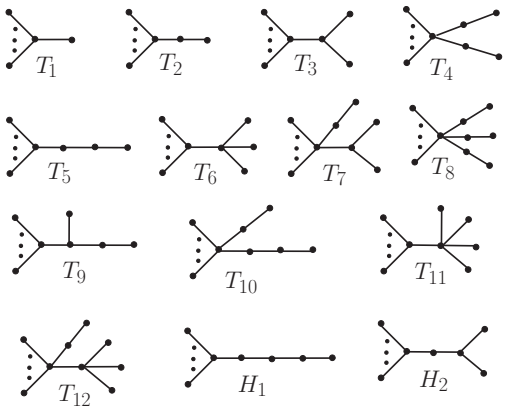


Fig. 2.3. The trees $T_1, T_2, \ldots, T_{12}, H_1$ and H_2 with $n \geq 12$ vertices.

$W_f(T^*_{\pi'})$, where the inequality is strict when $f(x)$ is strictly decreasing. (ii) If $f(x)$ is nondecreasing, then $W_f(T^*_{\pi}) \geq W_f(T^*_{\pi'})$, where the inequality is strict when $f(x)$ is strictly increasing.

Proof. Suppose that T^*_{π} and $T^*_{\pi'}$ are two trees with n vertices. By Theorem 1.1, $P_r(T^*_{\pi}) \leq P_r(T^*_{\pi'})$ and the inequality is strict for at least one $r \geq 1$. Now, (1.1) indicates that $Q_r(T^*_{\pi}) \geq Q_r(T^*_{\pi'})$ and $Q_r(T^*_{\pi}) > Q_r(T^*_{\pi'})$ holds for at least one $r \geq 1$. Thus, the result follows from (1.2). □

Since the greedy tree also has largest number of unordered pairs of vertices with distance not larger than r (i.e., $P_r(T)$) among all trees with given degree sequence [26], from (1.2) we can easily deduce that

Proposition 2.6. *[17,18] Let $f(x)$ be a nonnegative, nonincreasing (resp. nondecreasing) function of x. Then the graph invariant $W_f(T)$ is maximized (resp. minimized) by the greedy tree among all trees with given degree sequence. Furthermore, if $f(x)$ is strictly decreasing/increasing, then the greedy tree is the unique extremal tree.*

The tree $B(n, k)$ on n vertices is called a *broom*, which is obtained from a star S_{k+1} by attaching one path P_{n-k-1} to a pendent vertex of S_{k+1}. The following result determines the unique extremal tree with largest (resp. smallest) Q-index among $\mathbb{T}(n, \Delta)$ when $f(x)$ is a nonnegative, nonincreasing (resp. nondecreasing) function of x.

Proposition 2.7. *Let T be a tree of $\mathbb{T}(n, \Delta)$ with $2 \leq k \leq \Delta \leq n-1$ and $T \ncong B(n, k)$, and let $f(x)$ be a nonnegative function of x. (i) If $f(x)$ is nonincreasing, then $W_f(T) \geq W_f(B(n, \Delta)) \geq W_f(B(n, k))$ for $\Delta > k$, where both inequalities are strict when $f(x)$ is strictly decreasing. (ii) If $f(x)$ is nonincreasing, then $W_f(T) \leq W_f(B(n, \Delta)) \leq W_f(B(n, k))$ for $\Delta > k$, where both inequalities are strict when $f(x)$ is strictly increasing.*

Proof. We may suppose that $f(x)$ is 'nonincreasing', since the case of 'nondecreasing' can be proved similarly. Since $T \ncong B(n, \Delta)$, we have $3 \leq \Delta \leq n-2$. Suppose T contains exactly s branching vertices. If $s = 1$, by Proposition 2.1, $W_f(T) \geq W_f(B(n, \Delta)) \geq W_f(B(n, k))$ for $\Delta > k$, where both inequalities are strict when $f(x)$ is strictly decreasing. Otherwise, $s \geq 2$. By Proposition 2.1, there exists another tree of $\mathbb{T}(n, \Delta)$, said T', with exactly $s-1$ branching vertices such that $W_f(T) \geq W_f(T') \geq W_f(B(n, \Delta))$, where the first inequality is strict when $f(x)$ is strictly decreasing. This completes the proof of this result. □

As shown in Fig. 2.3, let $T_1, T_2, \ldots, T_{12}, H_1$ and H_2 be the trees with $n \geq 12$ vertices. Let $T_n(s_1, s_2, \ldots, s_k)$ denote the *starlike tree* of order n obtained by inserting $s_1 - 1, s_2 - 1, \ldots, s_k - 1$ vertices into k edges of the star S_{k+1} of order $k+1$ respectively, where $s_1 + s_2 + \cdots + s_k = n - 1$. From the definition, every tree with only one branching point is a starlike tree. It is easy to see that $T_1 \cong S_n$ and $B(n, 3) \cong T_n(n-3, 1, 1)$. In [18], it is shown that $W_f(P_n)$ is minimized and $W_f(S_n)$ is maximized when $f(x)$ is nonnegative nonincreasing function of x, and $W_f(P_n)$ is maximized and $W_f(S_n)$ is minimized when $f(x)$ is nonnegative nondecreasing function of x. Now, by Propositions 2.5–2.7, we can deduce the following:

Proposition 2.8. *Let T be a tree with n vertices and $f(x)$ a nonnegative function of x. Then, different from those occurring in the below inequalities, we have (i) If $f(x)$ is strictly decreasing, then $W_f(T_1) > W_f(T_2) > W_f(T_3) > \max\{W_f(T_4), W_f(T_6)\} > W_f(T) > \min\{W_f(T_n(1, 1; 1, 1)), W_f(T_n(n-4, 2, 1))\} > W_f(B(n, 3)) > W_f(P_n)$; (ii) If $f(x)$ is strictly increasing, then $W_f(T_1) < W_f(T_2) < W_f(T_3) < \min\{W_f(T_4), W_f(T_6)\} < W_f(T) < \max\{W_f(T_n(1, 1; 1, 1)), W_f(T_n(n-4, 2, 1))\} < W_f(B(n, 3)) < W_f(P_n)$.*

Proof. We may suppose that $f(x)$ is 'strictly decreasing', since the case of 'strictly increasing' can be proved similarly. Obviously, T_1 is the unique tree with $\Delta = n-1$, T_2 is the unique tree with $\Delta = n-2$, T_3, T_4, T_5 are all the trees with $\Delta = n-3$. If $T \cong T_5$, then Propositions 2.5–2.6 imply that $W_f(T_1) > W_f(T_2) > W_f(T_3) > W_f(T_4) > W_f(T_5)$. Otherwise, $\Delta(T) \leq n-4$.



Fig. 3.1. The trees W_n and W'_n with $n \geq 10$ vertices.

Let $\pi_1 = (n-4, 4, 1^{(n-2)})$ and let π be the degree sequence of T. Since T_6 is the unique greedy tree of $\Gamma(\pi_1)$ and $\pi \lhd \pi_1$, and hence Proposition 2.5 implies that $W_f(T_1) > W_f(T_2) > W_f(T_3) > W_f(T_6) > W_f(T)$.

If T has exactly one branching vertices, then $W_f(T) > W_f(T_n(n-4, 2, 1)) > W_f(B(n, 3)) > W_f(P_n)$ by Proposition 2.1. If T has exactly two branching vertices, then $W_f(T) > W_f(T_n(1, 1; 1, 1)) > W_f(B(n, 3)) > W_f(P_n)$ by Propositions 2.1 and 2.3. This completes the proof. □

3. New results on the ordering of Harary index of $\mathbb{T}(n)$

In [19], the eight largest Harary indices of $\mathbb{T}(n)$ have been determined for $n \geq 14$, the following results extends this ordering to the twelve largest Harary indices of $\mathbb{T}(n)$ for $n \geq 22$.

Theorem 3.1. *If T is a tree of order $n \geq 22$, then different from those occurring in the below inequalities, we have $H(T_1) > H(T_2) > \cdots > H(T_{12}) > H(T)$.*

Proof. Obviously, T_1 is the unique tree with $\Delta = n-1$, T_2 is the unique tree with $\Delta = n-2$, T_3, T_4, T_5 are all the trees with $\Delta = n-3$, $T_6, T_7, \ldots, T_{10}$, H_1 and H_2 are all the trees with $\Delta = n-4$. If $T \in \mathbb{T}(n) \setminus \{T_1, T_2, \ldots, T_{10}, H_1, H_2\}$, then $\Delta(T) \leq n-5$. Let $\pi_1 = (n-5, 5, 1^{(n-2)})$ and let $\pi_2 = (n-5, 4, 2, 1^{(n-3)})$. Then, $\Gamma(\pi_1) = \{T_{11}\}$ and T_{12} is the unique greedy tree of $\Gamma(\pi_2)$. For any $T \in \mathbb{T}(n) \setminus \{T_1, T_2, \ldots, T_{12}, H_1, H_2\}$ with $\pi \neq \pi_2$, it is easy to see that $\pi \lhd \pi_2 \lhd \pi_1$, and hence $H(T) < H(T_{12}) < H(T_{11})$ by Propositions 2.5–2.6, where π is the degree sequence of T. Furthermore, it has been proved that $H(T_1) > H(T_2) > \cdots > H(T_8) > H(T)$ for any $T \in \mathbb{T}(n) \setminus \{T_1, T_2, \ldots, T_8\}$ [19]. Thus, to complete the proof of this result, it suffices to show that $H(T_9) > H(T_{10}) > \cdots > H(T_{12}) > H(H_2)$, as $H(H_2) > H(H_1)$ by Proposition 2.1.

By an elementary computation, we have

$$H(T_9) = \frac{3n^2-4n+25}{12}, \quad H(T_{10}) = \frac{15n^2-20n+102}{60}, \quad H(T_{11}) = \frac{3n^2-5n+42}{12},$$

$$H(T_{12}) = \frac{3n^2-5n+33}{12}, \quad \text{and} \quad H(H_2) = \frac{3n^2-5n+30}{12}.$$

Thus, $H(T_9) - H(T_{10}) = \frac{23}{60} > 0$, $H(T_{10}) - H(T_{11}) = \frac{5n-108}{60} > 0$, $H(T_{11}) - H(T_{12}) = \frac{3}{4}$, and $H(T_{12}) - H(H_2) = \frac{1}{4}$. This completes the proof of this result. □

In [19], Xu has also identified the seven smallest Harary indices of trees with $n \geq 16$ vertices. In the following, we shall extend this ordering to the eighteen smallest Harary indices of trees with $n \geq 38$ vertices, that is

Theorem 3.2. *(i) If T is a tree with $n \geq 66$ vertices, then different from those occurring in the below inequalities, we have $H(T) > H(T_n(n-6, 1; 1, 1)) > \max\{H(T_n(n-10, 8, 1)), H(T_n(4, 1; 1, 1))\} > \min\{H(T_n(n-10, 8, 1)), H(T_n(4, 1; 1, 1))\} > H(T_n(n-9, 7, 1)) > H(T_n(2, 1; 2, 1)) > H(T_n(n-5, 1; 1, 1)) > \max\{H(T_n(3, 1; 1, 1)), H(T_n(n-8, 6, 1))\} > \min\{H(T_n(3, 1; 1, 1)), H(T_n(n-8, 6, 1))\} > H(B(n, 4)) > H(T_n(n-7, 5, 1)) > H(T_n(n-5, 2, 2)) > H(T_n(2, 1; 1, 1)) > H(T_n(n-6, 4, 1)) > H(T_n(n-5, 3, 1)) > H(T_n(1, 1; 1, 1)) > H(T_n(n-4, 2, 1)) > H(B(n, 3)) > H(P_n)$. (ii) If T is a tree with $38 \leq n \leq 65$ vertices, then different from those occurring in the below inequalities, we have $H(T) > \min\{H(T_n(n-11, 9, 1)), H(T_n(n-6, 1; 1, 1))\} > H(T_n(4, 1; 1, 1)) > H(T_n(n-10, 8, 1)) > H(T_n(2, 1; 2, 1)) > H(T_n(n-5, 1; 1, 1)) > H(T_n(n-9, 7, 1)) > H(T_n(3, 1; 1, 1)) > H(T_n(n-8, 6, 1)) > H(B(n, 4)) > H(T_n(n-7, 5, 1)) > H(T_n(n-5, 2, 2)) > H(T_n(2, 1; 1, 1)) > H(T_n(n-6, 4, 1)) > H(T_n(n-5, 3, 1)) > H(T_n(1, 1; 1, 1)) > H(T_n(n-4, 2, 1)) > H(B(n, 3)) > H(P_n)$.*

To prove Theorem 3.2, we shall introduce more notations and lemmas in the following. Let W_n and W'_n be the two trees with $n \geq 10$ vertices as shown in Fig. 3.1. Since $H(P_n) = \sum_{i=2}^{n} \frac{n}{i}$ (See Corollary 4.6 of [18]), it is not difficult to obtain the following equations:

$$H(B(n, \Delta)) = \sum_{i=2}^{n+1-\Delta} \frac{n}{i} + \frac{(\Delta-1)(\Delta+2)}{4}, \quad (\Delta \geq 2),$$

$$H(T_n(n-k-3, k, 2)) = \sum_{i=2}^{n-2} \frac{(n-2)}{i} + \sum_{i=1}^{n-k-1} \frac{2}{i} + \sum_{i=2}^{k+1} \frac{1}{i} + \sum_{i=3}^{k+2} \frac{1}{i} - \frac{1}{n-k-1}, \quad (4 \leq 2k \leq n-3),$$

$$H(T_n(n-k-2,k,1)) = \sum_{i=2}^{n-1}\frac{(n-1)}{i} + \sum_{i=1}^{n-k-1}\frac{1}{i} + \sum_{i=2}^{k+1}\frac{1}{i}, \quad (2 \le 2k \le n-2),$$

$$H(T_n(k,1;1,1)) = \sum_{i=2}^{n-3}\frac{(n-1)}{i} + \sum_{i=1}^{n-k-2}\frac{1}{i} + \sum_{i=1}^{k+1}\frac{1}{i} + \frac{3}{2} + \frac{1}{n-k-2}, \quad (2k \le n-3).$$

Lemma 3.1. (*i*) *If* $n \ge 34$, *then* $\min\{H(B(n,5)), H(T_n(n-5,2,1,1))\} > H(T_n(1^{(3)};1^{(2)})) > H(T_n(n-6,1;1,1))$ *and* $\min\{H(T_n(n-6,3,2)), H(T_n(5,1;1,1)), H(W_n), H(W_n'), H(T_n(2,2;1,1)), H(T_n(3,1;2,1))\} > H(T_n(n-6,1;1,1))$. (*ii*) *If* $20 \le n \le 56$, *then* $\min\{H(B(n,5)), H(T_n(n-5,2,1,1))\} > H(T_n(1^{(3)};1^{(2)})) > H(T_n(n-11,9,1))$ *and* $\min\{H(T_n(n-6,3,2)), H(T_n(5,1;1,1)), H(W_n), H(W_n'), H(T_n(2,2;1,1)), H(T_n(3,1;2,1))\} > H(T_n(n-11,9,1))$. (*iii*) *If* $20 \le n \le 49$, *then* $H(T_n(n-11,9,1)) < H(T_n(n-6,1;1,1))$. (*iv*) *If* $n \ge 50$, *then* $H(T_n(n-6,1;1,1)) < H(T_n(n-11,9,1))$.

Proof. By an elementary computation, it follows that

$$H(T_n(1^{(3)};1^{(2)})) = \sum_{i=2}^{n-4}\frac{n}{i} + 6 + \frac{2}{n-4}, \quad H(T_n(n-6,1;1,1)) = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{35}{6} + \frac{2}{n-3} - \frac{1}{n-4},$$

$$H(W_n') = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{19}{3} + \frac{1}{n-6} - \frac{1}{n-5}, \quad H(T_n(2,2;1,1)) = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{71}{12} + \frac{1}{n-5},$$

$$H(W_n) = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{37}{6} + \frac{1}{n-5}, \quad H(T_n(3,1;2,1)) = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{71}{12} + \frac{1}{n-3} + \frac{1}{n-6} - \frac{1}{n-4},$$

$$H(T_n(n-5,2,1,1)) = \sum_{i=2}^{n-4}\frac{n}{i} + \frac{37}{6} + \frac{1}{n-3}.$$

When $n \ge 20$, it is easy to check the required inequalities. □

Lemma 3.2. *Let* T *be a tree of* $\mathbb{T}(n,\Delta)$ *with* $n \ge 34$ *and* $\Delta \ge 4$. *If* $T \notin \{B(n,4), T_n(1^{(3)};1^{(2)})\}$, *then* $H(T) > H(T_n(1^{(3)};1^{(2)}))$.

Proof. If $\Delta \ge 5$, by Proposition 2.7 and Lemma 3.1, we have $H(T) \ge H(B(n,5)) > H(T_n(1^{(3)};1^{(2)}))$. Otherwise, $\Delta = 4$. We may suppose that T contains exactly k branching vertices.

If $k = 1$, since $T \ncong B(n,4)$, we have $H(T) \ge H(T_n(n-5,2,1,1))$ by Proposition 2.1.

If $k = 2$, we may suppose that $T \cong T_n(p_1,p_2,p_3;q_1,q_2,\ldots,q_{t-1})$, where $t \in \{3,4\}$ and $p_1 \ge p_2 \ge p_3 \ge 1$. When $p_1 \ge 2$, since $n - p_1 - p_2 - p_3 - 1 \ge 3$, we have $H(T) > H(T_n(p_1,p_2,p_3,n-p_1-p_2-p_3-1)) \ge H(T_n(n-5,2,1,1))$ by Proposition 2.1. When $p_1 = 1$, then $p_2 = p_3 = 1$, since $T \ncong T_n(1^{(3)};1^{(2)})$, Propositions 2.1 and 2.3 imply that $H(T) > H(T_n(1^{(3)};1^{(2)}))$.

Thus, the result also holds for $1 \le k \le 2$ by Lemma 3.1.

If $k \ge 3$, by Propositions 2.1, there exists another tree T' with $k-1$ branching vertices such that $H(T) > H(T') \ge H(T_n(1^{(3)};1^{(2)}))$. □

Lemma 3.3. *Let* T *be a tree of* $\mathbb{T}(n,3)$ *with exactly three branching vertices.* (*i*) *If* $n \ge 50$, *then* $H(T) > H(T_n(n-6,1;1,1))$. (*ii*) *If* $20 \le n \le 56$, *then* $H(T) > H(T_n(n-11,9,1))$.

Proof. Let w_1, w_2 and w_3 be the three branching vertices of T. We suppose that w_2 lies on the path from w_1 to w_3, and the orders of three branchings of $T - w_2$ are p_1, p_2 and p_3, respectively, where $p_1 \ge p_2 \ge p_3 \ge 1$. If $p_3 \ge 2$, then $H(T) > H(T_n(p_1,p_2,p_3)) \ge H(T_n(n-6,3,2))$ by Proposition 2.1, since $p_1 \ge p_2 \ge 3$. Otherwise, $p_3 = 1$.

If $p_2 \ge 9$, then $H(T) > H(T_n(p_1,p_2,1)) \ge H(T_n(n-11,9,1))$ by Proposition 2.1.

If $5 \le p_2 \le 8$, then $H(T) > H(T_n(p_2,1;1,1) \ge H(T_n(5,1;1,1))$ by Propositions 2.1–2.2.

If $3 \le p_2 \le 4$, then $H(T) \ge \min\{H(W_n'), H(W_n)\}$ by Propositions 2.1–2.3.

Now, the result follows from Lemma 3.1. □

Lemma 3.4. *Suppose that* $T \cong T_n(p_1,p_2;q_1,q_2)$ *and* $T \notin \{T_n(n-6,1;1,1), T_n(n-5,1;1,1), T_n(1,1;1,1), T_n(2,1;1,1), T_n(2,1;2,1), T_n(3,1;1,1), T_n(4,1;1,1)\}$. (*i*) *If* $n \ge 50$, *then* $H(T) > H(T_n(n-6,1;1,1))$. (*ii*) *If* $20 \le n \le 49$, *then* $H(T) > H(T_n(n-11,9,1))$.

Proof. For convenience, we may suppose that $p_1 \ge p_2$ and $p_1 \ge q_1 \ge q_2$. If either $p_2 \ge 3$ or $q_2 \ge 3$, then Proposition 2.1 implies that $H(T) > H(T_n(n-7,3,3)) > H(T_n(n-6,3,2))$ and hence the result follows from Lemma 3.1. Thus, it suffices to consider the case of $p_2 \le 2$ and $q_2 \le 2$. Since $T \notin \{T_n(n-5,1;1,1), T_n(1,1;1,1)\}$, we have $2 \le p_1 \le n-6$. We divide the proof into the following two cases:

Case 1. $p_2 = 2$. If $p_1 \ge 3$, since $n - p_1 - 3 \ge 3$, we have $H(T) > H(T_n(p_1,n-p_1-3,2)) \ge H(T_n(n-6,3,2))$ by Proposition 2.1. Otherwise, $p_1 = 2$. By Proposition 2.3, $H(T) \ge H(T_n(2,2;1,1))$.

Case 2. $p_2 = 1$.

By the choice of T and Case 1, we may suppose that $p_1 \geq q_1 \geq p_2 = q_2 = 1$ and $p_1 \geq 3$. If $9 \leq p_1 \leq n-11$, then $H(T) > H(T_n(n-11, 9, 1))$ by Proposition 2.1. If $5 \leq p_1 \leq 8$, by Propositions 2.2–2.3, we have $H(T) \geq H(T_n(p_1, 1; 1, 1)) \geq H(T_n(5, 1; 1, 1))$.

In what follows, we may suppose that $3 \leq p_1 \leq 4$ or $n-10 \leq p_1 \leq n-6$.

Subcase 2.1. $n-10 \leq p_1 \leq n-6$.

If $n-10 \leq p_1 \leq n-7$, by Proposition 2.3 it follows that $H(T) \geq H(T_n(p_1, 1; 1, 1))$. Since $n-10 \leq p_1 \leq n-7$, Proposition 2.4 implies that $H(T_n(p_1, 1; 1, 1)) > H(T_n(n-6, 1; 1, 1))$.

Otherwise, $p_1 = n-6$. Since $T \ncong T_n(n-6, 1; 1, 1)$, by Proposition 2.2 we have $H(T) > H(T_n(n-6, 1; 1, 1))$.

Subcase 2.2. $3 \leq p_1 \leq 4$.

Since $T \notin \{T_n(3, 1; 1, 1), T_n(4, 1; 1, 1)\}$, we have $2 \leq q_1 \leq p_1 \leq 4$. By Propositions 2.2–2.3, $H(T) \geq H(T_n(3, 1; 2, 1))$.

Now, the result follows from Lemma 3.1. □

Lemma 3.5. *Suppose that* $T \cong T_n(s_1, s_2, s_3)$ *and* $T \notin \{T_n(n-3, 1, 1), T_n(n-4, 2, 1), \ldots, T_n(n-10, 8, 1), T_n(n-5, 2, 2)\}$. *(i) If* $n \geq 50$, *then* $H(T) > H(T_n(n-6, 1; 1, 1))$. *(ii) If* $20 \leq n \leq 56$, *then* $H(T) \geq H(T_n(n-11, 9, 1))$, *with equality if and only if* $T \cong T_n(n-11, 9, 1)$.

Proof. We may suppose that $s_1 \geq s_2 \geq s_3 \geq 1$. If $s_3 \geq 2$, by Proposition 2.1 and the choice of T, we have $H(T) \geq H(T_n(n-6, 3, 2))$ and hence the result already holds by Lemma 3.1. Otherwise, $s_3 = 1$. By the definition of T and Proposition 2.1, we have $H(T) \geq H(T_n(n-11, 9, 1))$, with equality if and only if $T \cong T_n(n-11, 9, 1)$. □

Proof of Theorem 3.2. By Lemmas 3.1–3.3 and Proposition 2.1 we can conclude that $H(T) > H(T_n(n-6, 1; 1, 1))$ when $n \geq 50$ and $H(T) > H(T_n(n-11, 9, 1))$ when $38 \leq n \leq 49$ for any tree T with at least three branching vertices or maximum degree at least four. By an elementary computation, it follows that

$$H(T_n(n-5, 1; 1, 1)) = \sum_{i=2}^{n-3} \frac{n}{i} + \frac{14}{3} - \frac{1}{n-3}, \quad H(T_n(2, 1; 2, 1)) = \sum_{i=2}^{n-4} \frac{n}{i} + \frac{17}{3} + \frac{1}{n-3} + \frac{1}{n-5}.$$

Now, the results follow from Lemmas 3.1, 3.4 and 3.5, and the formulas for $H(T_n(n-5, 1; 1, 1))$, $H(T_n(2, 1; 2, 1))$, $H(T_n(n-k-3, k, 2))$, $H(T_n(n-k-2, k, 1))$, $H(T_n(k, 1; 1, 1))$ and $H(T_n(n-6, 1; 1, 1))$. □

4. New relations involving Wiener index, hyper-Wiener index and Harary index

In [19], Xu asked the following four questions (See Remarks 5.1–5.4 of [19]):

Problem 4.1. In what set $\mathcal{G}(n)$ of connected graphs of order n, are the extremal (maximal or minimal) Harary index and the extremal (minimal or maximal) hyper-Wiener index attained at the same graph?

Problem 4.2. In what set $\mathcal{G}(n)$ of connected graphs of order n, are the extremal (maximal or minimal) Harary index and the extremal (minimal or maximal) Wiener index attained at the same graph?

Problem 4.3. In what set $\mathcal{G}(n)$ of connected graphs of order n, are the extremal (maximal or minimal) hyper-Wiener index and the extremal (maximal or minimal) Wiener index attained at the same graph?

Problem 4.4. Which are the further relations among these three topological indices: Wiener index, hyper-Wiener index and Harary index, especially between (hyper-)Wiener index and Harary index?

In [16], Schmuck has shown that the complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ gives the minimal Wiener index for all connected bipartite graphs of order n. From the definitions of hyper-Wiener index and Harary index, one can easily prove that

$$WW(G) \geq WW(K_{a,b}) = \frac{3n(n-1)}{2} - 2ab \geq \frac{3n(n-1)}{2} - 2\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \quad \left(a+b=n,\ G \in \mathcal{B}(n)\right)$$

with equality holding if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$, and

$$H(G) \leq H(K_{a,b}) = \frac{n(n-1)}{4} + \frac{ab}{2} \leq \frac{n(n-1)}{4} + \frac{1}{2}\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \quad \left(a+b=n,\ G \in \mathcal{B}(n)\right)$$

with equality holding if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

From [16,23] with the above results, we make the following Tables 1 and 2 (In both tables, we only consider all the graphs of order $n \geq 7$). From these tables, we can obtain partial answer to Problems 4.1–4.3. Now, we introduce some notation for Tables 1 and 2. Denote by C_g a cycle with g vertices. Let $C_{n,g}$ be a unicyclic graph with n vertices and girth g, which is obtained by attaching one path P_{n-g} to one vertex of C_g. Let $B_n^{(0)}$ be a bicyclic graph obtained from $C_{n,4}$ by adding one edge between two non-adjacent vertices of degrees two in the cycle C_4 of $C_{n,4}$, and let $S_n^{(k)}$ be a graph obtained from S_n by adding any k edges among these pendent vertices of S_n. From the definition, $S_n^{(1)}$ is unique, while $S_n^{(2)}$ is not unique for $n \geq 5$. Let $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ be the completed bipartite graph with almost equal number of vertices in each part.

Table 1
Maximal (hyper-)Wiener index & minimal Harary index for the class of graphs $\mathcal{G}(n)$, $\mathcal{B}(n)$, $\mathbb{T}(n)$, $\mathbb{U}(n)$ and $\mathbb{B}(n)$.

	Maximal Wiener index	Maximal hyper-Wiener index	Minimal Harary index
$\mathcal{G}(n)$	P_n	P_n	P_n
$\mathcal{B}(n)$	P_n	P_n	P_n
$\mathbb{T}(n)$	P_n	P_n	P_n
$\mathbb{U}(n)$	$C_{n,3}$	$C_{n,3}$	$C_{n,3}$
$\mathbb{B}(n)$	$B_n^{(0)}$	$B_n^{(0)}$	$B_n^{(0)}$

Table 2
Minimal (hyper-)Wiener index & maximal Harary index for the class of graphs $\mathcal{G}(n)$, $\mathcal{B}(n)$, $\mathbb{T}(n)$, $\mathbb{U}(n)$ and $\mathbb{B}(n)$.

	Minimal Wiener index	Minimal hyper-Wiener index	Maximal Harary index
$\mathcal{G}(n)$	K_n	K_n	K_n
$\mathcal{B}(n)$	$K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$	$K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$	$K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$
$\mathbb{T}(n)$	S_n	S_n	S_n
$\mathbb{U}(n)$	$S_n^{(1)}$	$S_n^{(1)}$	$S_n^{(1)}$
$\mathbb{B}(n)$	$S_n^{(2)}$	$S_n^{(2)}$	$S_n^{(2)}$

In what follows, we shall give a partial answer to Problem 4.4 by presenting some relations between these three topological indices: Wiener index, hyper-Wiener index and Harary index. To do this, we need the following two lemmas:

Lemma 4.1. *(Radon's inequality) [9] If $a_k > 0$, $x_k > 0$, $p > 0$, and $k \in \{1, 2, \ldots, r\}$, then the following inequality holds:*

$$\sum_{k=1}^{r} \frac{x_k^{p+1}}{a_k^p} \geq \frac{\left(\sum_{k=1}^{r} x_k\right)^{p+1}}{\left(\sum_{k=1}^{r} a_k\right)^p}$$

with equality holding if and only if $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_r}{a_r}$.

Lemma 4.2. *(Reverse Radon's inequality) [9] If $a_k > 0$, $x_k > 0$, $0 \leq p \leq 1$, and $k \in \{1, 2, \ldots, r\}$, then the following inequality holds:*

$$\sum_{k=1}^{r} \frac{x_k^{p}}{a_k^{p-1}} \leq \frac{\left(\sum_{k=1}^{r} x_k\right)^{p}}{\left(\sum_{k=1}^{r} a_k\right)^{p-1}}.$$

Theorem 4.1. *Let G be a connected graph with m edges. Then,*

$$(H(G) - m)\,(2WW(G) - W(G) - m)^2 \geq (W(G) - m)^3 \tag{4.1}$$

with equality holding if and only if G is a graph of diameter at most 2.

Proof. Suppose that G is a graph with n vertices and the diameter G is d. For $d = 1$, we have $H(G) = W(G) = WW(G) = m = \frac{n(n-1)}{2}$. Hence the equality holds in (4.1). Otherwise, $d \geq 2$.

Let $\mathscr{D}$ be the set of pairs $\{u, v\}$ of vertices of G with $d(u, v) \geq 2$. Then, $r = |\mathscr{D}| = \frac{n(n-1)}{2} - m$. We set $p = 2$, $x_k = d(u, v)$ and $a_k = d^2(u, v)$ in Lemma 4.1, where $\{u, v\} \in \mathscr{D}$ and $k = 1, 2, \ldots, r$. Then,

$$\sum_{\{u,v\}\in\mathscr{D}} \frac{d^3(u, v)}{d^4(u, v)} \geq \frac{\left(\sum_{\{u,v\}\in\mathscr{D}} d(u, v)\right)^3}{\left(\sum_{\{u,v\}\in\mathscr{D}} d^2(u, v)\right)^2} \tag{4.2}$$

with equality holding if and only if $d(u, v) = d(y, z)$ for any two pairs $\{u, v\} \in \mathscr{D}$ and $\{y, z\} \in \mathscr{D}$ of vertices.

Using the definition of the Wiener index, hyper-Winer index and Harary index, from the above, we get

$$(2WW(G) - W(G) - m)^2 = \left(\sum_{\{u,v\}\in\mathscr{D}} d^2(u, v)\right)^2 \geq \frac{(W(G) - m)^3}{H(G) - m}, \tag{4.3}$$

and hence (4.1) holds.

It is easy to see that equality holds in (4.1) if and only if equality holds in (4.3). While lemma 4.1 implies that equality holds in (4.3) if and only if $d(u, v) = d(y, z)$ holds for any two pairs $\{u, v\} \in \mathscr{D}$ and $\{y, z\} \in \mathscr{D}$ of vertices, and hence G is a graph with diameter two. □

If we consider all pairs $\{u, v\}$ of vertices of G in (4.2), then we can obtain:

Corollary 4.1. *If G is a connected graph with n vertices, then*

$$H(G)\,(2WW(G)-W(G))^2 \geq W^3(G)$$

with equality holding if and only if $G \cong K_n$.

Theorem 4.2. *Let G be a connected graph with n vertices and m edges. Then,*

$$(2WW(G)-W(G)-m)\,(n(n-1)-2m) \geq 2(W(G)-m)^2 \tag{4.4}$$

with equality holding if and only if G is a graph of diameter at most 2.

Proof. Suppose that the diameter G is d. For $d=1$, it is easy to check equality (4.4) holds. Otherwise, $d \geq 2$. Similar with the proof of Theorem 4.1, by setting $p=1$, $x_k = d(u,v)$ and $a_k = d^2(u,v)$ in Lemma 4.1, where $\{u,v\} \in \mathscr{D}$ and $k = 1, 2, \ldots, \frac{n(n-1)}{2} - m$. Then,

$$\frac{n(n-1)}{2} - m = \sum_{\{u,v\}\in\mathscr{D}} 1 \geq \frac{\left(\sum\limits_{\{u,v\}\in\mathscr{D}} d(u,v)\right)^2}{\sum\limits_{\{u,v\}\in\mathscr{D}} d^2(u,v)} = \frac{(W(G)-m)^2}{2WW(G)-W(G)-m}$$

with equality holding if and only if $d(u,v) = d(y,z)$ for any two pairs $\{u,v\} \in \mathscr{D}$ and $\{y,z\} \in \mathscr{D}$ of vertices, and hence G is a graph with diameter two. This completes the proof. □

Theorem 4.3. *Let G be a connected graph with n vertices and m edges. Then,*

$$4(W(G)-m)\,(H(G)-m) \geq (n(n-1)-2m)^2.$$

Proof. Similar with the proof of Theorem 4.1, by setting $p=1/2$, $x_k = d(u,v)$ and $a_k = 1/d(u,v)$ in Lemma 4.2, where $\{u,v\} \in \mathscr{D}$ and $k = 1, 2, \ldots, \frac{n(n-1)}{2} - m$. Then,

$$\left(\sum_{\{u,v\}\in\mathscr{D}} 1\right)^2 \leq \left(\sum_{\{u,v\}\in\mathscr{D}} d(u,v)\right)\left(\sum_{\{u,v\}\in\mathscr{D}} \frac{1}{d(u,v)}\right), \tag{4.5}$$

that is,

$$(W(G)-m)\,(H(G)-m) \geq \left(\frac{n(n-1)}{2} - m\right)^2,$$

which gives the required result. □

If we consider all pairs $\{u,v\}$ of vertices of G in (4.5), then we can obtain:

Corollary 4.2. *If G is a connected graph with n vertices, then* $4W(G)H(G) \geq n^2(n-1)^2$.

5. Further discussion

By comparing the methods to dealt with the largest and smallest ordering of Harary indices in the class of trees with n vertices, it is not difficult to find that the largest ordering is easier than the smallest ordering. The main reason is that majorization theorem is effective for degree sequence with large maximum degree, since these trees with such degree sequences are easily determined. Actually, we can employ the similar method to extend the ordering of Theorem 3.1 by considering the trees with degree sequences such that $\Delta \geq n-6$, as the tree with degree sequence $(n-6, 6, 1^{(n-2)})$ is unique. With the similar reason, we can conclude that it is not a difficult task to consider the largest (resp. smallest) ordering of Q-indices in the class of trees with n vertices when $f(x)$ is nonnegative strictly decreasing (resp. increasing) function of x by employing Propositions 2.5–2.6.

Note that the twelve smallest Wiener indices of $\mathbb{T}(n)$ had been determined in [6,8,14] for $n \geq 24$, and the seven smallest hyper-Wiener indices of $\mathbb{T}(n)$ had been determined in [8,10] for $n \geq 17$ ($WW(T) > WW(T_5) > WW(T_8)$ in Theorem 3.4 (2) of [23] should be $WW(T) > WW(T_8)$). In what follows, as an illustrating example, we shall use majorization theorem to determined the ten smallest hyper-Wiener indices of $\mathbb{T}(n)$ for $n \geq 18$, that is,

Theorem 5.1. *If T is a tree of order* $n \geq 18$, *then different from those occurring in the below inequalities, we have* $WW(T) > WW(T_{12}) > WW(T_{11}) > WW(T_5) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.

Proof. Let $\pi_1 = (n-5, 5, 1^{(n-2)})$, $\pi_2 = (n-5, 4, 2, 1^{(n-3)})$ and let π be the degree sequence of T. If $T \in \mathbb{T}(n) \setminus \{T_1, T_2, \ldots, T_{12}, H_1, H_2\}$ with $\pi \neq \pi_2$, then $\pi \lhd \pi_2 \lhd \pi_1$, and hence $WW(T) > WW(T_{12}) > WW(T_{11})$ by Propositions 2.5–2.6.

It has been proved that $WW(T) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$ for any $T \in \mathbb{T}(n) \setminus \{T_1, T_2, T_3, T_4, T_6, T_7, T_8\}$ [8,10].

By an elementary computation, we have

$$WW(T_5) = \frac{3n^2+13n-70}{2}, \quad WW(T_9) = \frac{3n^2+19n-114}{2},$$
$$WW(T_{10}) = \frac{3n^2+19n-82}{2}, \quad WW(T_{11}) = \frac{3n^2+17n-140}{2},$$
$$WW(T_{12}) = \frac{3n^2+17n-98}{2}, \quad WW(H_1) = \frac{3n^2+37n-190}{2},$$
$$\text{and} \quad WW(H_2) = \frac{3n^2+27n-154}{2}.$$

From the above equations, we can conclude that $WW(T_{11}) > WW(T_5)$ and $\min\{WW(T_9), WW(T_{10}), WW(H_1), WW(H_2)\} > WW(T_{12})$, and hence the result holds. □

As referred before, we can employ the majorization theorem to extend these smallest ordering of Winer index and hyper-Wiener index (resp. largest ordering of Harary index), and hence the majorization theorem is a good and effective tool to deal with the largest (resp. smallest) ordering of Q-indices in the class of trees with n vertices when $f(x)$ is nonnegative strictly decreasing (resp. increasing) function of x. Actually, we can also employ the similar method to extend the ordering result of Theorem 3.2 by more complex analyze (By Lemma 3.2, it suffices to consider the ordering of trees of $\mathbb{T}(n,3)$). However, it is not an easy task for us to obtain a general method to consider the smallest (resp. largest) ordering of Q-indices in the class of trees with n vertices when $f(x)$ is nonnegative strictly decreasing (resp. increasing) function of x.

By the former discussion, we can conclude that the majorization theorem is a good tool to deal with the ordering problem of Q-index among trees with n vertices. Actually, many extremal problems for other topological indices or comparison problem between different topological indices among some graph categories has also been considered [20–22]. Thus, it is natural for us to consider the following problem [12]: whether we can also employ this method to deal with the ordering problem of Q-index or the comparison problem between different topological indices among some graph categories?

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Which cospectral graphs have same degree sequences☆

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ABSTRACT

Two graphs are said to be L-cospectral (respectively, Q-cospectral) if they have the same (respectively, signless) Laplacian spectra, and a graph G is said to be $L-DS$ (respectively, $Q-DS$) if there does not exist other non-isomorphic graph H such that H and G are L-cospectral (respectively, Q-cospectral). Let $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$ be the degree sequence of a graph G with n vertices. In this paper, we prove that except for two exceptions (respectively, the graphs with $d_1(G) \in \{4, 5\}$), if H is L-cospectral (respectively, Q-cospectral) with a connected graph G and $d_2(G) = 2$, then H has the same degree sequence as G. A spider graph is a unicyclic graph obtained by attaching some paths to a common vertex of the cycle. As an application of our result, we show that every spider graph and its complement graph are both $L-DS$, which extends the corresponding results of Haemers et al. (2008), Liu et al. (2011), Zhang et al. (2009) and Yu et al. (2014).
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1. Introduction

Throughout this paper, G is an undirected simple graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let $d_G(v)$ and $N_G(v)$ be the degree and neighbor set of vertex v in G, respectively. If $d_G(v) = 1$, then we call v a *pendent vertex*. A vertex with maximum degree of G is always referred to be a *maximum vertex*. In the sequel, we enumerate the degrees of G in non-increasing order, i.e., $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$.

As usual, $K_{1,n-1}$, K_n, C_n and P_n denote the star, complete graph, cycle and path with n vertices, respectively. A connected graph G with n vertices and $n + c - 1$ edges is called a *c-cyclic graph*. An *s-rose graph* is a graph with s (≥ 2) cycles that all meet in one vertex. Clearly, an s-rose graph is connected and the maximum vertex has degree $2s$ and the other vertices have degree 2. Let $R(p, q)$ be a 2-rose graph with two cycles C_p and C_q.

Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal degree matrix of G, respectively. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$, and the *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. It is easy to see that $Q(G)$ is positive semidefinite (see [18]) and hence its eigenvalues can be arranged as:

$$\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) \geq 0.$$

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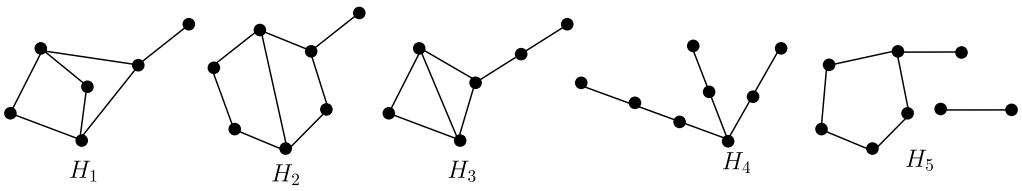


Fig. 1.1. The graphs H_1, H_2, H_3, H_4 and H_5.

Note that $L(G)$ is a positive semidefinite matrix with all row sums being equal to zero. Thus, we can use

$$\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0$$

to denote the eigenvalues of $L(G)$. For the sake of brevity, if there is no risk of confusion, we always simplify $d_i(G)$, $d_G(v)$, $N_G(v)$, $\lambda_i(G)$ and $\mu_i(G)$ as d_i, $d(v)$, $N(v)$, λ_i and μ_i, respectively.

Two graphs are said to be *A-cospectral* (respectively, *Q-cospectral*, *L-cospectral*) if they have the same adjacency (respectively, signless Laplacian, Laplacian) spectra. Similarly, two graphs are said to be *co-degree* if they have the same degree sequences. A graph G is said to be $A - DS$ (respectively, $Q - DS$, $L - DS$) if there does not exist other non-isomorphic graph H such that H and G are A-cospectral (respectively, Q-cospectral, L-cospectral).

Which graphs are determined by their spectra? This question was proposed by Günthard and Primas [4] more than 50 years ago in the context of Hückel's theory in chemistry, and had drawn more and more attention recently. For details, we refer the readers to [2,16] and the references therein. In this line, it is an interesting and challenging problem that

Problem 1.1 (*[2]*)**.** How much is the ratio between these *DS* graphs and all graphs with n vertices when n tends to infinity?

Furthermore, as discovered in [23], when we want to prove that G is $Q - DS$ (respectively, $L - DS$), we always first prove that H and G are co-degree under the supposition of G and H being Q-cospectral (respectively, L-cospectral), and then prove that G and H are isomorphic. But the first step is not an easy task, and we always have to spend a large amount of energy (sometimes with the similar method) to solve it. Thus, one of the present authors and his cooperators put forward the following problem:

Problem 1.2 (*[23]*)**.** Which graphs satisfy the property "every Q-cospectral graph of G is also co-degree with G"?

Up to now, few results have been determined for Problem 1.1 [2], and it is far to be solved. Motivated by Problems 1.1 and 1.2, the following two problems are also interesting and they are much easier than Problem 1.1:

Problem 1.3. How much is the ratio between these graphs satisfying Problem 1.2 and all graphs with n vertices when n tends to infinity?

Problem 1.4. How much is the ratio between these degree sequences whose corresponding graphs have the same (respectively, signless) Laplacian spectra and all the graphic degree sequences for graphs with n vertices when n tends to infinity?

It is natural for us to consider the similar problems for adjacency spectra. There is exactly one connected graph with n vertices and $d_2 = 1$, that is $K_{1,n-1}$. It has been proved that $K_{1,n-1}$ is $L - DS$ (respectively, $Q - DS$ for $n \neq 4$) [14]. However, there are infinite connected graphs with n vertices and $d_2 = 2$ when n tends to infinity, and we shall prove the following two results in the sequel.

Theorem 1.1. *Let G be a connected graph with $d_2 = 2$ and $G \notin \{R(3, 4), R(3, 5)\}$. If G and H are L-cospectral, then H is connected and H is co-degree with G.*

Theorem 1.2. *Let G be a connected graph with $d_2 = 2$ and $d_1(G) \notin \{4, 5\}$. If G and H are Q-cospectral, then H is co-degree with G.*

Remark 1.1. Let $H_1, H_2, \ldots, H_5$ be the graphs as shown in Fig. 1.1. It has been shown that $R(3, 4)$ and H_1 are L-cospectral [8], $R(3, 5)$ and H_2 are L-cospectral [8], $R(3, 4)$ and H_3 are Q-cospectral [12]. Furthermore, there are infinite pairs of non-isomorphic graphs such that they are both Q-cospectral and co-degree [19]. For instance, H_4 and H_5 are such a pair of graphs.

Let G be a graph such that every Q-cospectral (respectively, L-cospectral) graph of G is also co-degree with G. If the degree sequence of G is π and the graph with π as its degree sequence is unique, then G is $Q - DS$ (respectively, $L - DS$). For instance, by Theorems 1.1 and 1.2, we can easily prove that: if G is a connected graph with n vertices, $d_1 = n - 1$ and $d_2 = 2$, then G is $Q - DS$ and $L - DS$. That is the main result of [14].

Let $\mathbf{a}(\mathbf{k}) = (a_1, a_2, \ldots, a_k)$ be a sequence of positive integers, where $a_1 \geq a_2 \geq \cdots \geq a_k \geq 1$. As in [16], a *butterfly-like graph* $W_{p^{(s)},\mathbf{a}(\mathbf{k})}$ is a graph with s cycles C_p and $k \geq 1$ paths $P_{a_1+1}, P_{a_2+1}, \ldots, P_{a_k+1}$, which all meet in one vertex. In what follows, $W_{p^{(1)},\mathbf{a}(\mathbf{k})}$ is always rewritten as $W_{p;\mathbf{a}(\mathbf{k})}$, and we call $W_{p;\mathbf{a}(\mathbf{k})}$ as a *spider graph*, namely, $W_{p;\mathbf{a}(\mathbf{k})}$ is a graph obtained by attaching $k \geq 1$ paths say $P_{a_1}, P_{a_2}, \ldots, P_{a_k}$, to one vertex of the cycle C_p. Note that $W_{p;\mathbf{a}(\mathbf{1})}$ is also called a lollipop graph [7]. Recently, the $L - DS$ problem of spider graphs draw much attention. For instance, Haemers et al. proved that all lollipop graphs are $L - DS$ [7], Liu et al. [17] proved that all $W_{p;\mathbf{a}(\mathbf{2})}$ are $L - DS$, Zhang et al. proved that all spider graphs obtained by attaching k pendent vertices to one vertex of the cycle C_p are $L - DS$ [24], and Yu et al. proved that all spider graphs with even cycle are $L - DS$ [22]. As an application of Theorems 1.1 and 1.2, we shall extend the corresponding results of [7,17,22,24] by showing the following Theorem 1.3.

Theorem 1.3. *Each spider graph and its complement graph are both $L - DS$.*

2. Proof of Theorem 1.1

Hereafter, let $\tau(G)$ denote the number of triangles of G, and let $n_j(G)$, n_j for short, be the number of vertices of G with degree j in $V(G) \setminus \{v_1\}$, where $j \in \{1, 2, \ldots, d_2(G)\}$ and $d_1(G) = d_G(v_1)$.

Lemma 2.1 ([11,16]). *For any graph G with at least three vertices, we have $\lambda_2 \geq d_2$. Furthermore, if G is a connected graph with $d_2 = 2$, then $\lambda_2 < 4$.*

Lemma 2.2 ([1,13]). *If G is a graph with n vertices, m edges, and τ triangles, then*

$$\sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} d_i = 2m, \quad \sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} \lambda_i^2 = 2m + \sum_{i=1}^{n} d_i^2,$$
$$\sum_{i=1}^{n} \lambda_i^3 = \sum_{i=1}^{n} d_i^3 + 3\sum_{i=1}^{n} d_i^2 - 6\tau, \ \sum_{i=1}^{n} \mu_i^3 = \sum_{i=1}^{n} d_i^3 + 3\sum_{i=1}^{n} d_i^2 + 6\tau.$$

Lemma 2.3 ([16]). *If G is a connected graph with $d_2 \leq 3$, then $\tau(G) \leq n_3 + \lfloor \frac{1}{2} d_1 \rfloor$.*

Lemma 2.4 (*See* [1,18]). *If G is a connected graph with n vertices and at least one edge, then*

$$d_1 + 1 \leq \lambda_1 \leq \mu_1 \leq d_1 + d_2,$$

where the first equality holds if and only if $d_1 = n - 1$, the second equality holds if and only if G is bipartite, and the third equality holds if and only if G is regular or $G \cong K_{1,n-1}$.

Lemma 2.5 (*See* [18]). *If G is a connected graph with n vertices, then $nt(G) = \lambda_1\lambda_2 \cdots \lambda_{n-1}$, where $t(G)$ is the number of spanning trees of G.*

Lemma 2.6 (*See* [2,14]). *For any n, C_n and P_n are both $L - DS$ and $Q - DS$, $K_{1,n-1}$ is $L - DS$.*

Lemma 2.7 ([8]). *For $k \geq 2$, all k-rose graphs, except for $R(3, 4)$ and $R(3, 5)$, are $L - DS$. Both $R(3, 4)$ and $R(3, 5)$ have one L-cospectral mate, respectively.*

Proof of Theorem 1.1. Since H and G are L-cospectral and G is connected, we have $\lambda_{n-1}(H) = \lambda_{n-1}(G) > 0$ and hence H is also connected [18]. Taking Lemma 2.6 into consideration, we may suppose that $d_1(G) \geq 3$ in the following.

By Lemma 2.4 we have $d_1(H) + 1 \leq \lambda_1(H) = \lambda_1(G) \leq d_1(G) + 2$, and hence $d_1(H) \leq d_1(G) + 1$. For $d_2(H)$, since Lemma 2.1, we have $d_2(H) \leq \lambda_2(H) = \lambda_2(G) < 4$, and so $d_2(H) \leq 3$. Now, we divide the proof into the following three cases.

Case 1: $d_1(H) \leq d_1(G) - 2$.

By Lemma 2.4, we have $d_1(G) + 1 \leq \lambda_1(G) = \lambda_1(H) \leq \mu_1(H) \leq d_1(H) + d_2(H) \leq d_1(G) - 2 + 3 = d_1(G) + 1$, it implies that $\lambda_1(G) = n = d_1(G) + 1$ and H is either isomorphic to $K_{1,n-1}$ or a bipartite regular graph with $3 = d_2(H) = d_1(H) = d_1(G) - 2 = n - 3$.

If H is isomorphic to $K_{1,n-1}$, then Lemma 2.6 implies that $G \cong K_{1,n-1}$, which is contrary with $d_2(G) = 2$.

If H is a bipartite regular graph with $3 = d_2(H) = d_1(H) = d_1(G) - 2 = n - 3$, then $d_1(G) = 5$ and $n = 6$. Since every L-cospectral graph with a regular graph is also regular (see Proposition 2 of [2]), G is also a regular graph with $n - 1 = d_1(G) = 5$, and hence $G \cong K_6$, contrary to $d_2(G) = 2$.

Case 2: $d_1(H) = d_1(G) + 1$.

By Lemma 2.4, $d_1(G) + 2 = d_1(H) + 1 \leq \lambda_1(H) = \lambda_1(G) \leq d_1(G) + d_2(G) = d_1(G) + 2$, it implies that $\lambda_1(G) = d_1(G) + d_2(G)$ and hence G is bipartite regular with $d_1(G) = d_2(G) = 2$, a contradiction.

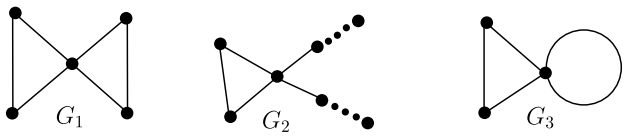


Fig. 2.1. The graphs G_1, G_2 and G_3.

Case 3: $d_1(G) - 1 \le d_1(H) \le d_1(G)$.
By Lemma 2.2, it follows that

$$\begin{cases} n_1(H) + n_2(H) + n_3(H) = n_1(G) + n_2(G), \\ n_1(H) + 2n_2(H) + 3n_3(H) + d_1(H) = n_1(G) + 2n_2(G) + d_1(G), \\ n_1(H) + 4n_2(H) + 9n_3(H) + d_1^2(H) = n_1(G) + 4n_2(G) + d_1^2(G). \end{cases} \tag{2.1}$$

From (2.1), we have

$$d_1(G)\big(d_1(G) - 3\big) = d_1(H)\big(d_1(H) - 3\big) + 2n_3(H). \tag{2.2}$$

Recall that $d_2(H) \le 3$ and $K_{1,n-1}$ is $L - DS$. Thus, we may suppose that $d_2(H) \in \{2, 3\}$, as H is connected.
Subcase 3.1: $d_2(H) = 2$.
In this case, $n_3(H) = 0$. If $d_1(H) = d_1(G) - 1$, then $d_1(G) = 2$ follows from (2.2), contrary with $d_2(G) \ge 3$. Otherwise, $d_1(H) = d_1(G)$. Now, by (2.1) we have $n_1(H) = n_1(G)$ and $n_2(H) = n_2(G)$, it implies that G and H are co-degree because of $d_2(G) = d_2(H) = 2$.
Subcase 3.2: $d_2(H) = 3$.
In this case, since $n_3(H) \ne 0$, by (2.2) it follows that $d_1(H) \ne d_1(G)$, and hence $d_1(H) = d_1(G) - 1$. By (2.1) and (2.2), we have

$$n_3(H) = d_1(G) - 2, \ \ n_2(H) = n_2(G) - 2d_1(G) + 5, \ \ n_1(H) = n_1(G) + d_1(G) - 3. \tag{2.3}$$

By $d_2(G) = 2$ we have $n_3(G) = 0$ and then $\tau(G) \le \frac{1}{2}d_1(G)$ follows from Lemma 2.3. On the other hand, by Lemma 2.2, we have

$$n_1(H) + 8n_2(H) + 27n_3(H) + d_1^3(H) - 6\tau(H) = n_1(G) + 8n_2(G) + d_1^3(G) - 6\tau(G).$$

Then, (2.3) implies that

$$\tau(H) + \frac{1}{2}\big(d_1(G) - 2\big)\big(d_1(G) - 3\big) = \tau(G) \le \frac{1}{2}d_1(G). \tag{2.4}$$

Since $3 = d_2(H) \le d_1(H) = d_1(G) - 1$, we have $d_1(G) \ge 4$. Combining with (2.4), it follows that $d_1(G) = 4$ and $1 \le \tau(G) = \tau(H) + 1 \le 2$. Combining with $d_1(G) = 4$ and (2.3), we have $n_3(H) = 2$, $n_2(H) = n_2(G) - 3$, and $n_1(H) = n_1(G) + 1$.

If $\tau(G) = 2$, then $G \cong G_1$ (see Fig. 2.1) by $d_1(G) = 4$ and $d_2(G) = 2$, and hence $H \cong G$ by Lemma 2.7, it contradicts with $d_1(H) = 3$ and $\tau(H) = 1$.
If $\tau(G) = 1$, then $G \cong G_2$ or $G \cong G_3$ (see Fig. 2.1) by $d_1(G) = 4$ and $d_2(G) = 2$.
When $G \cong G_2$, then Lemma 2.5 implies that $t(H) = t(G) = 3$. Since H is a connected graph with n vertices and n edges by Lemma 2.2, the unique cycle of H is a triangle, contrary with $\tau(H) = 0$.
When $G \cong G_3$, then G is a 2-rose. Since $G \notin \{R(3, 4), R(3, 5)\}$, Lemma 2.7 implies that $H \cong G$, which is contrary with $d_1(H) = 3$ and $\tau(H) = 0$. ■

3. Proof of Theorem 1.2

Lemma 3.1 (*[16]*). *If G is a graph with $d_2 = 4 < 6 \le d_1$, then $\mu_2 \ge 4$.*

Lemma 3.2 (*See [3,16]*). *If G is a graph with at least two vertices, then*

$$\mu_2 \ge \frac{1}{2}\left(d_1 + d_2 - \sqrt{(d_1 - d_2)^2 + 4}\right) \ge d_2 - 1.$$

Furthermore, if G is a connected graph with $d_2 = 2$, then $\mu_2 < 4$.

Lemma 3.3 (*[15]*). *Suppose that G is connected with $\mu_2 < 4$, and G and H are Q-cospectral.*
(i) *If G is non-bipartite, then H is connected.*
(ii) *If G is bipartite, then either H is connected or $H = H_1 \cup P$, where P is a path and H_1 is a connected non-bipartite graph.*

Lemma 3.4 ([20]). *Let G be a c-cyclic graph. If $c \in \{3, 4\}$, then $\tau(G) \leq c + 1$.*

Corollary 3.1. *Let $1 \leq c \leq 3$, G be a c-cyclic graph with $d_2(G) = 2$ and H be Q-cospectral with G. Then we have*

(i) *If $c \in \{1, 2\}$, then either H is a c-cyclic graph with $\tau(H) \leq c$ or $H = H_1 \cup P$, where H_1 is a $(c + 1)$-cyclic non-bipartite graph with $\tau(H) \leq 2\left\lceil \frac{c+1}{2} \right\rceil$ and P is a path.*

(ii) *If $c = 3$, then either H is a 3-cyclic graph with $\tau(H) \leq 4$ or $H = H_1 \cup P$, where H_1 is a 4-cyclic non-bipartite graph with $\tau(H) \leq 5$ and P is a path.*

Proof. Since G is a c-cyclic graph, G is a connected graph with n vertices and $n + c - 1$ edges. Note that H is Q-cospectral with G. Thus, Lemma 2.2 implies that H also has n vertices and $n + c - 1$ edges. Now, (i) and (ii) follow from Lemmas 3.2–3.4. ■

Proof of Theorem 1.2. Suppose that G is a c-cyclic graph with n vertices. Since $d_2(G) = 2$ and G is connected, we have

$$c \leq \left\lfloor \frac{1}{2} d_1(G) \right\rfloor, \tag{3.1}$$

where the equality implies that $d_{n-1}(G) = 2$.

Since H and G are Q-cospectral and G is connected, H contains at most one bipartite component by Lemmas 3.2 and 3.3. Taking Lemma 2.6 into consideration, we may suppose that $d_1(G) \geq 3$ in the following.

By Lemma 3.2, we have $d_2(H) - 1 \leq \mu_2(H) = \mu_2(G) < 4$, and hence $d_2(H) \leq 4$. From Lemma 2.4, it follows that $d_1(H) + 1 \leq \mu_1(H) = \mu_1(G) \leq d_1(G) + 2$, and hence $d_1(H) \leq d_1(G) + 1$.

Furthermore, by Lemmas 2.2 and 3.3, we have $n_0(H) \in \{0, 1\}$ and

$$\begin{cases} n_0(H) + n_1(H) + n_2(H) + n_3(H) + n_4(H) = n_1(G) + n_2(G), \\ n_1(H) + 2n_2(H) + 3n_3(H) + 4n_4(H) + d_1(H) = n_1(G) + 2n_2(G) + d_1(G), \\ n_1(H) + 4n_2(H) + 9n_3(H) + 16n_4(H) + d_1^2(H) = n_1(G) + 4n_2(G) + d_1^2(G), \\ n_1(H) + 8n_2(H) + 27n_3(H) + 64n_4(H) + d_1^3(H) + 6\tau(H) = n_1(G) + 8n_2(G) + d_1^3(G) + 6\tau(G). \end{cases} \tag{3.2}$$

Now, we complete the proof by considering the following four cases.

Case 1: $d_1(H) \leq d_1(G) - 3$.

In this case, we have $d_1(G) + 1 \leq \lambda_1(G) \leq \mu_1(G) = \mu_1(H) \leq d_1(H) + d_2(H) \leq d_1(G) - 3 + 4$ by Lemma 2.4, which implies that $G \cong K_{1,n-1}$, contrary to $d_2(G) = 2$.

Case 2: $d_1(H) = d_1(G) + 1$.

In this case, we have $d_1(G) + 2 = d_1(H) + 1 \leq \lambda_1(H) \leq \mu_1(H) = \mu_1(G) \leq d_1(G) + d_2(G) = d_1(G) + 2$ by Lemma 2.4, which implies that G is regular with $d_1(G) = d_2(G) = 2$, contrary to $d_1(G) \geq 3$.

Case 3: $d_1(H) = d_1(G)$.

If $n_0(H) = 1$, then $n_3(H) + 3n_4(H) = -1$ follows from the first three equations of (3.2), a contradiction. Thus, $n_0(H) = 0$. By the first three equations of (3.2), we have $n_3(H) + 3n_4(H) = 0$, and hence $n_3(H) = n_4(H) = 0$, $n_1(H) = n_1(G)$ and $n_2(H) = n_2(G)$, that is, H is co-degree with G.

Case 4: $d_1(G) - 2 \leq d_1(H) \leq d_1(G) - 1$.

Now by the first three equations of (3.2), we have

$$2n_3(H) + 2n_0(H) + 6n_4(H) = d_1(G)\big(d_1(G) - 3\big) - d_1(H)\big(d_1(H) - 3\big). \tag{3.3}$$

Since $d_2(H) \leq 4$, it suffices to consider the following two subcases.

Subcase 4.1: $d_2(H) \leq 3$.

If $d_1(H) = d_1(G) - 2$, then $d_1(G) + 1 \leq \lambda_1(G) \leq \mu_1(G) = \mu_1(H) \leq d_1(H) + d_2(H) \leq d_1(G) - 2 + 3$ by Lemma 2.4. In this case, Lemma 2.4 implies that $G \cong K_{1,n-1}$, contrary with $d_2(G) = 2$. Otherwise, $d_1(H) = d_1(G) - 1$.

By (3.3) we have

$$n_3(H) + n_0(H) = d_1(G) - 2. \tag{3.4}$$

By Lemma 3.3, either H is connected or $H = H_1 \cup P$, where P is a path and H_1 is a connected non-bipartite graph. Thus, $0 \leq n_0(H) \leq 1$.

Subcase 4.1.1: $n_0(H) = 0$.

By (3.2) and (3.4) we have $n_3(H) = d_1(G) - 2$, $n_2(H) = n_2(G) + 5 - 2d_1(G)$, and $n_1(H) = n_1(G) + d_1(G) - 3$. In this case, the fourth equation of (3.2) and Lemma 2.3 imply that

$$\tau(G) + \frac{1}{2}\left(d_1(G) - 2\right)\left(d_1(G) - 3\right) = \tau(H) = \tau(H_1) \leq \frac{1}{2}\big(3d_1(G) - 5\big). \tag{3.5}$$

Solving (3.5), we have $d_1(G) \in \big\{3, 4, 5, 6\big\}$. Since $d_1(G) \notin \big\{4, 5\big\}$, it suffices to consider the cases of $d_1(G) = 3$ or $d_1(G) = 6$.

If $d_1(G) = 3$, then $d_1(H) = 2$ and $n_3(H) = d_1(G) - 2 = 1$ by (3.4), a contradiction.

If $d_1(G) = 6$, then (3.5) implies that $\tau(H) \geq 6$, which is contrary to (3.1) and Corollary 3.1.

Subcase 4.1.2: $n_0(H) = 1$.

By (3.2) and (3.3) we have $n_3(H) = d_1(G) - 3$, $n_2(H) = n_2(G) + 8 - 2d_1(G)$, and $n_1(H) = n_1(G) + d_1(G) - 6$. In this case, the fourth equation of (3.2) and Lemma 2.3 imply that

$$\tau(G) + \frac{1}{2}\left(d_1^2(G) - 5d_1(G) + 8\right) = \tau(H) = \tau(H_1) \leq \frac{1}{2}\left(3d_1(G) - 7\right). \tag{3.6}$$

Solving (3.6), we have $d_1(G) \in \{3, 4, 5\}$. We only need to consider the case of $d_1(G) = 3$, as $d_1(G) \notin \{4, 5\}$. By Lemma 2.4 and $d_1(H) = d_1(G) - 1 = 2$, we have $4 = d_1(G) + 1 \leq \lambda_1(G) \leq \mu_1(G) = \mu_1(H) \leq d_1(H) + d_2(H) \leq 4$. Now, Lemma 2.4 implies that $G \cong K_{1,3}$, which is contrary with $d_2(G) = 2$.

Subcase 4.2: $d_2(H) = 4$.

Since Lemma 3.2 and G and H are Q-cospectral, we have $\mu_2(H) = \mu_2(G) < 4$. Combining with Lemma 3.1 and $d_2(H) = 4$, it follows that $d_1(H) \in \{4, 5\}$. Recall that $d_1(G) - 2 \leq d_1(H) \leq d_1(G) - 1$ and $d_1(G) \notin \{4, 5\}$. Thus, $d_1(G) \in \{6, 7\}$. Now, (3.1) implies that $c \leq 3$, and hence $\tau(H) \leq 5$ by Corollary 3.1.

On the other hand, from (3.2) we have

$$\begin{aligned} &6\left(n_4(H) + \tau(H) - \tau(G) - n_0(H)\right) \\ =&\left(d_1(G) - d_1(H)\right)\left(d_1^2(H) + d_1^2(G) - 6\left(d_1(G) + d_1(H)\right) + d_1(G)d_1(H) + 11\right). \end{aligned} \tag{3.7}$$

Subcase 4.2.1: $d_1(G) = 7$.

In this case, we have $d_1(H) = 5$, and hence $n_4(H) \leq 3$ by (3.3). Thus, (3.7) yields that $\tau(H) = 16 + \tau(G) + n_0(H) - n_4(H) \geq 13$, which is contrary with $\tau(H) \leq 5$.

Subcase 4.2.2: $d_1(G) = 6$.

Then, $d_1(H) \in \{4, 5\}$.

If $d_1(H) = 4$, then we have $n_4(H) \leq 2$ by (3.3). Now, (3.7) implies that $\tau(H) = 9 + \tau(G) + n_0(H) - n_4(H) \geq 7$, which is contrary with $\tau(H) \leq 5$.

If $d_1(H) = 5$, then (3.3) yields that $n_4(H) \leq 1$, and thus $\tau(H) = 6 + \tau(G) + n_0(H) - n_4(H) \geq 5$ by (3.7). Now Corollary 3.1 and (3.1) imply that $c = 3$ and hence G is a 3-rose graph by $d_1(G) = 6$ and $d_2(G) = 2$. It has been proved that all 3-rose graphs are $Q - DS$ [20], and hence $H \cong G$, which is contrary with $d_1(H) \neq d_1(G)$. ■

4. Proof of Theorem 1.3

Let $M_n^{(1)}$ be the matrix of order n obtained from $L(P_{n+1})$ by deleting the row and column corresponding to one end vertex of P_{n+1}, and let $M_n^{(2)} = 2I_n - A(P_n)$, where I_n is the identity matrix of order n. For a real symmetry matrix M of order n, we use $\theta_1(M) \geq \theta_2(M) \geq \cdots \geq \theta_n(M)$ to define the eigenvalues of M.

Lemma 4.1 ([5]). *Let $P_{k+1} = w_1w_2\cdots w_{k+1}$ be a pendent path (i.e., a path with exactly one end vertex of degree being at least three) of the graph G such that $d(w_1) = 1$ and $d(w_{k+1}) \geq 3$. If $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ is a unit eigenvector corresponding to a nonzero eigenvalue λ of $L(G)$, then for any $i \in \{2, 3, \ldots, k+1\}$, we have*

$$\varphi(w_i) = \varphi(w_1)\prod_{j=1}^{i-1}\left(\theta_j(M_{i-1}^{(1)}) - \lambda\right).$$

Lemma 4.2 ([9]). *Let $\delta_j = \frac{j\pi}{n+1}$ and $M = [M_1, M_2, \ldots, M_n]$, where $M_j^T = [x_{j1}, x_{j2}, \ldots, x_{jn}]$ with $x_{ji} = \sin(i\delta_j)$ for $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, n$. Then $\rho_j = 2\cos(\delta_j)$ is an eigenvalue of $A(P_n)$ and M_j is the corresponding eigenvector of ρ_j, where $j = 1, 2, \ldots, n$.*

A *starlike tree* is a tree with exactly one vertex of degree being at least three [10]. Hereafter, we use the notation $q^{(s)}$ to define s copies of a real number q, and we use $S_L(G)$ to define the set of eigenvalues of $L(G)$.

Lemma 4.3. *Let G be a connected graph with at least two vertices, G^* be a graph obtained from G by attaching p (≥ 2) paths, says $P_q^{(i)} = w_1^{(i)}w_2^{(i)}\cdots w_q^{(i)}$ ($1 \leq i \leq p$), of order q to the vertex v of G. For any $j \in \{1, 2, \ldots, q\}$, let G_j be a graph obtained from G^* by adding any t edges among $\left\{w_j^{(1)}, w_j^{(2)}, \ldots, w_j^{(p)}\right\}$, where $1 \leq t \leq \frac{p(p-1)}{2}$. Let λ be a nonzero eigenvalue of $L(G^*)$ with the corresponding unit eigenvector $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$, where $\lambda \notin \left\{\theta_1(M_q^{(1)}), \theta_2(M_q^{(1)}), \ldots, \theta_q(M_q^{(1)})\right\}$. Then λ is also an eigenvalue of $L(G_j)$ and $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ is also a unit eigenvector corresponding to λ of $L(G_j)$. Furthermore,*

$$\varphi\left(w_j^{(1)}\right) = \varphi\left(w_j^{(2)}\right) = \cdots = \varphi\left(w_j^{(p)}\right) \text{ for } j = 1, 2, \ldots, q. \tag{4.1}$$

Proof. For $i \in \{1, 2, \ldots, p\}$, we may suppose that $vw_q^{(i)} \in E(G_j)$. Firstly, we show $\varphi(w_1^{(1)}) = \varphi(w_1^{(2)}) = \cdots = \varphi(w_1^{(p)})$ by considering the following two cases.

Case 1: $\varphi(w_1^{(i)}) = 0$ holds for some $i \in \{1, 2, \ldots, p\}$.
Then, $\varphi(v) = 0$ and hence $\varphi(w_1^{(1)}) = \varphi(w_1^{(2)}) = \cdots = \varphi(w_1^{(p)}) = 0$ by Lemma 4.1.
Case 2: $\varphi(w_1^{(i)}) \neq 0$ holds for all $i \in \{1, 2, \ldots, p\}$.
Then, $\varphi(v) \neq 0$ by $\lambda \notin \left\{\theta_1(M_q^{(1)}), \theta_2(M_q^{(1)}), \ldots, \theta_q(M_q^{(1)})\right\}$ and hence $\varphi(w_1^{(1)}) = \varphi(w_1^{(2)}) = \cdots = \varphi(w_1^{(p)})$ by Lemma 4.1.

Now, since $\varphi(w_1^{(1)}) = \varphi(w_1^{(2)}) = \cdots = \varphi(w_1^{(p)})$, we can conclude that (4.1) holds by Lemma 4.1. By (4.1), it is easy to check that λ is also an eigenvalue of $L(G_j)$ and $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ is also a unit eigenvector corresponding to λ of $L(G_j)$. ■

Now, we are ready to prove the following result, which has interest in its ownright.

Theorem 4.1. *Let G be a starlike tree obtained from $W_{(2q+1)^{(s)},\mathbf{a}(\mathbf{k})}$ by deleting s edges on s cycles, whose end vertices are vertices at distance q from the maximum vertex of $W_{(2q+1)^{(s)},\mathbf{a}(\mathbf{k})}$. If $s \geq 1$, then $A_1 \subseteq S_L(G)$ and $\left(S_L(G) \cup A_2\right) \setminus A_1 = S_L\left(W_{(2q+1)^{(s)},\mathbf{a}(\mathbf{k})}\right)$, where*

$$A_1 = \left\{\left(\theta_j\left(M_q^{(1)}\right)\right)^{(s)} : j = 1, 2, \ldots, q\right\} \text{ and } A_2 = \left\{\left(2 - 2\cos\left(\frac{2j\pi}{2q+1}\right)\right)^{(s)} : j = 1, 2, \ldots, q\right\}.$$

Proof. In the proof of this result, we rewrite $W_{(2q+1)^{(s)},\mathbf{a}(\mathbf{k})}$ as G^*, and we suppose that G contains n vertices and v is the maximum vertex of G. Let $L_v(G)$ be the matrix obtained from $L(G)$ by deleting the row and column corresponding to the maximum vertex v in $L(G)$. Then, $L_v(G)$ is a principal matrix of $L(G)$ and there are at least $2s$ disjointed copies of $M_q^{(1)}$ in $L_v(G)$. Since the eigenvalues of any principal submatrix of $L(G)$ interlace the eigenvalues of $L(G)$ (see [6]) and there are $2s$ disjointed copies of $M_q^{(1)}$ in $L_v(G)$, we can conclude that

$$\left(\theta_1\left(M_q^{(1)}\right)\right)^{(s)}, \left(\theta_2\left(M_q^{(1)}\right)\right)^{(s)}, \ldots, \left(\theta_q\left(M_q^{(1)}\right)\right)^{(s)}$$

are also the eigenvalues of $S_L(G)$, namely, $A_1 \subseteq S_L(G)$.

Note that there are s disjoint copies of $M_{2q}^{(2)} = 2I_{2q} - A(P_{2q})$ being a principal matrix of $L(G^*)$. By Lemma 4.2, for each $j \in \{1, 2, \ldots, q\}$, $2 - \delta_{2j} = 2 - 2\cos\left(\frac{2j\pi}{2q+1}\right)$ is an eigenvalue of $M_{2q}^{(2)}$ with the corresponding eigenvector

$$M_{2j} = \left[\sin\left(\frac{2j\pi}{2q+1}\right), \sin\left(\frac{4j\pi}{2q+1}\right), \ldots, \sin\left(\frac{4qj\pi}{2q+1}\right)\right]^T \tag{4.2}$$

For $t \in \{1, 2, \ldots, s\}$, we may suppose that $C_{2q+1}^{(t)} = vu_1^{(t)}u_2^{(t)}\cdots u_{2q}^{(t)}v$ is the t-th cycle of G^*, and we can construct a vector $\left(\psi_{tj}(v_1), \psi_{tj}(v_2), \ldots, \psi_{tj}(v_n)\right)$ by setting $\psi_{tj}(u_i^{(t)}) = \sin\left(\frac{2ji\pi}{2q+1}\right)$ for $i = 1, 2, \ldots, 2q$ and $\psi_{tj}(w) = 0$ for all $w \notin \left\{u_1^{(t)}, u_2^{(t)}, \ldots, u_{2q}^{(t)}\right\}$, where $j \in \{1, 2, \ldots, q\}$.

For each $j \in \{1, 2, \ldots, q\}$ and $t \in \{1, 2, \ldots, s\}$, since

$$\sin\left(\frac{2jp\pi}{2q+1}\right) + \sin\left(\frac{2j(2q+1-p)\pi}{2q+1}\right) = 0$$

holds for $p \in \{1, 2, \ldots, q\}$, we have $\psi_{tj}(v_1) + \psi_{tj}(v_2) + \cdots + \psi_{tj}(v_n) = 0$. Recall that 0 is an eigenvalue of $L(G^*)$ with the corresponding vector $(1^{(n)})$. Thus, $2 - \delta_{2j}$ is also an eigenvalue of $L(G^*)$ with the corresponding eigenvector $\left(\psi_{tj}(v_1), \psi_{tj}(v_2), \ldots, \psi_{tj}(v_n)\right)$, that is,

$$A_2 \subseteq S_L\left(G^*\right). \tag{4.3}$$

Let $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ be a unit eigenvector corresponding to a nonzero eigenvalue λ of $L(G)$ such that $\lambda \notin \left\{\theta_1(M_q^{(1)}), \theta_2(M_q^{(1)}), \ldots, \theta_q(M_q^{(1)})\right\}$, that is $\lambda \in S_L(G) \setminus \left(A_1 \cup \{0\}\right)$. By Lemma 4.3, it is easy to check that $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ is also a unit eigenvector corresponding to the eigenvalue λ of $L(G^*)$ such that (4.1) holds. Thus,

$$S_L(G) \setminus A_1 \subseteq S_L\left(G^*\right). \tag{4.4}$$

By (4.1) and (4.2), it is easy to see that $\left(\psi_{tj}(v_1), \psi_{tj}(v_2), \ldots, \psi_{tj}(v_n)\right)$ is orthogonal with each eigenvector $\left(\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_n)\right)$ corresponding to a nonzero eigenvalue λ of $S_L(G) \setminus \left(A_1 \cup \{0\}\right)$. Furthermore, since $\psi_{tj}(v_1) + \psi_{tj}(v_2) + \cdots + \psi_{tj}(v_n) = 0$ and $(1^{(n)})$ is the corresponding vector of the eigenvalue 0 of $L(G^*)$, we can conclude that

$$A_2 \cap \left(S_L(G) \setminus A_1\right) = \emptyset. \tag{4.5}$$

By combining with (4.3)–(4.5), it follows that $\left(S_L(G) \cup A_2\right) \setminus A_1 = S_L\left(G^*\right)$. ■

Proof of Theorem 1.3. Let $G = W_{p;\mathbf{a}(\mathbf{k})}$ be a spider graph on n vertices, $\overline{G}$ be the complement graph of G. Since $S_L(\overline{G}) = \left\{0, n - \lambda_1(G), n - \lambda_2(G), \ldots, n - \lambda_{n-2}(G), n - \lambda_{n-1}(G)\right\}$ [18], to complete the proof of this result, it suffices to prove that every spider graph is $L - DS$.

Let H be L-cospectral with $W_{p;\mathbf{a}(\mathbf{k})}$. By Theorem 1.1, H is connected and co-degree with $W_{p;\mathbf{a}(\mathbf{k})}$. Furthermore, Lemma 2.5 implies that $H \cong W_{p;\mathbf{b}(\mathbf{k})}$, where $\mathbf{b}(\mathbf{k}) = \{b_1, b_2, \ldots, b_k\}$ with $b_1 \geq b_2 \geq \cdots \geq b_k \geq 1$ and $b_1+b_2+\cdots+b_k = a_1+a_2+\cdots+a_k$. Now, we show $W_{p;\mathbf{b}(\mathbf{k})} \cong W_{p;\mathbf{a}(\mathbf{k})}$ by considering the following two cases and then complete the proof.

Case 1: $p = 2q + 1$.

Then we can construct two starlike trees, say H_1 and H_2, obtained from $W_{p;\mathbf{a}(\mathbf{k})}$ and $W_{p;\mathbf{b}(\mathbf{k})}$ by deleting one edge on the unique cycle, whose two end vertices of the edge are vertices with distance q to the maximum vertex of $W_{p;\mathbf{a}(\mathbf{k})}$ and $W_{p;\mathbf{b}(\mathbf{k})}$, respectively. By Theorem 4.1, $S_L(H_1) = S_L(H_2)$. Note that two starlike trees are L-cospectral if and only if they are isomorphic [10]. Thus, $H_1 \cong H_2$, which implies that $W_{p;\mathbf{b}(\mathbf{k})} \cong W_{p;\mathbf{a}(\mathbf{k})}$.

Case 2: $p = 2q$.

Then $S_Q(H) = S_L(H) = S_L(W_{p;\mathbf{a}(\mathbf{k})}) = S_Q(W_{p;\mathbf{a}(\mathbf{k})})$. It is well-known that G_1 and G_2 are Q-cospectral if and only if $S(G_1)$ and $S(G_2)$ are A-cospectral [21], where $S(G)$ is the subdivision graph of G (namely, $S(G)$ is obtained by inserting an additional vertex into each edge of G). Furthermore, since $W_{p^{(s)},\mathbf{a}(\mathbf{k})}$ and $W_{p^{(s)},\mathbf{b}(\mathbf{k})}$ are A-cospectral if and only if they are isomorphic [16], we can conclude that $W_{p;\mathbf{b}(\mathbf{k})} \cong W_{p;\mathbf{a}(\mathbf{k})}$. ■

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The spectral characterization of butterfly-like graphs ☆

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Wind-wheel graph

ABSTRACT

Let $\mathbf{a}(\mathbf{k}) = (a_1, a_2, \ldots, a_k)$ be a sequence of positive integers. A *butterfly-like graph* $W_{p^{(s)};\mathbf{a}(\mathbf{k})}$ is a graph consisting of s (≥ 1) cycle of lengths $p+1$, and k (≥ 1) paths P_{a_1+1}, P_{a_2+1}, …, P_{a_k+1} intersecting in a single vertex. The *girth* of a graph G is the length of a shortest cycle in G. Two graphs are said to be *A-cospectral* if they have the same adjacency spectrum. For a graph G, if there does not exist another non-isomorphic graph H such that G and H share the same Laplacian (respectively, signless Laplacian) spectrum, then we say that G is $L-DS$ (respectively, $Q-DS$). In this paper, we firstly prove that no two non-isomorphic butterfly-like graphs with the same girth are A-cospectral, and then present a new upper and lower bounds for the i-th largest eigenvalue of $L(G)$ and $Q(G)$, respectively. By applying these new results, we give a positive answer to an open problem in Wen et al. (2015) [17] by proving

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that all the butterfly-like graphs $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ are both $Q-DS$ and $L-DS$.

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1. Introduction

Throughout this paper, G is an undirected simple graph with $V(G)=\{v_1,v_2,\ldots,v_n\}$. Let $d_G(v)$ and $N_G(v)$ be the degree and neighbor set of vertex v in G, respectively. If $d_G(v)=1$, then we call v a *pendent vertex*. In the sequel, we enumerate the degrees of G in non-increasing order, i.e., $d_1(G)\geq d_2(G)\geq\cdots\geq d_n(G)$, where $d_G(v_i)=d_i(G)$ for $i\in\{1,2,...,n\}$. Sometimes, we call a vertex with maximum degree, i.e., v_1, as a *maximum degree vertex* of G.

As usual, $K_{1,n-1}$, K_n, C_n and P_n denote the star, complete graph, cycle and path with n vertices, respectively. In what follows, let $\mathbf{a}(\mathbf{k})=(a_1,a_2,\ldots,a_k)$ and $\mathbf{b}(\mathbf{k})=(b_1,b_2,\ldots,b_k)$ be two sequences of positive integers.

Suppose that $G_i\cong C_{p+1}$ with $v_i\in V(G_i)$ and $H_j\cong P_{a_j+1}$ with $u_j\in V(H_j)$, where $i=1,2,\ldots,s$ and $j=1,2,\ldots,k$. As shown in Fig. 1.1, a *butterfly-like graph* $W_{p^{(s)};\mathbf{a}(\mathbf{k})}$ is a graph obtained from $G_1,G_2,\cdots,G_s$ and $H_1,H_2,\cdots,H_k$ by identifying the vertices $v_1,v_2,\cdots,v_s$ and $u_1,u_2,\cdots,u_k$ (i.e., "coalescing" these vertices into a single vertex). In particular, $W_{2^{(s)};\mathbf{a}(\mathbf{1})}$ is called a *wind-wheel graph* (see [17]).

Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal degree matrix of G, respectively. The *Laplacian matrix* of G is $L(G)=D(G)-A(G)$, and the *signless Laplacian matrix* of G is $Q(G)=D(G)+A(G)$. It is easy to see that $Q(G)$ is positive semidefinite (see [13]) and hence its eigenvalues can be arranged as:

$$\mu_1(G)\geq\mu_2(G)\geq\cdots\geq\mu_n(G)\geq 0.$$

Note that $L(G)$ is positive semidefinite matrix with all row sums being equal to zero. Thus, we can use

$$\lambda_1(G)\geq\lambda_2(G)\geq\cdots\geq\lambda_{n-1}(G)\geq\lambda_n(G)=0$$

to denote the eigenvalues of $L(G)$. For the sake of brevity, if there is no risk of confusion, we always simplify $d_i(G)$, $d_G(v)$, $N_G(v)$, $\lambda_i(G)$ and $\mu_i(G)$ as d_i, $d(v)$, $N(v)$, λ_i and μ_i, respectively.

Two graphs are said to be *A-cospectral* (respectively, *Q-cospectral*, *L-cospectral*) if they have the same adjacency (respectively, signless Laplacian, Laplacian) spectrum. Similarly, two graphs are said to be *co-degree* if they have the same degree sequences. A graph G is said to be $A-DS$ (respectively, $Q-DS$, $L-DS$) if there does not

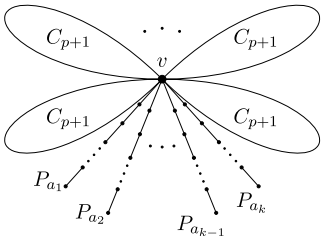


Fig. 1.1. $W_{p^{(s)};\mathbf{a(k)}}$.

exist other non-isomorphic graph H such that H and G are A-cospectral (respectively, Q-cospectral, L-cospectral).

Which graphs are determined by their spectra? This question was proposed by Günthard and Primas [6] more than 50 years ago in the context of Hückel's theory in chemistry, and had drawn more and more attention recently. For detail, we refer the readers to [5,17] and the references therein. In this line, all wind-wheel graphs are proved to be both $Q-DS$ and $L-DS$ [17], and all butterfly-like graphs $W_{2^{(s)};\mathbf{a(k)}}$ are proved to be both $Q-DS$ and $L-DS$ for $1 \leq a_i \leq 2$ and $s \geq 1$, where $1 \leq i \leq k$ [11,12]. Inspired by these results, Wen et al. [17] put forwards the following problem:

Problem 1.1. [17] Whether all butterfly-like graphs $W_{2^{(s)};\mathbf{a(k)}}$ are both $Q-DS$ and $L-DS$?

The *girth* of graph G is the length of a shortest cycle of G. In this paper, we will firstly prove that two butterfly-like graphs with the same girth are A-cospectral if and only if they are isomorphic, and then list a new upper and lower bounds for $\mu_i(G)$ and $\lambda_i(G)$, respectively. After that, we give a positive answer to Problem 1.1 by proving that all butterfly-like graphs are both $Q-DS$ and $L-DS$.

2. No two non-isomorphic butterfly-like graphs with the same girth are A-cospectral

Let $I_k = \{0,1\}^k$. Denote by $I_k^{(1)} = I_k \backslash \{(0,0,\ldots,0)\}$ and $I_k^{(2)} = \{\mathbf{x} \in I_k \text{ with } ||\mathbf{x}|| \geq 2\}$. Let

$$\chi(t) = \sum_{\mathbf{x} \in I_k^{(1)}} (-1)^{k-||\mathbf{x}||} \psi(||\mathbf{x}||, k, t) \left(t^{\sum_{i=1}^k x_i(a_i+1)} - t^{\sum_{i=1}^k x_i(b_i+1)} \right),$$

where $\psi(||\mathbf{x}||, k, t)$ is a polynomial on variables $||\mathbf{x}||$, k and t.

By the definition of $\chi(t)$, it is easy to see that $\chi(t) = \chi_1(t) + \chi_2(t)$, where

$$\chi_1(t) = (-1)^{k-1} \psi(1, k, t) \left(\sum_{i=1}^k t^{a_i+1} - \sum_{i=1}^k t^{b_i+1} \right), \text{ and}$$

$$\chi_2(t) = \sum_{\mathbf{x} \in I_k^{(2)}} (-1)^{k-||\mathbf{x}||} \psi(||\mathbf{x}||, k, t) \left(t^{\sum_{i=1}^k x_i(a_i+1)} - t^{\sum_{i=1}^k x_i(b_i+1)} \right).$$

For a polynomial $f(t)$ on variable t, let $c_j(t)$ be the coefficient of t^j in $f(t)$.

Lemma 2.1. *If there exists an index j $(1 \leq j \leq k)$ such that $a_s = b_s$ holds for any $s > j$ and $a_j \geq b_j$, then $c_q(\chi_2(t)) = 0$ holds for any $q \leq b_j + 2$.*

Proof. It suffices to show that $\mathbf{x}$ contributes 0 to $c_q(\chi_2(t))$ for any $\mathbf{x} \in I_k^{(2)}$.

Suppose that for some $\mathbf{x} \in I_k^{(2)}$, $\sum_{i=1}^k x_i(a_i+1) \leq b_j + 2$. We may suppose that $\psi(||\mathbf{x}||, k, t) \neq 0$ (otherwise, $\mathbf{x}$ only contributes 0 to $c_q(\chi_2(t))$, as desired). If $x_i = 1$ holds for some $i \leq j$, since $||\mathbf{x}|| \geq 2$, $a_1 \geq a_2 \geq \cdots \geq a_k \geq 1$ and $a_j \geq b_j$, we have $\sum_{i=1}^k x_i(a_i+1) \geq a_j + a_k + 2 > b_j + 2$, a contradiction. Thus, $x_i = 0$ holds for any $i \leq j$. With the similar reason, if $\mathbf{x} \in I_k^{(2)}$ with $\psi(||\mathbf{x}||, k, t) \neq 0$ such that $\sum_{i=1}^k x_i(b_i+1) \leq b_j + 2$, then $x_i = 0$ holds for any $i \leq j$.

For each $\mathbf{x} \in I_k^{(2)}$ with $\psi(||\mathbf{x}||, k, t) \neq 0$, if $\sum_{i=1}^k x_i(a_i+1) \leq b_j+2$ and $\sum_{i=1}^k x_i(b_i+1) \leq b_j + 2$, since $x_i = 0$ holds for any $i \leq j$ and $a_s = b_s$ holds for any $s > j$, we have

$$t^{\sum_{i=1}^k x_i(a_i+1)} - t^{\sum_{i=1}^k x_i(b_i+1)} = t^{\sum_{i=j+1}^k x_i(a_i+1)} - t^{\sum_{i=j+1}^k x_i(b_i+1)} = 0.$$

Thus, $\mathbf{x}$ contributes 0 to $c_q(\chi_2(t))$, as desired. By the arbitrariness of $\mathbf{x}$, the result follows. □

Theorem 2.1. *If $\chi(t) = 0$ and $\psi(1, k, 0) \neq 0$, then $a_i = b_i$ holds for any $i = 1, 2, \ldots, k$.*

Proof. Assume that there exists an index j $(1 \leq j \leq k)$ such that $a_j \neq b_j$. Without loss of generality we may suppose that $a_j > b_j$ and $a_i = b_i$ for $i > j$. Let r and s be the number of times of the term b_j occurs in $(a_1, a_2, \ldots, a_k)$ and $(b_1, b_2, \ldots, b_k)$, respectively. Since $a_1 \geq a_2 \geq \cdots \geq a_k$ and $b_1 \geq b_2 \geq \cdots \geq b_k$, we have $s > r$. By Lemma 2.1, $c_{b_j+1}(\chi_2(t)) = 0$. Thus,

$$c_{b_j+1}(\chi(t)) = c_{b_j+1}(\chi_1(t)) = (-1)^k(s-r)\psi(1, k, 0) \neq 0,$$

a contradiction. □

Let $\Phi(G) = \Phi(G, x) = \det(xI_n - A(G))$ be the polynomial of $A(G)$.

Lemma 2.2. [15] *Let G be a graph with $v \in V(G)$. If C_v denotes the set of all cycles containing the vertex v in G, then*

$$\Phi(G, x) = x\Phi(G - v, x) - \sum_{w \sim v} \Phi(G - v - w, x) - 2 \sum_{C \in C_v} \Phi(G - V(C), x).$$

Lemma 2.3. [9] *By setting* $t^{\frac{1}{2}} = e^{i\theta}$, *and* $\mathscr{X}_i = \{1, 2, \ldots, k\}\backslash\{i\}$, *we have*

$$\Phi(P_n, t^{\frac{1}{2}} + t^{-\frac{1}{2}}) = \frac{t^{-\frac{n}{2}}}{t-1}\left(t^{n+1}-1\right), \prod_{i=1}^{k}\left(t^{a_i+1}-1\right) = \sum_{\mathbf{x}\in I_k}(-1)^{k-||\mathbf{x}||}t^{\sum_{i=1}^{k}x_i(a_i+1)},$$

$$t\sum_{i=1}^{k}\left(\left(t^{a_i}-1\right)\prod_{j\in\mathscr{X}_i}\left(t^{a_j+1}-1\right)\right) = \sum_{\mathbf{x}\in I_k}(-1)^{k-||\mathbf{x}||}((k-||\mathbf{x}||)t+||\mathbf{x}||)t^{\sum_{i=1}^{k}x_i(a_i+1)}.$$

As in [14], let $N_G(H)$ be the number of subgraphs H in graph G, and let $N_G(i)$ be the number of closed walks of length i in G.

Lemma 2.4. [2,14] *If* G *and* G' *are* A*-cospectral, then* $|V(G)| = |V(G')|$, $|E(G)| = |E(G')|$ *and* $N_{G'}(4) = N_G(4) = 2|E(G)| + 4N_G(P_3) + 8N_G(C_4)$.

Theorem 2.2. $W_{p^{(s)};\mathbf{a}(\mathbf{k})}$ *and* $W_{p^{(s)};\mathbf{b}(\mathbf{k}')}$ *are* A-cospectral *if and only if they are isomorphic.*

Proof. In the proof of this result, we rewrite $W_{p^{(s)};\mathbf{a}(\mathbf{k})}$ and $W_{p^{(s)};\mathbf{b}(\mathbf{k}')}$ as G_1 and G_2, respectively. The sufficiency is clearly, and it suffices to prove the necessity. Now, we suppose that G_1 and G_2 are *A-cospectral*. By Lemma 2.4, it follows that

$$\begin{aligned}
0 &= N_{G_1}(4) - N_{G_2}(4)\\
&= \left(2|E(G_1)| + 4\sum_{i=1}^{n}\binom{d_i(G_1)}{2} + 8N_{G_1}(C_4)\right)\\
&\quad - \left(2|E(G_2)| + 4\sum_{i=1}^{n}\binom{d_i(G_2)}{2} + 8N_{G_2}(C_4)\right)\\
&= 4\left(\binom{2s+k}{2} + (n-k-1) - \binom{2s+k'}{2} - (n-k'-1)\right)\\
&= 2(k-k')(k+k'+4s-3),
\end{aligned}$$

and hence $k = k'$. Since $|V(G_1)| = |V(G_2)|$ by Lemma 2.4, we have $\sum_{i=1}^{k} a_i = \sum_{i=1}^{k} b_i$.

If we apply Lemma 2.2 to the maximum degree vertex of G_1, then we have

$$\begin{aligned}
\Phi(G_1) &= x\left(\Phi(P_p)\right)^s\prod_{i=1}^{k}\Phi(P_{a_i}) - 2s\left(\Phi(P_p)\right)^{s-1}\Phi(P_{p-1})\prod_{i=1}^{k}\Phi(P_{a_i})\\
&\quad - \left(\Phi(P_p)\right)^s\left(\sum_{i=1}^{k}\frac{\Phi(P_{a_i-1})}{\Phi(P_{a_i})}\right)\prod_{i=1}^{k}\Phi(P_{a_i}) - 2s\left(\Phi(P_p)\right)^{s-1}\prod_{i=1}^{k}\Phi(P_{a_i})\\
&= \left(\Phi(P_p)\right)^s\prod_{i=1}^{k}\Phi(P_{a_i})\left(x - \sum_{i=1}^{k}\frac{\Phi(P_{a_i-1})}{\Phi(P_{a_i})}\right)\\
&\quad - 2s\left(\Phi(P_{p-1}) + 1\right)\left(\Phi(P_p)\right)^{s-1}\prod_{i=1}^{k}\Phi(P_{a_i}).
\end{aligned}$$

Denote by

$$\Psi(G_1,x)=(x\Phi(P_p)-2s(\Phi(P_{p-1})+1))\prod_{i=1}^{k}\Phi(P_{a_i})$$
$$-\left(\sum_{i=1}^{k}\frac{\Phi(P_{a_i-1})}{\Phi(P_{a_i})}\right)\Phi(P_p)\prod_{i=1}^{k}\Phi(P_{a_i}).$$

So, $\Phi(G_1)=\Phi(P_p)^{s-1}\Psi(G_1,x)$.

Set $f_1(t)=(t^{p+1}-1)(t+1)-2st(t^p-1)-2s(t-1)t^{\frac{p+1}{2}}$. By Lemma 2.3,

$$\Psi(G_1,t^{\frac{1}{2}}+t^{-\frac{1}{2}})=t^{-\frac{p+1}{2}-\sum_{i=1}^{k}\frac{a_i}{2}}(t-1)^{-k-1}\chi(G_1,t),$$

where

$$\chi(G_1,t)=f_1(t)\prod_{i=1}^{k}\left(t^{a_i+1}-1\right)-t(t^{p+1}-1)\sum_{i=1}^{k}(t^{a_i}-1)\prod_{j\in\mathscr{X}_i}\left(t^{a_j+1}-1\right)$$
$$=\sum_{\mathbf{x}\in I_k}(-1)^{k-||\mathbf{x}||}t^{\sum_{i=1}^{k}x_i(a_i+1)}\left(((k-||\mathbf{x}||)t+||\mathbf{x}||)(t^{p+1}-1)+f_1(t)\right).$$

Similarly with the corresponding definition of G_1, we define $\Psi(G_2,x)$ and $\chi(G_2,t)$ such that $\Phi(G_2)=\Phi(P_p)^{s-1}\Psi(G_2,x)$ and $\Psi(G_2,t^{\frac{1}{2}}+t^{-\frac{1}{2}})=t^{-\frac{p+1}{2}-\sum_{i=1}^{k}\frac{b_i}{2}}(t-1)^{-k-1}\times\chi(G_2,t)$. Since G_1 and G_2 are A-cospectral, we have $\Phi(G_1)=\Phi(G_2)$, and hence $\Psi(G_1,x)=\Psi(G_2,x)$. Combining with $\sum_{i=1}^{k}a_i=\sum_{i=1}^{k}b_i$, we get $\chi(G_1,t)=\chi(G_2,t)$. It is easy to see that

$$0=\chi(t)=\chi(G_1,t)-\chi(G_2,t)$$
$$=\sum_{\mathbf{x}\in I_k^{(1)}}(-1)^{k-||\mathbf{x}||}\psi_1(||\mathbf{x}||,k,t)\left(t^{\sum_{i=1}^{k}x_i(a_i+1)}-t^{\sum_{i=1}^{k}x_i(b_i+1)}\right),$$

where $\psi_1(||\mathbf{x}||,k,t)=((k-||\mathbf{x}||)t+||\mathbf{x}||)(t^{p+1}-1)+f_1(t)$.

Note that $\psi_1(1,k,0)=-1+f_1(0)=-2\neq 0$. Thus, $G_1\cong G_2$ by Theorem 2.1. □

The subdivision graph $S(G)$ of G is obtained by inserting an additional vertex into each edge of G. The following result is well-known:

Lemma 2.5. [16] *G and G' are Q-cospectral if and only if $S(G)$ and $S(G')$ are A-cospectral.*

Corollary 2.1. *Two butterfly-like graphs with the same girth are Q-*cospectral *if and only if they are isomorphic.*

Proof. By Lemma 2.5 and Theorem 2.2, the result clearly follows. □

3. Upper and lower bounds for $\mu_i(G)$ and $\lambda_i(G)$

Let $\theta_i(M)$ be the i-th largest eigenvalue of M and let $R_i(M)$ be the sum of i-th row of M, where M is a symmetric real matrix of order n and $1 \leq i \leq n$.

Lemma 3.1. [7] *Let M and N be two symmetric real matrices of order n. For $1 \leq i, j \leq n$, we have*

(i) If $i + j - 1 \leq n$, then $\theta_{i+j-1}(M + N) \leq \theta_i(M) + \theta_j(N)$;
(ii) If $i + j - 1 \geq n$, then $\theta_{i+j-n}(M + N) \geq \theta_i(M) + \theta_j(N)$.

Lemma 3.2. [7] *If M is a symmetric real matrix of order n and N is a principal submatrix of order k of M, then $\theta_i(M) \geq \theta_i(N) \geq \theta_{n-k+i}(M)$ holds for any $i = 1, 2, \ldots, k$.*

In the following, let $\mathrm{diag}\{p_1, p_2, \ldots, p_k\}$ denote a diagonal matrix of order k with its i-th diagonal entry being equal to p_i, where $1 \leq i \leq k$.

Theorem 3.1. *Let G be a graph with $X \subseteq V(G)$ and let $H \cong G[X]$. If $X = \{u_1, u_2, \ldots, u_k\}$, then for any $i \in \{1, 2, \ldots, k\}$ and $0 \leq p_i \leq d_G(u_i)$ we have*

$$\mu_i(G) \geq \theta_i\left(A(H) + \mathrm{diag}\{p_1, p_2, \ldots, p_k\}\right), \quad \textit{and}$$

$$\lambda_i(G) \geq \theta_i\left(\mathrm{diag}\{p_1, p_2, \ldots, p_k\} - A(H)\right).$$

Proof. We only prove the case of λ_i, since the case of μ_i can be proved similarly. Since $\mathrm{diag}\{d_G(u_1), d_G(u_2), \ldots, d_G(u_k)\} = \mathrm{diag}\{p_1, p_2, \ldots, p_k\} + \mathrm{diag}\{d_G(u_1) - p_1, d_G(u_2) - p_2, \ldots, d_G(u_k) - p_k\}$ and since $L(G)$ contains $\mathrm{diag}\{d_G(u_1), d_G(u_2), \ldots, d_G(u_k)\} - A(H)$ as its principal submatrix, by Lemmas 3.1 (ii) and 3.2 it follows that

$$\begin{aligned}
\lambda_i(G) &\geq \theta_i\left(\mathrm{diag}\{d_G(u_1), d_G(u_2), \ldots, d_G(u_k)\} - A(H)\right) \\
&\geq \theta_i\left(\mathrm{diag}\{p_1, p_2, \ldots, p_k\} - A(H)\right) \\
&\quad + \theta_k\left(\mathrm{diag}\{d_G(u_1) - p_1, d_G(u_2) - p_2, \ldots, d_G(u_k) - p_k\}\right) \\
&\geq \theta_i\left(\mathrm{diag}\{p_1, p_2, \ldots, p_k\} - A(H)\right).
\end{aligned}$$

This completes the proof of this result. □

Corollary 3.1. *If G is a graph with $d_2 = 4 < 6 \leq d_1$, then $\mu_2 \geq 4$.*

Proof. By contradiction, assume that $\mu_2 < 4$, and hence $v_1v_2 \in E(G)$ by Theorem 3.1. Let

$$B_1 = \begin{pmatrix} 6 & 1 & 1 & 1 & 1 & 0 \\ 1 & 4 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}, B_2 = \begin{pmatrix} 6 & 1 & 1 & 1 \\ 1 & 4 & 1 & 1 \\ 1 & 1 & 3 & 1 \\ 1 & 1 & 1 & 3 \end{pmatrix}, B_3 = \begin{pmatrix} 6 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 4 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

By using 'Matlab', we have $\theta_2(B_1) = \theta_2(B_2) = \theta_2(B_3) = 4$.

If there exists some vertex $u_1 \in N(v_2) \setminus \{N(v_1) \cup \{v_1\}\}$, then there exist vertices $\{u_2, u_3, u_4\}$ such that $\{u_2, u_3, u_4\} \subseteq N(v_1) \setminus \{N(v_2) \cup \{v_2\}\}$, as $d_1 \geq 6$. By Theorem 3.1, we have $\mu_2 \geq \theta_2(B_1) = 4$, contrary to $\mu_2 < 4$. This contradiction implies that $N(v_2) \cup \{v_2\} \subseteq N(v_1) \cup \{v_1\}$.

Let $X = \{v_1, v_2, u, w\}$ and let $H \cong G[X]$. If there exist two vertices $\{u, w\} \subseteq N(v_1) \cap N(v_2)$ such that $H \cong K_4$, then by Theorem 3.1 we have $\mu_2 \geq \theta_2(B_2) = 4$, a contradiction. Thus, $d_H(u) = d_H(w) = 2$ holds for any $\{u, w\} \subseteq N(v_1) \cap N(v_2)$. Since $d_1 \geq 6$, we have $\mu_2 \geq \theta_2(B_3) = 4$ by Theorem 3.1, a contradiction. □

Lemma 3.3. [7] *For any irreducible non-negative matrix M, we have*

$$\min\{R_i(M) : 1 \leq i \leq n\} \leq \theta_1(M) \leq \max\{R_i(M) : 1 \leq i \leq n\},$$

where either equality holds if and only if $R_1(M) = R_2(M) = \cdots = R_n(M)$.

Theorem 3.2. *If G is a graph of order n, then for any $i \in \{1, 2, \ldots, n\}$ we have*

$$\max\{\mu_i, \lambda_i\} \leq d_i + \theta_1(A(H)) \leq d_i + d_1(H) \leq d_i + n - i, \tag{3.1}$$

where $H \cong G[\{v_i, v_{i+1}, \ldots, v_n\}]$. Furthermore, if $\max\{\mu_i, \lambda_i\} = d_i + n - i$, then H is a complete graph.

Proof. Since $\mu_n < d_n$ holds for any connected graph of order $n \geq 2$ [4], the result follows for $i = n$. Thus, we may suppose that $1 \leq i \leq n - 1$ in the following.

Since $\theta_1(A(H))$ is equal to the maximum eigenvalue of adjacency matrix of each component of H, by Lemma 3.3 it follows that $\theta_1(A(H)) \leq d_1(H) \leq n - i$. Furthermore, if $\theta_1(A(H)) = n - i$, then $d_1(H) = n - i = |V(H)| - 1$, and hence H is a complete graph by Lemma 3.3 (note that the sum of each row of $A(H)$ is not larger than $n - i$).

Let $M = \mathrm{diag}\{d_i, d_{i+1}, \ldots, d_n\}$. Since $Q(G)$ contains $M + A(H)$ as its principal matrix, by Lemmas 3.1 (i) and 3.2 we have $\mu_i \leq \theta_1(M + A(H)) \leq \theta_1(M) + \theta_1(A(H)) \leq d_i + d_1(H) \leq d_i + n - i$. Note that $L(G)$ contains $M - A(H)$ as its principal matrix. Thus,

by Lemmas 3.1 (i) and 3.2, we have $\lambda_i \leq \theta_1(M - A(H)) \leq \theta_1(M) + \theta_1(-A(H)) \leq \theta_1(M) + \theta_1(A(H)) \leq d_i + d_1(H) \leq d_i + n - i$, and hence inequality (3.1) holds.

Now, we suppose that $\max\{\mu_i, \lambda_i\} = d_i + n - i$. Then, $\theta_1(A(H)) = n - i$ and hence H is a complete graph by the former argument. □

Corollary 3.2. *If G is a connected graph with n vertices and i pendent vertices, then* $\max\{\mu_{n-i+1}, \lambda_{n-i+1}\} \leq 1$.

Proof. Since G contains i pendent vertices, $H \cong G[\{v_{n-i+1}, v_{n-i+2}, \ldots, v_n\}]$ is an empty graph. Thus, $\theta_1(A(H)) = 0$. Now, the result follows from Theorem 3.2. □

Corollary 3.3. *If G is a connected graph with $d_2 = 2$, then* $\max\{\mu_2, \lambda_2\} < 4$.

Proof. By Theorem 3.2 and Lemma 3.3, $\max\{\mu_2, \lambda_2\} \leq d_2 + \theta_1(A(G - v_1)) < 4$. □

4. All butterfly-like graphs $W_{\mathbf{2^{(s)};a(k)}}$ are both $Q - DS$ and $L - DS$

Let $\tau(G)$ denote the number of triangles of G, and let $n_j(G)$ be the number of vertices of G with degree j in $V(G) \setminus \{v_1\}$, where $j \in \{1, 2, \ldots, d_2(G)\}$. If there is no risk of confusion, we always simplify $\tau(G)$ and $n_j(G)$ as τ and n_j, respectively.

Lemma 4.1. [1,11] *If G is a graph with n vertices, m edges, and τ triangles, then*

$$\sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n} d_i = 2m, \quad \sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2, \tag{4.1}$$

$$\sum_{i=1}^{n} \mu_i^3 = \sum_{i=1}^{n} d_i^3 + 3\sum_{i=1}^{n} d_i^2 + 6\tau, \quad \sum_{i=1}^{n} \lambda_i^3 = \sum_{i=1}^{n} d_i^3 + 3\sum_{i=1}^{n} d_i^2 - 6\tau. \tag{4.2}$$

Lemma 4.2. *If G is a connected graph $d_2 \leq 3$, then* $\tau(G) \leq n_3 + \lfloor \frac{1}{2} d_1 \rfloor$.

Proof. In the proof of this result, we suppose that G contains n vertices, and we simplify $n_i(G)$ and $d_i(G)$ as n_i and d_i respectively. Let G be a minimum counterexample with as little number of edges as possible. Since G is connected, we have $n \geq 5$.

We first suppose that there exists some edge, say e, such that $G - e$ is disconnected. Then, $\tau(G) = \tau(G - e)$ and $G - e$ contains exactly two components, say G_1 and G_2 with $d_1(G_1) \geq d_1(G_2)$. Note that $n \geq 5$. Thus, $d_1(G_2) \leq 3$ and $d_1(G_1) \geq 2$.

If $d_1(G_2) \leq 2$, then $\tau(G_2) \leq 1$, where equality holding implies that $G_2 \cong K_3$ and exactly one vertex of G_2 is a vertex with degree three in G. When $d_1(G_1) = 2$, it is easy to check that $\tau(G) \leq n_3 + \lfloor \frac{1}{2} d_1 \rfloor$, a contradiction. When $d_1(G_1) \geq 3$, by the choice of G, we have $\tau(G) = \tau(G - e) = \tau(G_1) + \tau(G_2) \leq n_3(G_1) + \lfloor \frac{1}{2} d_1(G_1) \rfloor + \tau(G_2) \leq n_3 + \lfloor \frac{1}{2} d_1 \rfloor$, a contradiction.

If $d_1(G_2) = 3$, then $d_1(G_1) \geq 3$ and hence $n_3 \geq n_3(G_1)+n_3(G_2)+1$. By the choice of G, we have $\tau(G) = \tau(G-e) = \tau(G_1)+\tau(G_2) \leq n_3(G_1)+\lfloor \frac{1}{2}d_1(G_1)\rfloor+n_3(G_2)+\lfloor \frac{1}{2}d_1(G_2)\rfloor = n_3(G_1)+n_3(G_2)+1+\lfloor \frac{1}{2}d_1(G_1)\rfloor \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction.

We secondly suppose that $G-e$ is connected for any $e \in G$. Let v be a vertex of G such that $d_G(v) = d_n$. Denote by $\tau_v(G)$ the number of triangles such that v is located in G. In the following, we may choose v such that $\tau_v(G)$ is as small as possible and $d_G(v) = d_n$. Since $d_n \leq 3$ and G contains no cut edge, $G-v$ is connected and $d_n \geq 2$. In this case, it is easy to check that

$$n_3(G-v) \leq n_3. \tag{4.3}$$

If $\tau_v(G) = 0$, by the choice of G and (4.3), we have $\tau(G) = \tau(G-v) \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction. Thus, $\tau_v(G) \geq 1$.

We claim that $d_n = 2$. Otherwise, assume that $d_n = 3$. Then, $1 \leq \tau_v(G) \leq 3$, $d_2 = d_3 = \cdots = d_n = 3$ and $n_3(G-v)+3 \leq n_3 \leq n_3(G-v)+4$. In this case, since v is contained in at most three triangles, we have $\tau(G) \leq \tau(G-v)+3 \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor+3 \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, contrary to the choice of G. Thus, $d_n = 2$.

Since v is contained in a triangle C_3 and $d_2 \leq 3$, C_3 must contain at least one vertex with degree being at least three in G. We consider the following tow cases.

Case 1. C_3 contains at least one vertex of degree three in G.

If the maximum degree vertex of G is not contained in C_3, then $n_3(G-v)+1 \leq n_3 \leq n_3(G-v)+2$ and hence $\tau(G) = \tau(G-v)+1 \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor+1 \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction. Thus, we may suppose that the maximum degree vertex of G is contained in C_3.

When $d_1 \geq 4$, then C_3 contains exactly one vertex of degree three in G, and hence $n_3 = n_3(G-v)+1$. In this case, $\tau(G) = \tau(G-v)+1 \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor+1 \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction. When $d_1 = 3$, since G contains no cut edge, C_3 contains exactly two vertices of degree three and one vertex of degree two. Thus, $n_3(G-v)+1 \leq n_3 \leq n_3(G-v)+2$ and hence $\tau(G) = \tau(G-v)+1 \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor+1 \leq n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction.

Case 2. The degree of any vertex of C_3 is not equal to three in G.

Then, C_3 must contain two vertices of degrees two, say u and v, and one maximum degree vertex of G.

If $d_1 \geq 5$, then $G \setminus \{u,v\}$ is also connected. In this case, $d_1 = d_1(G \setminus \{u,v\})+2$ and $n_3 = n_3(G \setminus \{u,v\})$, which implies that $\tau(G) = \tau(G \setminus \{u,v\})+1 \leq n_3(G \setminus \{u,v\})+\lfloor \frac{1}{2}d_1(G \setminus \{u,v\})\rfloor+1 = n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction.

If $d_1 = 4$, then $G-v$ is connected with $d_1(G-v) = 3$. In this case, $n_3 = n_3(G-v)$, and hence $\tau(G) = \tau(G-v)+1 \leq n_3(G-v)+\lfloor \frac{1}{2}d_1(G-v)\rfloor+1 = n_3+\lfloor \frac{1}{2}d_1\rfloor$, a contradiction. □

Lemma 4.3. (See [1,13]) *Let G be a graph. Then, G is connected if and only if $\lambda_{n-1} > 0$, and the multiplicity of the eigenvalue 0 of $Q(G)$ is equal to the number of bipartite components of G.*

Lemma 4.4. [4,10] *For any graph G with at least two vertices, we have*

$$\mu_2 \geq \frac{1}{2}\left(d_1 + d_2 - \sqrt{(d_1 - d_2)^2 + 4}\right) \geq d_2 - 1 \text{ and } \lambda_2 \geq d_2.$$

Lemma 4.5. [3,13] *If G is a connected graph with n vertices and at least one edge, then*

$$d_1 + 1 \leq \lambda_1 \leq \mu_1 \leq d_1 + d_2,$$

where the first equality holds if and only if $d_1 = n-1$, the second equality holds if and only if G is bipartite, and the third equality holds if and only if G is regular or $G \cong K_{1,n-1}$.

Lemma 4.6. [11,17] *If $1 \leq a_1 \leq 2$ or $k = 1$, then $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ is $Q - DS$ and $L - DS$.*

Lemma 4.7. *If G and $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ are Q-cospectral, then G is connected and G is co-degree with $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$.*

Proof. In the proof of this result, we simplify $\mu_i(G)$, $n_i(G)$ and $d_i(G)$ as μ_i, n_i and d_i, respectively, and we write $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ as W. By Lemma 4.3 and Corollary 3.3, every component of G is non-bipartite and $\mu_2 = \mu_2(W) < 4$, which implies that G is connected and $d_2 \leq 4$ by Lemma 4.4. From Lemma 4.6, we may suppose that $a_1 \geq 3$ and $k \geq 2$ in the following.

By (4.1) and (4.2), it follows that

$$\begin{cases} n_1 + n_2 + n_3 + n_4 = n - 1 \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n + s - 1) - d_1 \\ n_1 + 4n_2 + 9n_3 + 16n_4 = 4n - 3k - 4 + (2s + k)^2 - d_1^2 \\ n_1 + 8n_2 + 27n_3 + 64n_4 = 8(n - 1) - 7k + (2s + k)^3 - d_1^3 + 6(\tau(W) - \tau(G)) \end{cases} \tag{4.4}$$

From Lemma 4.5 we can conclude that $2s + k + 1 < \mu_1 = \mu_1(W) < 2s + k + 2$, and hence $2s + k - 2 \leq d_1 \leq 2s + k$ by Lemma 4.5 and $d_2 \leq 4$.

If $d_1 = 2s + k$, by the first three equations of (4.4) we have

$$\begin{cases} n_1 + n_2 + n_3 + n_4 = n - 1 \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - k - 2 \\ n_1 + 4n_2 + 9n_3 + 16n_4 = 4n - 3k - 4 \end{cases} \tag{4.5}$$

Now, from (4.5), it is easy to see that G and W are co-degree. Thus, we may suppose that

$$2s + k - 2 \leq d_1 \leq 2s + k - 1 \tag{4.6}$$

in the following. We consider the following two cases.

Case 1. $d_2 \leq 3$.

By Lemma 4.5 and (4.6), we have $d_1 = 2s + k - 1$. From (4.4), it follows that

$$2n_3 = (2s+k)^2(7-2s-k) + 14(d_1 - k) - 28s + d_1^2(d_1 - 7) + 6(\tau(G) - \tau(W)). \tag{4.7}$$

From the first three equations of (4.4), it follows that

$$\begin{cases} n_1 + n_2 + n_3 = n - 1 \\ n_1 + 2n_2 + 3n_3 = 2n - k - 1 \\ n_1 + 4n_2 + 9n_3 = 4n + 4s - k - 5 \end{cases} \tag{4.8}$$

and hence $n_1 = 2k + 2s - 3$, $n_2 = n + 4 - 4s - 3k$, and $n_3 = 2(s-1) + k$. Combining with (4.7), we have

$$\tau(G) = \tau(W) + \frac{1}{2}(2s+k-3)(2s+k-2) = 2s(s+k-2) + \frac{1}{2}(k-2)(k-3). \tag{4.9}$$

If $s = 1$, since G is connected, we have $\tau(G) \leq 1$ by (4.1), which is contrary to (4.9) and $k \geq 2$. Thus, $s \geq 2$. In this case, since $d_2 \leq 3$, by Lemma 4.2 we have

$$\tau(G) \leq n_3 + \frac{1}{2}d_1 = 3s + \frac{3}{2}k - \frac{5}{2} < 2s(s+k-2) + \frac{1}{2}(k-2)(k-3),$$

which contradicts (4.9).

Case 2. $d_2 = 4$.

By Corollaries 3.1 and 3.3, $4 \leq d_1 \leq 5$. Combining with (4.6) and $k \geq 2$, it follows that $1 \leq s \leq 2$. Since G is connected and $1 \leq s \leq 2$, $\tau(G) \leq s = \tau(W)$. From (4.7), we have

$$\begin{aligned} 2n_3 &= (2s+k)^2(7-2s-k) + 14(d_1 - k) - 28s + d_1^2(d_1 - 7) + 6(\tau(G) - \tau(W)) \\ &\leq (2s+k)^2(7-2s-k) + 14(d_1 - k - 2s) + d_1^2(d_1 - 7). \end{aligned} \tag{4.10}$$

If $s = 1$, by (4.6) we have $k \leq d_1 \leq k+1$. If $s = 2$, by (4.6) we have $k+2 \leq d_1 \leq k+3$. Now, from (4.10) and $4 \leq d_1 \leq 5$, we have the following table

(s, k, d_1)	$(1,3,4)$	$(1,4,4)$	$(1,4,5)$	$(1,5,5)$	$(2,2,4)$	$(2,2,5)$	$(2,3,5)$
n_3	≤ -6	≤ -20	≤ -14	≤ -39	≤ -20	≤ -14	≤ -39

which is impossible. □

Lemma 4.8. *If G is L-cospectral with $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$, then G is connected and G is co-degree with $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$.*

Proof. In the proof of this result, we simplify $\lambda_i(G)$, $n_i(G)$ and $d_i(G)$ as λ_i, n_i and d_i, respectively, and we rewrite $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ as W. Since W is connected, by Lemma 4.3, we have $\lambda_{n-1} = \lambda_{n-1}(W) > 0$ and hence G is connected. From Corollary 3.3 it follows that $\lambda_2 = \lambda_2(W) < 4$, and hence $d_2 \leq 3$ by Lemma 4.4. Taking Lemmas 4.6 into consideration, we may suppose that $a_1 \geq 3$ and $k \geq 2$ in the following. Now, from Lemma 4.5 it follows that $2s + k + 1 < \lambda_1 = \lambda_1(W) < 2s + k + 2$, and hence $2s + k - 1 \leq d_1 \leq 2s + k$ by Lemma 4.5. If $d_1 = 2s + k$, (4.5) also holds by (4.1), and hence G and W are co-degree. Thus, we may suppose that $d_1 = 2s + k - 1$ in the following. In this case, taking (4.1) in mind, (4.8) also holds and hence $n_1 = 2k + 2s - 3$, $n_2 = n + 4 - 4s - 3k$, and $n_3 = 2(s-1) + k$. Combining this with (4.2), it follows that

$$s = \tau(W) = \tau(G) + \frac{1}{2}(2s + k - 3)(2s + k - 2),$$

which implies that $s = 1$, $k = 2$ and $\tau(G) = 0$. Let $t(G)$ be the number of spanning trees of G. It is famous that (see [13]) $nt(G) = \lambda_1\lambda_2 \cdots \lambda_{n-1}$. Thus, $t(G) = t(W) = 3$. Since $t(G) = 3$ and G is a connected graph with n vertices and n edges, we have $\tau(G) = 1$, a contradiction. □

Lemma 4.9. [3] *Let G be a graph with $N_G(u_1) = N_G(u_2) = \cdots = N_G(u_k) = \{w_1, w_2, \ldots, w_p\}$. If G^* is the graph obtained from G by adding any q $(1 \leq q \leq \frac{k(k-1)}{2})$ edges among $\{u_1, u_2, \ldots, u_k\}$, then the eigenvalues of $L(G^*)$ are as follows: those eigenvalues of $L(G)$ which are equal to p $(k-1$ in number$)$ are incremented by $\lambda_i(G^*[X])$, $i = 1, 2, \ldots, k-1$, and the remaining eigenvalues are the same, where $X = \{u_1, u_2, \ldots, u_k\}$.*

Theorem 4.1. *The butterfly-like graph $W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ is both $Q - DS$ and $L - DS$.*

Proof. Suppose that G and $W \cong W_{2^{(s)};\mathbf{a}(\mathbf{k})}$ are either L-cospectral or Q-cospectral. By Lemmas 4.7–4.8 and (4.2), we can conclude that G is connected with $\tau(G) = s$ and G and W are co-degree. Thus, $G \cong W_{2^{(s)};\mathbf{b}(\mathbf{k})}$. By Corollary 2.1, $G \cong W$ if G and W are $Q - DS$. In the following, we shall prove that $G \cong W$ if G and W are $L - DS$.

Let G^* be the starlike tree (a starlike tree is a tree consisting of $t \geq 3$ paths intersecting in a single vertex) obtained from G by deleting s edges, whose end vertices are vertices of degrees two on s triangles of G. Similarly, we can define W^*. By Lemma 4.9, G^* and W^* are L-cospectral. Note that two starlike trees are L-cospectral if and only if they are isomorphic [8]. Thus, $G^* \cong W^*$, which implies that $G \cong W$. □

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The (signless) Laplacian spectral radii of c-cyclic graphs with n vertices, girth g and k pendant vertices

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ABSTRACT

Let $\Gamma_g(n,k;c)$ denote the class of c-cyclic graphs with n vertices, girth $g \geq 3$ and $k \geq 1$ pendant vertices. In this paper, we determine the unique extremal graph with largest signless Laplacian spectral radius and Laplacian spectral radius in the class of connected c-cyclic graphs with $n \geq c(g-1)+1$ vertices, girth g and at most $n-c(g-1)-1$ pendant vertices, respectively, and the unique extremal graph with largest signless Laplacian spectral radius of $\Gamma_g(n,k;c)$ when $n \geq c(g-1)+k+1$ and $c \geq 1$, and we also identify the unique extremal graph with largest Laplacian spectral radius in $\Gamma_g(n,k;c)$ in the case $c \geq 1$ and either $n \geq c(g-1)+k+1$ and g is even or $n \geq \frac{1}{2}(g-1)k+cg$ and g is odd. Our results extends the corresponding results of [Sci. Sin. Math. 2010;40:1017–1024, Electron. J. Combin. 2011; 18:p.183, Comput. Math. Appl. 2010;59:376–381, Electron. J. Linear Algebra. 2011;22:378–388 and J. Math. Res. Appl. 2014;34:379–391].

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1. Introduction

Throughout this paper, unless specially indicated, we are concerned with connected undirected simple graph only. Suppose G is a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For a vertex v of G, we use $N_G(v)$ and $d_G(v)$ to denote the neighbour set and degree of v in G, respectively. If there is no confusion, we always simply write $d(u)$ and $N(u)$ instead of $d_G(u)$ and $N_G(u)$, respectively. The sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v_i)$ holds for $1 \leq i \leq n$. Throughout this paper, we enumerate the degrees in non-increasing order, i.e. $d_1 \geq d_2 \geq \cdots \geq d_n$, and we suppose that $d(v_i) = d_i$, where $1 \leq i \leq n$. Especially, we use $\Delta(G)$ to denote the maximum degree of G. From the definition, it follows that $\Delta(G) = d_1(G)$. We call u a *pendant vertex* if $d(u) = 1$, and call u a *maximum degree vertex* if $d(u) = \Delta(G)$. Suppose that P is a path. If one end vertex of P is a pendant vertex while all the internal vertices of P are vertices with degrees two, then P is called a *pendant path*.

Throughout this paper, k and c are two nonnegative integers, and n is a positive integer. If G is connected with n vertices and $n+c-1$ edges, then G is called a *c-cyclic graph*. In particular, G is called a tree, unicyclic graph, bicyclic graph or a tricyclic graph if $c = 0$,

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1, 2 or 3, respectively. The length of a shortest cycle of G is called the *girth* of G and denoted by $g(G)$. Let $\Gamma(n,k;c)$ denote the class of c-cyclic graphs with n vertices and k pendant vertices, let $\Gamma_g(n;c)$ denote the class of c-cyclic graphs with n vertices and girth g, and let $\Gamma_g(n,k;c)$ denote the class of c-cyclic graphs with n vertices, k pendant vertices and girth g, where g is an integer being at least three hereafter. It is easy to see that $\Gamma(n,k;c)=\bigcup_{g=3}^{n}\Gamma_g(n,k;c)$ and $\Gamma_g(n;c)=\bigcup_{k=0}^{n-1}\Gamma_g(n,k;c)$. For simplification, let $\mathbb{T}(n,k)$, $\mathbb{U}(n,k)$, $\mathbb{B}(n,k)$ and $\mathbb{S}(n,k)$ be the class of trees, unicyclic graphs, bicyclic graphs and tricyclic graphs with n vertices and k pendant vertices, respectively.

As usual, K_n, C_n, P_n and $K_{s,n-s}$ define, respectively, the complete graph, cycle, path and complete bipartite graph on n vertices. Suppose v is a vertex of G, and $P_s=w_1w_2\cdots w_s$, where $V(P_s)\cap V(G)=\emptyset$. If we obtain a new graph G^* from G and P_s by adding two edges vw_1 and vw_s, then we say that G^* is obtained from G by *sewing* the path P_s to v of G. If we obtain a new graph G' from G and P_s by adding one edge vw_1, then we say that G' is obtained from G by *attaching* the path P_s to v of G. In the sequel, if we say that we attach or sew k paths to one vertex of G, then we agree that these k paths are vertex disjoint each other, and they are also vertex disjoint with G.

If q is a positive integer and G is a connected graph, qG denote the graph consisting of q copies of the graph G, and $q^{(p)}$ means p copies of the integer q, where p is a nonnegative integer. Paths $P_{l_1}, P_{l_2}, \ldots, P_{l_k}$ are said to *have almost equal lengths* if $l_1, l_2, \ldots, l_k$ satisfy $|l_i-l_j|\le 1$ for $1\le i\le j\le k$. Denoted by $C(q_1,q_2,\ldots,q_c)$, the graph on $\sum_{i=1}^{c}(q_i-1)+1$ vertices obtained by sewing the paths $P_{q_1-1}, P_{q_2-1}, \ldots, P_{q_c-1}$, to a common vertex, where $q_i\ge 2$ and $1\le i\le c$. Let $F_n(k,C_{q_1}^{(s)},C_{q_2}^{(c-s)})$ be the c-cyclic graph on n vertices obtained from $C(q_1^{(s)},q_2^{(c-s)})$ by attaching k paths of almost equal lengths to the maximum degree vertex of $C(q_1^{(s)},q_2^{(c-s)})$. In particular, we always simply write $F_n(k,C_{q_1}^{(c)},C_{q_2}^{(0)})$ and $F_n(k,C_{q_1}^{(0)},C_{q_2}^{(c)})$ as $F_n(k,C_{q_1}^{(c)})$ and $F_n(k,C_{q_2}^{(c)})$, respectively. Furthermore, we use the symbol $F_n(k)$ ($\cong F_n(k,C_g^{(0)})$) to denote the unique tree on n vertices obtained by attaching k paths of almost equal lengths to a common vertex. If all cycles of G have exactly one common vertex, then G is called a *bundle graph* (see, e.g. [1]). From the definitions, both $C(q_1,q_2,\ldots,q_c)$ and $F_n(k,C_{q_1}^{(s)},C_{q_2}^{(c-s)})$ are bundle graphs.

Let $D(G)$ be the diagonal matrix of vertex degrees, and $A(G)$ be the adjacency matrix of G. The *Laplacian matrix* and *signless Laplacian matrix* of G are, respectively, defined as $L(G)=D(G)-A(G)$ and $Q(G)=D(G)+A(G)$. The maximum eigenvalues of $L(G)$ and $Q(G)$ are denoted by $\lambda(G)$ and $\mu(G)$, respectively. Furthermore, $\mu(G)$ and $\lambda(G)$ are called, respectively, the *signless Laplacian spectral radius* and *Laplacian spectral radius* of G. For the relation between $\mu(G)$ and $\lambda(G)$, it is well known that

Theorem 1.1 ([2]): *If G is a connected graph on $n\ge 2$ vertices, then*

$$\Delta(G)+1\le\lambda(G)\le\mu(G),$$

where the first equality holds if and only if $\Delta(G)=n-1$, and the second equality holds if and only if G is bipartite.

If G has the largest (signless) Laplacian spectral radius in some given category of graphs, then we call G a (*signless*) *Laplacian largest extremal graph*.

Recently, the work on determining the signless Laplacian largest extremal graph, and/or Laplacian largest extremal graph in $\Gamma(n,k;c)$, has attained much attention. For any fixed positive number n and k, it is proved that: $F_n(k)$ is the unique Laplacian largest extremal tree (also the signless Laplacian largest extremal tree by Theorem 1.1) of $\mathbb{T}(n,k)$,[3,4] $F_n(k,C_3^{(1)})$ is the unique signless Laplacian largest extremal unicyclic graph of $\mathbb{U}(n,k)$ [5,6] when $n \geq k+3$ and $F_n(k,C_4^{(1)})$ is the unique Laplacian largest extremal unicyclic graph of $\mathbb{U}(n,k)$ [5,7] when $n \geq k+4$; $F_n(k,C_3^{(2)})$ is the unique signless Laplacian largest extremal bicyclic graph of $\mathbb{B}(n,k)$ [8–10] when $n \geq k+5$ and $F_n(k,C_4^{(2)})$ is the unique Laplacian largest extremal bicyclic graph of $\mathbb{B}(n,k)$ [5,7] when $n \geq k+7$; $F_n(k,C_3^{(3)})$ is the unique signless Laplacian largest extremal tricyclic graph of $\mathbb{S}(n,k)$ [3,9,11] when $n \geq k+7$ and $F_n(k,C_4^{(3)})$ is the unique Laplacian largest extremal tricyclic graph of $\mathbb{S}(n,k)$ [12] when $n \geq k+10$.

In the sequel, one of the present authors extended the above referred results of [3–12] by determining the unique signless Laplacian and Laplacian largest extremal graphs of $\Gamma(n,k;c)$ for $c \geq 0$, $k \geq 1$ and $n \geq 2c+k+1$, namely, he proved that

Theorem 1.2 ([13]): *If $k \geq 1$, $c \geq 0$ and $n \geq 2c+k+1$, then $F_n(k,C_3^{(c)})$ is the unique signless Laplacian largest extremal graph of $\Gamma(n,k;c)$.*

Theorem 1.3: ([13]) *Suppose that $k \geq 1$, $c \geq 0$ and G is a Laplacian largest extremal graph of $\Gamma(n,k;c)$. (i) If $n \geq 3c+k+1$, then $G \cong F_n(k,C_4^{(c)})$. (ii) If $n = 2c+k+1+t$ and $0 \leq t \leq c-1$, then $G \cong F_n(k,C_4^{(t)},C_3^{(c-t)})$. (iii) If $k+1 \leq n \leq 2c+k$, then G is any graph with $\Delta(G) = n-1$.*

At the same time, the extremal graphs with largest (signless) Laplacian spectral radii in the class of $\Gamma_g(n,k;c)$ and/or $\Gamma_g(n;c)$ were also studied by some scholars. Up to now, for any fixed positive number n, k and $g \geq 3$, the following results are identified: $F_n(k,C_g^{(1)})$ is the unique Laplacian largest extremal unicyclic graph of $\Gamma_g(n,k;1)$ for any $k \geq 1$ and $n \geq k+g$ [14]; $F_n(n-g,C_g^{(1)})$ is the unique signless Laplacian largest extremal unicyclic graph of $\Gamma_g(n;1)$ for any $n \geq g$ [15]; $F_n(n-2g+1,C_g^{(2)})$ is the unique signless Laplacian and Laplacian largest extremal bicyclic graph in the class of bicyclic bundle graphs with n vertices and girth g for any $n \geq 2g-1$, respectively, [15–17]; $F_n(n-3g+2,C_g^{(3)})$ is the unique signless Laplacian largest extremal tricyclic graph in the class of tricyclic bundle graphs with n vertices and girth g for any $n \geq 3g-2$.[18] In this paper, we will extend the corresponding results of [15–18] by showing the following theorem:

Theorem 1.4: *Let $\mathcal{G}$ be the class of graphs pertaining to $\Gamma_g(n;c)$, which contain at most $n-c(g-1)-1$ pendant vertices. If $g \geq 3$, $c \geq 1$ and $n \geq \max\{c(g-1)+1,6\}$, then $F_n(n-c(g-1)-1,C_g^{(c)})$ is the unique signless Laplacian and Laplacian largest extremal graph of $\mathcal{G}$, respectively.*

Remark 1.1: Since $\lambda(K_{2,3}) = \lambda(F_5(0,C_3^{(2)})) = 5$, the condition '$n \geq 6$' in Theorem 1.4 is necessary. Let H_1 be the bicyclic graph with six vertices obtained from $K_4 - e$ by attaching two isolated vertices to one vertex of degree three of $K_4 - e$. Since $\lambda(F_6(1,C_3^{(2)})) = \lambda(H_1) = 6$, the condition 'contain at most $n-c(g-1)-1$ pendant vertices' in Theorem 1.4 is also necessary.

We will also extend the corresponding result of [14] by proving the following theorem:

Theorem 1.5: *Let $c \geq 1$, $g \geq 3$ and $k \geq 1$, and let G be the Laplacian largest extremal graph of $\Gamma_g(n,k;c)$. (i) If g is even and $n \geq c(g-1)+k+1$, then $G \cong F_n(k, C_g^{(c)})$. (ii) If g is odd and $n \geq \frac{1}{2}(g-1)k+cg$, then $G \cong F_n(k, C_g^{(1)}, C_{g+1}^{(c-1)})$.*

Remark 1.2: Since $\lambda(F_{13}(2, C_5^{(1)}, C_6^{(1)})) < 7.166 < 7.192 < \lambda(F_{13}(2, C_5^{(2)}))$, the condition '$n \geq \frac{1}{2}(g-1)k+cg$' in Theorem 1.5 (*ii*) is necessary.

One can also easily see that Theorem 1.5 extends partially result of Theorem 1.3. Furthermore, the following theorem extends partially result of Theorem 1.2.

Theorem 1.6: *If $k \geq 1$, $g \geq 3$, $c \geq 1$ and $n \geq c(g-1)+k+1$, then $F_n(k, C_g^{(c)})$ is the unique signless Laplacian largest extremal graph of $\Gamma_g(n,k;c)$.*

2. The proof of Theorem 1.6

Let uv be an edge of G and v be a vertex of G. Let $m(v)$ denote the average of the degrees of the vertices being adjacent to v, i.e. $m(v) = \sum_{u \in N(v)} d(u)/d(v)$. Denote by

$$\Psi(uv) = \frac{d(u)(d(u)+m(u)) + d(v)(d(v)+m(v))}{d(u)+d(v)}.$$

Theorem 1.1 presents a well-known lower bound to $\lambda(G)$, while the following result gives a famous upper bound for $\mu(G)$.

Lemma 2.1 ([19]): *Let G be a connected graph with at least three vertices, and let $s = \Psi(u_0v_0) = \max\{\Psi(uv) : uv \in E(G)\}$ and $t = \max\{\Psi(uv) : uv \in E(G) \setminus \{u_0v_0\}\}$. Then*

$$\mu(G) \leq 2 + \sqrt{(s-2)(t-2)}$$

with equality holding if and only if G is a regular graph or a bipartite semiregular graph or a path with four vertices.

When G is connected, by the Perron–Frobenius Theorem of non-negative matrices (see e.g. [20]), it follows that

Lemma 2.2: *If G is connected and $G' \subset G$, then $\mu(G') < \mu(G)$ and $\lambda(G') \leq \lambda(G)$.*

Furthermore, by the Perron–Frobenius Theorem of non-negative matrices, there also exists a unique positive unit eigenvector corresponding to $\mu(G)$. In the sequel, we use $f = (f(v_1), f(v_2), \ldots, f(v_n))^T$ to indicate the unique positive unit eigenvector corresponding to $\mu(G)$, and call f the *Perron vector* of G. As we will see later, the following three operations will play an important role in our proofs.

Let $G-uv$ be the graph obtained from G by deleting the edge $uv \in E(G)$, and let $G+uv$ be the graph obtained from G by adding an edge $uv \notin E(G)$. Similarly, $G-v$ denoted the graph obtained from G by deleting the vertex $v \in V(G)$.

Lemma 2.3 ([4]): *Suppose that u, v are two vertices of a connected graph G, and $w_1, w_2, \ldots, w_k$ $(1 \leq k \leq d(v))$ are some vertices of $N(v) \setminus (N(u) \cup \{u\})$. Let $G' = G + w_1u + w_2u + \cdots + w_ku - w_1v - w_2v - \cdots - w_kv$. If f is the Perron vector of G with $f(u) \geq f(v)$, then $\mu(G') > \mu(G)$.*

Let $G_{u,v}$ define a new graph obtained from G by subdividing the edge uv, i.e. adding a new vertex w and two edges wu, wv in $G - uv$, where $uv \in E(G)$. An *internal path*, say $P = w_1w_2\cdots w_s$ ($s \geq 2$), is a path joining w_1 and w_s (which need not be distinct) such that the degrees of w_1 and w_s are greater than 2, while all other vertices (if exist) $w_2, w_3, \ldots, w_{s-1}$ are of degree 2.

Lemma 2.4 ([5]): *If G is a connected graph and uv is an edge in an internal path of G, then $\mu(G) > \mu(G_{u,v})$.*

Suppose v is a vertex of a connected graph G with at least two vertices. Let $G_{s,t}$ ($t \geq s \geq 1$) be the graph obtained from G by attaching two new paths $P_s = w_1w_2\cdots w_s$ and $P_t = u_1u_2\cdots u_t$, respectively, to v of G. Let $G_{s-1,t+1} = G_{s,t} - w_{s-1}w_s + u_tw_s$.

Lemma 2.5 ([5]): *Let G be a connected graph with at least two vertices. If $t \geq s \geq 1$, then $\mu(G_{s,t}) > \mu(G_{s-1,t+1})$.*

To prove our results, we need to extend Lemma 3.1 of [13] as follows.

Lemma 2.6: *Let G be a graph of $\Gamma(n, k; c)$ and $G \notin \{K_{2,3}, C_n\}$, where $c \geq 1$ and $k \geq 0$. If $\lambda(G) \geq k + 2c + 1$ or $\mu(G) \geq k + 2c + 1$, then G is one of the following candidates: (i) G is obtained by attaching k paths and then sewing another c paths, respectively, to a common vertex; (ii) G is obtained by adding an edge joining one vertex of a cycle to one vertex of degree two of a path; (iii) G is obtained by attaching one path to each of two adjacent vertices of a cycle, respectively; (iv) G is obtained by adding one edge to two nonadjacent vertices of C_n; (v) G is obtained by adding one edge joining one vertex of C_s with one vertex of C_{n-s}, where $n - s \geq s \geq 3$.*

Proof: Suppose the degree sequence of G is $(d_1, d_2, \ldots, d_n)$ and $G \notin \{K_{2,3}, C_n\}$. Since $G \in \Gamma(n, k; c)$, we have

$$2(n + c - 1) = \sum_{i=1}^{n} d_i. \tag{2.1}$$

If $d_1 + d_2 \geq k + 2c + 3$, then

$$2(n + c - 1) = \sum_{i=1}^{n} d_i \geq k + 2c + 3 + 2(n - 2 - k) + k = 2n + 2c - 1, \text{ a contradiction.}$$

If $k \geq 1$ and $d_1 + d_2 \leq k + 2c + 1$, then G is neither regular nor bipartite semiregular. By Theorem 1.1 and Lemma 2.1,

$$\lambda(G) \leq \mu(G) < 2 + \sqrt{(d_1 + d_2 - 2)^2} = d_1 + d_2 \leq k + 2c + 1, \text{ a contradiction.}$$

If $k = 0$ and $d_1 + d_2 \leq 2c$, then by Theorem 1.1 and Lemma 2.1, we have

$$\lambda(G) \leq \mu(G) \leq d_1 + d_2 \leq 2c, \text{ a contradiction.}$$

If $k = 0$ and $d_1 + d_2 = 2c + 1$, then by (2.1), we have $d_1 > d_2 \geq d_3 = 3$. By Theorem 1.1 and Lemma 2.1,

$$\lambda(G) \leq \mu(G) \leq d_1 + d_2 \leq 2c + 1.$$

Furthermore, by Lemma 2.1, $\mu(G) = 2c + 1$ implies that $d_1 = 2c - 2$ and $d_2 = d_3 = \cdots = d_n = 3$, which contradicts (2.1).
Therefore, if $\lambda(G) \geq k + 2c + 1$ or $\mu(G) \geq k + 2c + 1$, then $d_1 + d_2 = k + 2c + 2$. Since G contains exactly k pendant vertices with (2.1), we have

$$d_1 + d_2 = k + 2c + 2, \ \ d_3 = d_4 = \cdots = d_{n-k} = 2 \ \text{ and } \ d_{n-k+1} = \cdots = d_n = 1. \quad (2.2)$$

If $d_1 \leq k + 2c - 2$, then by Theorem 1.1 and Lemma 2.1 with (2.2),

$$\lambda(G) \leq \mu(G) \leq 2 + \sqrt{(d_1 + d_2 - 2)(d_1 + d_3 - 2)} = 2 + \sqrt{(k + 2c)d_1} < k + 2c + 1,$$

a contradiction. If $d_1 = k + 2c$, by (2.2) we have $d_2 = d_3 = \cdots = d_{n-k} = 2$ and $d_{n-k+1} = d_{n-k+2} = \cdots = d_n = 1$, then G is a graph of (i). Notice that $d_1 = k + 2c + 2 - d_2 \leq k + 2c$ by (2.2). Thus, the final possibility is $d_1 = k + 2c - 1$. By (2.2) it follows that $d_2 = 3$. Next, we shall prove that

$$\mu(G) < \max\{\Psi(uv) : uv \in E(G)\}. \quad (2.3)$$

If $c \geq 2$, since $d_1 = k + 2c - 1 \geq 3 = d_2 > d_3 = 2$ and $G \ncong K_{2,3}$, then G is neither regular nor bipartite semiregular. In this case, (2.3) follows from Lemma 2.1. Now, we consider the case $c = 1$. Since $G \ncong C_n$, $d_n = 1$. Thus, G is neither regular nor bipartite semiregular, and hence (2.3) follows from Lemma 2.1.

Suppose $\Psi(u_0v_0) = \max\{\Psi(uv) : uv \in E(G)\}$, where $d(u_0) \geq d(v_0)$. Since G is connected and $c \geq 1$, $d(u_0) \in \{k + 2c - 1, 3, 2\}$. If $d_1 = k + 2c - 1 = 3 = d_2$, then either $c = 2$ and $k = 0$ or $c = 1$ and $k = 2$. If $v_1v_2 \notin E(G)$, then by Theorem 1.1 and (2.3) we have $\lambda(G) \leq \mu(G) < \Psi(u_0v_0) \leq 5$, a contradiction. Thus, $v_1v_2 \in E(G)$. If $c = 2$ and $k = 0$, then G is one graph of (iv) or (v). If $c = 1$ and $k = 2$, then G is one graph of (ii) or (iii). In the following, we only need to consider the case $d_1 = k + 2c - 1 \geq 4$:
Case 1 $d(u_0) = d_1 = k + 2c - 1 \geq 4$. If $d(v_0) = 3$, then $d(u_0) = d_1$ and $d(v_0) = d_2$ by (2.2). Therefore,

$$\begin{aligned}\Psi(u_0v_0) &\leq \frac{d_1^2 + d_2 + 2(d_1 - 1) + d_2^2 + d_1 + 2(d_2 - 1)}{d_1 + d_2} \\ &= k + 2c - 1 + \frac{14}{k + 2 + 2c} \\ &\leq k + 2c + 1.\end{aligned}$$

If $d(v_0) = 2$, then

$$\Psi(u_0v_0) \leq \frac{d_1^2 + 3 + 2(d_1 - 1) + 4 + d_1 + 3}{d_1 + 2} = k + 2c + \frac{6}{k + 2c + 1} \leq k + 2c + 1.$$

If $d(v_0) = 1$, then

$$\Psi(u_0v_0) \leq \frac{d_1^2 + 1 + 3 + 2(d_1 - 2) + 1 + d_1}{d_1 + 1} = k + 2c + 1 - \frac{1}{k + 2c} < k + 2c + 1.$$

Case 2 $d(u_0) = 3$. By (2.2), we have $d_1 \geq 4$ and $d(u_0) = 3 = d_2 > d_3$, which implies that $1 \leq d(v_0) \leq 2$. If $d(v_0) = 2$, then

$$\Psi(u_0v_0) \leq \frac{d_2^2 + d_1 + 2(d_2 - 1) + 4 + d_1 + d_2}{d_2 + 2} = \frac{2(k + 2c) + 18}{5} < k + 2c + 1.$$

If $d(v_0) = 1$, then

$$\Psi(u_0v_0) \leq \frac{d_2^2 + d_1 + 2 + 1 + 1 + d_2}{d_2 + 1} = \frac{k + 2c + 15}{4} < k + 2c + 1.$$

Case 3 $d(u_0) = 2$. Then, $1 \leq d(v_0) \leq 2$. If $d(v_0) = 2$, then

$$\Psi(u_0v_0) \leq \frac{2(4 + d_1 + 2)}{2 + 2} = \frac{k + 2c + 5}{2} < k + 2c + 1.$$

If $d(v_0) = 1$, then

$$\Psi(u_0v_0) \leq \frac{4 + d_1 + 1 + 1 + 2}{2 + 1} = \frac{k + 2c + 7}{3} < k + 2c + 1.$$

Now, from Theorem 1.1 with (2.3) and the above discussion, we can conclude that $\lambda(G) \leq \mu(G) < \Psi(u_0v_0) \leq k + 2c + 1$, a contradiction. □

Lemma 2.7: *If G is one graph of (ii) or (iii) as defined in Lemma 2.6 and $g(G) = g$, then $\mu(G) < \mu(F_n(2, C_g^{(1)}))$.*

Proof: Let f be the Perron vector of G. We first suppose that G is a graph of (*iii*). Without loss of generality, we may suppose that $f(v_1) \geq f(v_2)$. Let u be a vertex of $N_G(v_2) \setminus V(C_g)$. Let $G' = G + v_1u - v_2u$. By Lemma 2.3, we have $\mu(G) < \mu(G')$. Since G' is obtained from a cycle C_g by attaching two paths to exactly one vertex of C_g, by Lemma 2.5 we have $\mu(G') \leq \mu(F_n(2, C_g^{(1)}))$. Therefore, $\mu(G) < \mu(F_n(2, C_g^{(1)}))$ holds.

We secondly suppose that G is a graph of (*ii*). Suppose that $v_1 \in V(C_g)$. Then, $v_2 \notin V(C_g)$. If $f(v_1) \geq f(v_2)$, since $d_G(v_2) = 3$, it can be proved similarly with the former case. If $f(v_1) < f(v_2)$, choose u as a vertex of $N_G(v_1) \cap V(C_g)$. Let $G' = G + v_2u - v_1u$. By Lemma 2.3, we have $\mu(G) < \mu(G')$. Suppose that $N_{G'}(u) = \{v_2, v\}$. Let $G_1 = G' + vv_2 - uv - uv_2$, $G_2 = G_1 - u$ and $G_3 = G_1 + xu$, where x is a pendant vertex of G_1. Since $d_{G_2}(v_2) = 4$, vv_2 lies in an internal path of G_2. By Lemma 2.4, $\mu(G') < \mu(G_2)$. Furthermore, since $G_1 \subset G_3$, by Lemma 2.2 we have $\mu(G_2) = \mu(G_1) < \mu(G_3)$, and hence $\mu(G') < \mu(G_3)$. Note that G_3 is obtained by attaching two paths to exactly one vertex of C_g. By Lemma 2.5, we have $\mu(G_3) \leq \mu(F_n(2, C_g^{(1)}))$.

Now, we can conclude that $\mu(G) < \mu(F_n(2, C_g^{(1)}))$ holds. □

Proof of Theorem 1.6: Suppose that G is a signless Laplacian largest extremal graph of $\Gamma_g(n, k; c)$. Since $F_n(k, C_g^{(c)}) \in \Gamma_g(n, k; c)$, by the choice of G and Theorem 1.1 it follows that $\mu(G) \geq \mu(F_n(k, C_g^{(c)})) > k + 2c + 1$. By Lemmas 2.5–2.7, we can conclude that G is obtained by attaching k paths of almost equal lengths to the maximum degree vertex of $C(q_1, q_2, \ldots, q_c)$, where $q_1 \geq q_2 \geq \cdots \geq q_{c-1} \geq q_c = g$.

If $q_1 = g$, then $q_1 = q_2 = \cdots = q_c = g$ and hence $G \cong F_n(k, C_g^{(c)})$, the result already holds. Thus, we only need to consider the case of $q_1 \geq g + 1$.

Suppose that $\{u, v, w\} \in V(C_{q_1})\backslash\{v_1\}$ such that $uv \in E(C_{q_1})$ and $vw \in E(C_{q_1})$. Let x be a pendant vertex of G. Let $G_1 = G + uw - uv - vw$, $G_2 = G_1 - v$ and $G_3 = G_1 + xv$. Then, $G_3 \in \Gamma_g(n, k; c)$. Since $d_G(v_1) = k + 2c \geq 3$, uw lies in an internal path of G_2. By Lemma 2.4, we have $\mu(G) < \mu(G_2)$. Note that $G_1 \subset G_3$. By Lemma 2.2, $\mu(G) < \mu(G_2) = \mu(G_1) < \mu(G_3)$, contradicting the choice of G. Thus, $G \cong F_n(k, C_g^{(c)})$. □

3. The proofs of Theorems 1.4–1.5

By Lemma 2.2, if we add some edges to a connected graph, the signless Laplacian spectral radius will increase strictly. However, the following result shows that additional edges to a connected graph can result for unchanged Laplacian spectral radius:

Lemma 3.1 ([21,22]): *Let v be a vertex of a connected graph G with at least two vertices and let G' be obtained from G by attaching k paths of equal lengths to v. If G'' is obtained from G by adding any s $(1 \leq s \leq \frac{k(k-1)}{2})$ edges among these pendant vertices of G'', which belong to the referred k paths, then $\lambda(G') = \lambda(G'')$.*

Lemma 3.2: *If $k \geq 1, c \geq s \geq 1$ and $n \geq c(g-1) + k + s + 1$, then*

$$\mu(F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)})) < \mu(F_n(k, C_{g+1}^{(s-1)}, C_g^{(c-s+1)})).$$

Proof: Suppose v_1 is the maximum degree vertex of $F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)})$, and suppose that $\{u, v, w\} \in V(C_{g+1})\backslash\{v_1\}$ such that $uv \in E(C_{g+1})$ and $vw \in E(C_{g+1})$ in $F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)})$. Let x be a pendant vertex of $F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)})$. Let $G_1 = F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)}) + uw - uv - vw$, $G_2 = G_1 - v$ and $G_3 = G_1 + xv$. Since $d_{G_2}(v_1) = k + 2c \geq 3$, uw is contained in an internal path of G_2. By Lemma 2.4, we have $\mu(F_n(k, C_{g+1}^{(s)}, C_g^{(c-s)})) < \mu(G_2)$. Note that $G_1 \subset G_3$. By Lemma 2.2, $\mu(G_2) = \mu(G_1) < \mu(G_3)$. Furthermore, since G_3 is obtained by attaching k paths to the maximum degree vertex of $C((g+1)^{(s-1)}, g^{(c-s+1)})$, by Lemma 2.5 we have $\mu(G_3) \leq \mu(F_n(k, C_{g+1}^{(s-1)}, C_g^{(c-s+1)}))$. Now, the result follows by combining the above discussion. □

Suppose that $g \geq 3$ is an odd number. Let $F_n^*(k, C_{g+1}^{(c-s)}, C_g^{(s)})$ be a graph obtained from $F_n(k, C_{g+1}^{(c-s)}, C_g^{(s)})$ by deleting every edge, which has the largest distance from the maximum degree vertex of $F_n(k, C_{g+1}^{(c-s)}, C_g^{(s)})$ in each cycle C_g. From the definition, $F_n^*(k, C_{g+1}^{(c-s)}, C_g^{(s)})$ can be also obtained from $F_{n-s(g-1)}(k, C_{g+1}^{(c-s)})$ by attaching $2s$ paths of length $\frac{1}{2}(g-1) - 1$ to the vertex of degree $k + 2(c-s)$ of $F_{n-s(g-1)}(k, C_{g+1}^{(c-s)})$. By Lemma 3.1, the following equation holds for any $c \geq s \geq 1$, $k \geq 1$ and $g \geq 3$:

$$\lambda(F_n^*(k, C_{g+1}^{(c-s)}, C_g^{(s)})) = \lambda(F_n(k, C_{g+1}^{(c-s)}, C_g^{(s)})). \tag{3.1}$$

Lemma 3.3: *Suppose that g is odd, and G is a c-cyclic graph on n vertices obtained by attaching k paths to the vertex with degree $2c$ of $C(g^{(s)}, q_1, q_2, \ldots, q_{c-s})$. If $c \geq s \geq 1$, $k \geq 1$ and $q_1 \geq q_2 \geq \cdots \geq q_{c-s} \geq g + 1$, then*

$$\lambda(G) \leq \lambda(F_n^*(k, C_{g+1}^{(c-s)}, C_g^{(s)})) = \lambda(F_n(k, C_{g+1}^{(c-s)}, C_g^{(s)})),$$

where the first equality holds if and only if $G \cong F_n(k, C_{g+1}^{(c-s)}, C_g^{(s)})$.

Proof: Since v_1 is the maximum degree vertex of G, we have $d_G(v_1) = k + 2c$. Let G_1 be a $(c-s)$-cyclic graph on n vertices obtained by deleting every edge, which has the largest distance from v_1 in each C_g. By Lemma 3.1, $\lambda(G) = \lambda(G_1)$.

First we assume that $c = s$. In this case, G_1 is a tree obtained by attaching $k + 2c$ paths (among which at least $2c$ paths are $P_{0.5(g-1)}$) to a common vertex. By (3.1) with Theorem 1.1 and Lemma 2.5, we have

$$\lambda(G) = \lambda(G_1) = \mu(G_1) \leq \mu(F_n^*(k, C_g^{(c)})) = \lambda(F_n^*(k, C_g^{(c)})).$$

If $\lambda(G) = \lambda(F_n^*(k, C_g^{(c)}))$, then $\mu(G_1) = \mu(F_n^*(k, C_g^{(c)}))$, and hence $G_1 \cong F_n^*(k, C_g^{(c)})$ by Lemma 2.5. By the definition of G_1, $G \cong F_n(k, C_g^{(c)})$. Conversely, if $G \cong F_n(k, C_g^{(c)})$, then by (3.1) we have $\lambda(G) = \lambda(F_n^*(k, C_g^{(c)}))$. So, the result holds for $c = s$.

Next, we assume that $c - s \geq 1$. In this case, $g(G_1) = q_{c-s} \geq g + 1$.

Case 1 $q_1 = g + 1$. Now, $q_1 = q_2 = \cdots = q_{c-s} = g + 1$ and G_1 is a $(c-s)$-cyclic graph obtained by attaching $k + 2s$ paths (among which at least $2s$ paths are $P_{0.5(g-1)}$) to the vertex of degree $2(c-s)$ of $C((g+1)^{(c-s)})$. By Lemma 2.5,

$$\mu(G_1) \leq \mu\left(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right)$$

with equality holding if and only if $G_1 \cong F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$. By Theorem 1.1 and Lemma 3.1, we have

$$\lambda(G) = \lambda(G_1) = \mu(G_1) \leq \mu\left(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right) = \lambda(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)).$$

If $\lambda(G) = \lambda(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right))$, then $\mu(G_1) = \mu(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right))$, and hence $G \cong F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$. Conversely, if $G \cong F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$, then by Lemma 3.1 implies that $\lambda(G) = \lambda(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right))$.

Case 2 $q_1 \geq g + 2$. Suppose that $\{u, v, w\} \in V(C_{q_1})\backslash\{v_1\}$ such that $uv \in E(C_{q_1})$ and $vw \in E(C_{q_1})$. Let x be a pendent vertex pertaining to a longest pendant path of G. Let $G_2 = G_1 + uw - uv - vw$, $G_3 = G_2 - v$ and $G_4 = G_2 + xv$. Since $d_{G_3}(v_1) = k + 2c \geq 3$, uw is contained in an internal path of G_3. By Lemma 2.4, we have $\mu(G_1) < \mu(G_3)$. Note that $G_2 \subset G_4$. By Lemma 2.2, $\mu(G_1) < \mu(G_3) = \mu(G_2) < \mu(G_4)$.

Note that G_4 contains exactly $k + 2s$ pendant vertices, and at least $2s$ pendant vertices are contained in $2s$ pendant paths of lengths $\frac{1}{2}(g-1)$ initial from the maximum degree vertex of G_4. By repeating the above operation, we can obtain a $(c-s)$-cyclic graph G_5 such that $\mu(G_4) \leq \mu(G_5)$, where G_5 is obtained by attaching $k + 2s$ paths (among which at least $2s$ paths are $P_{0.5(g-1)}$) to the vertex of degree $2(c-s)$ of $C((g+1)^{(c-s)})$. By Lemma 2.5, $\mu(G_5) \leq \mu(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right))$. Now, from Theorem 1.1, we have $\lambda(G) = \lambda(G_1) \leq \mu(G_1) < \mu(G_5) \leq \mu(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)) = \lambda(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right))$. □

Lemma 3.4: *If g is odd, $c \geq s \geq 1$, $k \geq 1$ and $n \geq \frac{1}{2}(g-1)k + cg + 2 - s$, then*

$$\lambda\left(F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right) < \lambda\left(F_n\left(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)}\right)\right).$$

Proof: Let P be a longest pendant path among these k pendant paths, which are initial from the maximum degree vertex (i.e. v_1) of $F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$, and let y be the pendant vertex of P. If $|V(P)| \leq \frac{1}{2}(g+1)$, then

$$n \leq s(g-1) + g(c-s) + 1 + \frac{1}{2}(g-1)k = \frac{1}{2}(g-1)k + gc + 1 - s, \text{ a contradiction.}$$

Thus, $|V(P)| \geq \frac{1}{2}(g+1)+1$. Let x be a pendant vertex of a pendant path with length $\frac{1}{2}(g-1)$, which is initial from v_1 in $F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$. By the definition of $F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$, such vertex x must exist.

Let $G_1 = F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right) + xy$. Then $g(G_1) \geq g+1$ and G_1 is a $(c-s+1)$-cyclic graph obtained by attaching $k + 2(s-1)$ paths (among which at least $2s-1$ paths are $P_{0.5(g-1)}$) to the maximum degree vertex of $C((g+1)^{(c-s)}, q)$, where $q \geq g+1$. By Lemmas 2.4 and 2.5, $\mu(G_1) \leq \mu(F_n^*(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)}))$. Since $g+1$ is even, by (3.1), we have

$$\mu(F_n^*(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)})) = \lambda(F_n^*(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)})).$$

Furthermore, since $F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right) \subset G_1$, by (3.1) with Theorem 1.1 and Lemma 2.2, we have

$$\begin{aligned}\lambda\left(F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right) &= \lambda(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)) = \mu(F_n^*\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)) \\ &< \mu(G_1) \leq \lambda(F_n^*(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)})) = \lambda(F_n(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)})).\end{aligned}$$

Thus, the required inequality holds. □

Lemma 3.5: *If G is one graph of (ii) or (iii) as defined in Lemma 2.6 and $g(G) = g$, then* $\lambda(G) < \lambda(F_n(2, C_g^{(1)}))$.

Proof: When g is even, by Lemma 2.7 and Theorem 1.1, the result already holds. Thus, we may suppose that g is odd and $n \geq 6$ in the following, as $n = 5$ can be checked easily. If $g = 3$ and G is a graph of (iii), it is well-known that [23]

$$\lambda(G) \leq \max\{|N(u) \cup N(v)| : uv \in E(G)\},$$

and hence $\lambda(G) \leq 5 < \lambda(F_n(2, C_g^{(1)}))$ by Theorem 1.1. If $g = 3$ and G is a graph of (ii), let G' be the graph obtained from G by deleting one edge with both end vertices are of degrees two in C_3. By Lemmas 2.1 and 3.1 with Theorem 1.1, we have

$$\lambda(G) = \lambda(G') \leq \max\{\Psi(uv) : uv \in E(G')\} = 5 < \lambda(F_n^*(2, C_g^{(1)})).$$

If $g \geq 5$, then by Lemmas 2.1–2.2 it follows that

$$\lambda(G) \leq \mu(G) \leq 2 + \sqrt{\left(\frac{16}{3} - 2\right)(5-2)} < 5.163 < \lambda(F_7^*(2, C_5^{(1)})) \leq \lambda(F_n^*(2, C_g^{(1)})). \tag{3.2}$$

Now, the result follows from (3.1). □

Proof of Theorem 1.5: When g is even, by Theorems 1.1 and 1.6, we have $\lambda(G) \leq \mu(G) \leq \mu(F_n(k, C_g^{(c)})) = \lambda(F_n(k, C_g^{(c)}))$, where $\lambda(G) = \lambda(F_n(k, C_g^{(c)}))$ holds if and only if $G \cong F_n(k, C_g^{(c)})$. Thus, (i) follows. Now, we turn to prove (ii).

Since $n \geq \frac{1}{2}(g-1)k + cg + 1$, $F_n(k, C_g, C_{g+1}^{(c-1)}) \in \Gamma_g(n, k; c)$. By Theorem 1.1 and the choice of G, $\lambda(G) \geq \lambda(F_n(k, C_g, C_{g+1}^{(c-1)})) \geq k + 2c + 1$. From Lemmas 2.6 and 3.5, it follows that G is obtained from $C(q_1, q_2, \ldots, q_c)$ by attaching k paths to the maximum degree vertex of $C(q_1, q_2, \ldots, q_c)$, where $q_1 \geq q_2 \geq \cdots \geq q_{c-1} \geq q_c = g$.

We suppose that G contains exactly s cycles C_g. By Lemma 3.3, we have

$$\lambda(G) \leq \lambda\left(F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right)$$

with equality holding if and only if $G \cong F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)$. If $s = 1$, then the result already holds. Otherwise, $s \geq 2$. By Lemma 3.4, it follows that

$$\lambda\left(F_n\left(k, C_{g+1}^{(c-s)}, C_g^{(s)}\right)\right) < \lambda\left(F_n\left(k, C_{g+1}^{(c-s+1)}, C_g^{(s-1)}\right)\right) \leq \cdots \leq \lambda(F_n(k, C_{g+1}^{(c-1)}, C_g^{(1)})).$$

Thus, $\lambda(G) < \lambda(F_n(k, C_{g+1}^{(c-1)}, C_g^{(1)}))$. This completes the proof of (ii). □

Lemma 3.6: *Let G be one graph of (iv) or (v) as defined in Lemma 2.6 and $g(G) = g$. If $n \geq 2g - 1$, then $\lambda(G) < \lambda(F_n(n - 2g + 1, C_g^{(2)}))$ and $\mu(G) < \mu(F_n(n - 2g + 1, C_g^{(2)}))$.*

Proof: In this case, G is neither regular nor bipartite semiregular. If $n - 2g + 1 \geq 1$, by Lemma 2.1 and Theorem 1.1, we have

$$\lambda(G) \leq \mu(G) < 6 \leq \lambda(F_n(n - 2g + 1, C_g^{(2)})) \leq \mu(F_n(n - 2g + 1, C_g^{(2)})),$$

and the result already holds.

If $n = 2g - 1$, it is easy to check the result holds for $g = 3$. Now, we suppose that $g \geq 4$. Since $F_7^*(2, C_5^{(1)}) \subset F_n(0, C_g^{(2)})$, by Theorem 1.1, Lemmas 2.1–2.2 and (3.2), we have

$$\lambda(G) \leq \mu(G) < 5.163 < \lambda(F_7^*(2, C_5^{(1)})) \leq \lambda(F_n(0, C_g^{(2)})) \leq \mu(F_n(0, C_g^{(2)})).$$

This completes the proof of this result. □

Proof of Theorem 1.4: Let G be a Laplacian or signless Laplacian largest extremal graph of $\mathcal{G}$. Since $F_n(k, C_g^{(c)}) \in \mathcal{G}$, by Lemmas 2.6–2.7 and Lemmas 3.5–3.6, G is obtained from $C(q_1, q_2, \ldots, q_c)$ by attaching k paths to the maximum degree vertex of $C(q_1, q_2, \ldots, q_c)$, where $q_1 \geq q_2 \geq \cdots \geq q_{c-1} \geq q_c = g$ and $0 \leq k \leq n - c(g-1) - 1$. Furthermore, when $n = c(g-1) + 1$, then $G \cong F_n(0, C_g^{(c)})$ and the result already holds. We may suppose that $n \geq c(g-1) + 2$ in the following.

If $k \leq n - c(g-1) - 2$, by Lemma 2.1 and Theorem 1.1, we have

$$\begin{aligned}\lambda(G) \leq \mu(G) &\leq d_1 + d_2 = 2c + k + 2 \leq 2c + n - c(g-1) \\ &\leq \lambda(F_n(n - c(g-1) - 1, C_g^{(c)})) \leq \mu(F_n(n - c(g-1) - 1, C_g^{(c)})).\end{aligned}$$

By the structure of G and Lemma 2.1, G is regular with $d_1 = 2c + k = 2 = d_2$. Thus, $c = 1$ and $k = 0$, which implies that $G \cong C_n$. In this case, $0 \leq k \leq n - c(g-1) - 2 = -1$, a contradiction. Therefore, $k = n - c(g-1) - 1$ and hence $G \cong F_n(n - c(g-1) - 1, C_g^{(c)})$. □

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On partitions of graphs under degree constraints

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ABSTRACT

Let s, t be two integers, and let $g(s, t)$ denote the minimum integer such that the vertex set of a graph of minimum degree at least $g(s, t)$ can be partitioned into two nonempty sets which induce subgraphs of minimum degree at least s and t, respectively. In this paper, it is shown that, (1) for positive integers s and t, $g(s, t) \leq s+t$ on (K_4-e)-free graphs except K_3, and (2) for integers $s \geq 2$ and $t \geq 2$, $g(s, t) \leq s + t - 1$ on triangle-free graphs in which no two quadrilaterals share edges. Our first conclusion generalizes a result of Kaneko (1998), and the second generalizes a result of Diwan (2000).

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1. Introduction

All graphs considered in this paper are finite and simple. Let G be a graph, let X be a subset of $V(G)$. We use $G[X]$ to denote the subgraph of G induced by X. For a vertex $x \in X$, we use $N_X(x)$ to denote the neighbor set of x in X, let $N_X[x] = N_X(x) \cup \{x\}$, and let $d_X(x) = |N_X(x)|$ (when $X = V(G)$, we simplify $N_X(x)$, $N_X[x]$ and $d_X(x)$ as $N(x)$, $N[x]$ and $d(x)$, respectively). Let A and B be two nonempty disjoint subsets of $V(G)$. If $A \cup B = V(G)$, then we call (A, B) a partition of $V(G)$. We also say that $V(G)$ is partitioned into A and B if (A, B) is a partition.

In 1972, Mader [6] showed that every graph of minimum degree at least $4k$ contains a k-connected subgraph. In 1982, Györi (see [4,8]) proposed a problem as follows: for given positive integers s and t, is there an integer $f(s, t)$ such that the vertex set of every $f(s, t)$-connected graph can be partitioned into two sets S and T which induce subgraphs of connectivity at least s and t respectively? Thomassen [8], and Szegedy independently (see [4]), proved the existence of the function $f(s, t)$, and Hajnal [4] improved the bound to $f(s, t) \leq 4s + 4t - 13$. In his proof, Thomassen proved a degree version of Györi's problem. He showed essentially that for positive integers s and t, there is an integer $g(s, t)$ such that the vertex set of every graph G with minimum degree at least $g(s, t)$ can be partitioned into S and T which induce subgraphs of minimum degree at least s and t, respectively. The complete graph K_{s+t+1} shows that $g(s, t) \geq s + t + 1$. Then, Thomassen conjectured that $g(s, t) = s + t + 1$.

In [7], Stiebitz confirmed Thomassen's conjecture with an elegant argument. In fact, Stiebitz proved a result stronger than the conjecture. Let $\mathbb{N}$ denote the set of nonnegative integers.

Theorem 1.1 ([7]). *Let G be a graph and $a, b : V(G) \longmapsto \mathbb{N}$ two functions. Suppose that $d(x) \geq a(x) + b(x) + 1$ for each vertex x of G. Then, there exists a partition of $V(G)$ into A and B such that*

(1) $d_A(x) \geq a(x)$ *for each* $x \in A$, *and*
(2) $d_B(y) \geq b(y)$ *for each* $y \in B$.

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Let (A, B) be a partition of $V(G)$, and let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. We say that (A, B) is an (a, b)-*feasible partition* if $d_A(x) \geq a(x)$ for each $x \in A$ and $d_B(y) \geq b(y)$ for each $y \in B$. Theorem 1.1 says that G admits an (a, b)-feasible partition if $d(x) \geq a(x) + b(x) + 1$ for each vertex x of G. Stiebitz [7] further asked a question if there are some pair of positive integers s and t and a triangle-free graph G of minimum degree $s + t$ such that G has no vertex disjoint subgraphs G_1 and G_2 with minimum degree at least s and t, respectively. In another words, is it true that, for any positive integers s and t, $g(s, t) \leq s+t$ on triangle-free graphs? The complete bipartite graph $K_{s+t,s+t}$ shows that $g(s, t) \geq s + t$ on triangle-free graphs, and every connected regular triangle-free graph requires s and t to be positive in order to have $g(s, t) \leq s + t$. Kaneko [5] answered Stiebitz's problem with a similar argument as that used in [7].

Theorem 1.2 ([5]). *Let s and t be two positive integers. Then, $g(s, t) \leq s + t$ on triangle-free graphs.*

As Stiebitz pointed out in his paper [7], K_{s+t+1} does not admit (s, t)-feasible partitions for any pair $s \geq 1$ and $t \geq 1$, and the icosahedron is 5-regular and does not admit $(4, 1)$-feasible partitions. Note that triangles appear densely in both K_{s+t+1} and the icosahedron (every set of three vertices of K_{s+t+1} spans a triangle, and every edge of the icosahedron is in two triangles). One may ask naturally whether the bound $g(s, t) \leq s+t$ holds on graphs in which the triangles are not dense. This is indeed the case. A cycle of length 4 is referred to as a *quadrilateral*, and $K_4 - e$ is the graph obtained from K_4 by removing one edge. A graph is said to be $(K_4 - e)$-*free* if it does not contain $K_4 - e$ as a subgraph (here $K_4 - e$ may not be induced, a $(K_4 - e)$-free graph is also K_4-free. The similar happens when we talk no two quadrilaterals sharing an edge later). We show that $g(s, t) \leq s + t$ on $(K_4 - e)$-free graphs except K_3.

Theorem 1.3. *Let G be a $(K_4 - e)$-free graph with at least four vertices, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ two functions. If $d(x) \geq a(x) + b(x)$ for each vertex x of G, then G admits an (a, b)-feasible partition.*

The requirement $(K_4 - e)$-free is necessary in Theorem 1.3 as evidenced by the icosahedron. Another example is $K_4 - e$ itself. Let $G = K_4 - e$, and let $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0\}$ be two functions such that $a(x) = d(x) - 1$ and $b(x) = 1$ for each vertex $x \in V(G)$. Then G has no (a, b)-feasible partition.

As usual, the length of a shortest cycle in a graph G is called the *girth* of G. In 2000, Diwan considered the problem that whether $g(s, t)$ can be reduced further by forbidding the existence of triangles and quadrilaterals in the graphs, and he succeeded in showing that

Theorem 1.4 ([2]). *Let $s \geq 2$ and $t \geq 2$ be two integers. Then, $g(s, t) \leq s + t - 1$ on the graphs of girth at least five.*

The cycle of length n ($n \geq 5$) shows that one cannot expect to omit the requirement of $s \geq 2$ and $t \geq 2$ by simply increasing the girth of graphs. In 2004, Gerber and Kobler generalized Theorem 1.4 and proved the following analogue of Theorem 1.1. Bazgan, Tuza and Vanderpooten [1] presented three polynomial time algorithms to find (a, b)-feasible partitions satisfying Theorems 1.1, 1.2 and 1.5, respectively.

Theorem 1.5 ([3]). *Let G be a graph of girth at least five, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ two functions. If $d(x) \geq a(x) + b(x) - 1$ for each vertex x of G, then G admits an (a, b)-feasible partition.*

Our next result generalizes Theorem 1.5 to triangle-free graphs that may contain quadrilaterals.

Theorem 1.6. *Let G be a triangle-free graph in which no two quadrilaterals share edges, and $a, b : V(G) \longmapsto \mathbb{N} \setminus \{0, 1\}$ two functions. If $d(x) \geq a(x) + b(x) - 1$ for each vertex x of G, then G admits an (a, b)-feasible partition.*

The complete bipartite graph $K_{3,3}$ shows that the restriction on the sparsity of quadrilaterals cannot be relaxed too much, since it does not admit $(2, 2)$-feasible partitions. We are not sure whether Theorem 1.6 can be improved further. It would be nice if someone can strengthen Theorem 1.6 to graphs with neither triangle nor $K_{2,3}$. Furthermore, up to our best knowledge, the following problem due to Diwan [2] is still open: whether the bound $s + t - 1$ in Theorem 1.4 can be improved further for graphs with larger girth.

As a direct corollary of Theorems 1.3 and 1.6, we have

Corollary 1.1. *Let s and t be two positive integers. Then, $g(s, t) \leq s+t$ on $(K_4 - e)$-free graphs except K_3, and $g(s, t) \leq s+t-1$ on triangle-free graphs in which no two quadrilaterals share edges if $s \geq 2$ and $t \geq 2$.*

Before proving our theorems, we still need to introduce some notations that are also used in [1–3,5,7]. Let G be a graph, and let S be a subset of $V(G)$. Recall that for each vertex x of S, $d_S(x)$ denotes the degree of x in $G[S]$. Let y be a vertex in $V(G) \setminus S$. We use $e_G(y, S)$ to denote the number of edges joining y to S.

Let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. We say that S is a-*satisfactory* if $d_S(x) \geq a(x)$ for each vertex x of S, and say that S is a-*degenerate* if for each nonempty subset S' of S there exists a vertex $x \in S'$ such that $d_{S'}(x) \leq a(x)$. By an (a, b)-*degenerate partition* we mean a partition (A, B) of $V(G)$ such that A is a-degenerate and B is b-degenerate.

As in [3,7,8], the weight $\omega(A, B)$ of an (a, b)-degenerate partition (A, B) is defined by

$$\omega(A, B) = |E(G[A])| + |E(G[B])| + \sum_{u \in A} b(u) + \sum_{v \in B} a(v).$$

Then, for each vertex x of A and each vertex $y \in B$,

$$\omega(A \setminus \{x\}, B \cup \{x\}) - \omega(A, B) = e_G(x, B) - d_A(x) + a(x) - b(x), \tag{1.1}$$

and

$$\omega(A \cup \{y\}, B \setminus \{y\}) - \omega(A, B) = e_G(y, A) - d_B(y) + b(y) - a(y). \tag{1.2}$$

Both proofs of Theorems 1.3 and 1.6 begin with Lemma 1.1, which was essentially proved by Stiebitz [7]. Let $a, b : V(G) \longmapsto \mathbb{N}$ be two functions. A pair (A, B) of disjoint subsets A and B of $V(G)$ is said to be (a, b)-*feasible* if A is a-satisfactory and B is b-satisfactory. An (a, b)-feasible partition is just an (a, b)-feasible pair (A, B) with $A \cup B = V(G)$. Suppose that $d(x) \geq a(x) + b(x) - 1$ for each vertex x, and suppose that G has a maximum (a, b)-feasible pair (A, B). If $A \cup B \neq V(G)$, then there exists a vertex $u \in V(G) \setminus (A \cup B)$ such that either $(A \cup \{u\}, B)$ or $(A, B \cup \{u\})$ is still an (a, b)-feasible pair. So, below Lemma 1.1 follows immediately.

Lemma 1.1. *For any two functions $a, b : V(G) \longmapsto \mathbb{N}$ such that $d(x) \geq a(x) + b(x) - 1$ for each vertex x, if G has an (a, b)-feasible pair, then it admits an (a, b)-feasible partition.*

2. Proofs of Theorems 1.3 and 1.6

This section is devoted to the proofs of Theorems 1.3 and 1.6. The main idea is an extension of that used in [2,5,7]. Let us prove Theorem 1.3 first.

Proof of Theorem 1.3. Suppose that the conclusion is not true. Then, we may suppose, by Lemma 1.1, that G has no (a, b)-feasible pair. We claim that

$$a(x) + a(y) \geq 3 \text{ and } b(x) + b(y) \geq 3 \text{ for each edge } xy \text{ of } G. \tag{2.1}$$

Suppose the contrary to (2.1), and suppose by symmetry that xy is an edge such that $b(x) = b(y) = 1$. If $N(x) \cap N(y) = \emptyset$, then for each vertex v in $V(G) \setminus \{x, y\}$, $d(v) - 1 \geq a(v)$ as $|N(v) \cap \{x, y\}| \leq 1$, which imply that $(V(G) \setminus \{x, y\}, \{x, y\})$ is an (a, b)-feasible partition. Therefore, $N(x) \cap N(y) \neq \emptyset$. Since G is $(K_4 - e)$-free, $N(x) \cap N(y)$ consists of a single vertex, say w, and $|N(u) \cap \{w, x, y\}| \leq 1$ for each vertex $u \in V(G) \setminus \{w, x, y\}$. If $b(w) = 1$, then $(V(G) \setminus \{w, x, y\}, \{w, x, y\})$ is an (a, b)-feasible partition (as $|N(u) \cap \{w, x, y\}| \leq 1$ for each vertex $u \in V(G) \setminus \{w, x, y\}$). Otherwise, we have $b(w) \geq 2$. Now, $a(w) \leq d(w) - 2$, and thus $(V(G) \setminus \{x, y\}, \{x, y\})$ is an (a, b)-feasible partition (again since $|N(u) \cap \{w, x, y\}| \leq 1$ for each vertex $u \in V(G) \setminus \{w, x, y\}$). These two contradictions prove (2.1).

If G has no (a, b)-degenerate partition, let A be an a-satisfactory subset of $V(G)$ of minimum size, and let $B = V(G) \setminus A$. Then, B is non-empty as $b(v) \geq 1$ for each $v \in V(G)$. By the choice of A, A is a-degenerate. So, B cannot be b-degenerate (for otherwise (A, B) was an (a, b)-degenerate partition), and there must be a non-empty subset B' of B such that $d_{B'}(v) > b(v)$ for every $v \in B'$. Now, (A, B') is an (a, b)-feasible pair, contradicting our assumption.

Therefore, G must have an (a, b)-degenerate partition, say (A, B).

Since G has no (a, b)-feasible pair by our assumption, either A is $(a-1)$-degenerate or B is $(b-1)$-degenerate. By symmetry, we suppose that B is $(b-1)$-degenerate. Now, (A, B) is an $(a, b-1)$-degenerate partition of $V(G)$.

We may choose (A, B), among all $(a, b-1)$-degenerate partitions of $V(G)$, such that

(1) $\omega(A, B)$ is maximum, and
(2) $|A|$ is minimum subject to (1).

First, we show that

$$|B| \geq 2. \tag{2.2}$$

If it is not the case, suppose that $B = \{y\}$. Since A is a-degenerate, there exists a vertex, say x, in A such that $d_A(x) \leq a(x)$. Then, $e_G(x, B) \geq b(x) \geq 1$, and so $b(x) = 1$ and $xy \in E(G)$ since $B = \{y\}$. By (2.1), $b(y) \geq 2$ which means $(A \setminus \{x\}, B \cup \{x\})$ is also an $(a, b-1)$-degenerate partition. But now, $\omega(A \setminus \{x\}, B \cup \{x\}) - \omega(A, B) \geq b(x) - a(x) + a(x) - b(x) = 0$ by (1.1), and $|A \setminus \{x\}| < |A|$. This contradicts the choice of (A, B), and therefore (2.2) holds.

Next, we will find a vertex u_0 in B with $d_B(u_0) \leq b(u_0) - 1$, and two vertices x_0, y_0 in A with $d_A(x_0) = a(x_0)$ and $d_A(y_0) = a(y_0)$ such that $u_0x_0y_0u_0$ is a triangle in G, and then complete the proof by showing that $(A \setminus \{x_0, y_0\}, B \cup \{x_0, y_0\})$ is an $(a, b-1)$-degenerate partition with $\omega(A \setminus \{x_0, y_0\}, B \cup \{x_0, y_0\}) > \omega(A, B)$.

Since B is $(b-1)$-degenerate, there is a vertex, say u_0, in B such that $d_B(u_0) \leq b(u_0) - 1$, and hence $e_G(u_0, A) \geq a(u_0) + 1$. This implies that $|A| \geq a(u_0) + 1 \geq 2$. Let $A' = A \cup \{u_0\}$, and $B' = B \setminus \{u_0\}$ ($B' \neq \emptyset$ by (2.2)). Applying (1.2) to (A, B) with $y = u_0$, we have $\omega(A', B') - \omega(A, B) \geq 2$. Note that B' is $(b-1)$-degenerate. The maximality of $\omega(A, B)$ indicates that A' cannot be a-degenerate. So, there exists a subset A_0 of A such that $A_0 \cup \{u_0\}$ is $(a+1)$-satisfactory. It follows that A_0 is a-satisfactory.

If A is not a-satisfactory, there must exist a vertex, say x, in $A \setminus A_0$ such that $d_A(x) \leq a(x) - 1$ and $e_G(x, B) \geq b(x) + 1$. Let $A'' = A \setminus \{x\}$ and $B'' = B \cup \{x\}$. It is clear that A'' is still a-degenerate. Since $A_0 \subseteq A''$ and G has no (a, b)-feasible pair, B''

must be $(b-1)$-degenerate. So, (A'', B'') is still an $(a, b-1)$-degenerate partition of $V(G)$. By applying (1.1) to (A, B), we have $\omega(A'', B'') - \omega(A, B) \geq 2$ because $d_A(x) \leq a(x) - 1$ and $e_G(x, B) \geq b(x) + 1$, contradicting the maximality of $\omega(A, B)$. Therefore, A is a-satisfactory.

Let $C = \{u \in A | d_A(u) = a(u)\}$. Since A is both a-degenerate and a-satisfactory, $C \neq \emptyset$. We claim that $C \subseteq A_0$. If it is not the case, there must exist some vertex, say w, in $A \setminus A_0$ such that $d_A(w) = a(w)$ and $e_G(w, B) \geq b(w)$. Let $A' = A \setminus \{w\}$ and $B' = B \cup \{w\}$. By applying (1.1) to (A, B) with $x = w$, we have that $\omega(A', B') \geq \omega(A, B)$. Since $A_0 \subseteq A'$ and A_0 is a-satisfactory, B' must be $(b-1)$-degenerate as G has no (a, b)-feasible pair. Now, either $\omega(A', B') > \omega(A, B)$ contradicting (1), or $\omega(A', B') = \omega(A, B)$ but $|A'| < |A|$ contradicting (2). So, $C \subseteq A_0$. Since $A_0 \cup \{u_0\}$ is $(a+1)$-satisfactory by the choice of A_0, $C \subseteq N(u_0)$. Therefore,

$$C \subseteq A_0 \cap N(u_0).$$

Let x_0 be a vertex in C. If $N_A(x_0) \subseteq A \setminus C$, let $A' = A \setminus \{x_0\}$ and $B' = B \cup \{x_0\}$, then A' is still a-satisfactory, and hence B' must be $(b-1)$-degenerate as G has no (a, b)-feasible pair. So, (A', B') is also an $(a, b-1)$-degenerate partition of $V(G)$. But now $\omega(A', B') \geq \omega(A, B)$ (by applying (1.1) to (A, B) with $x = x_0$) and $|A'| < |A|$, contradicting the choice of (A, B). Therefore, $N_A(x_0) \cap C \neq \emptyset$. Let $y_0 \in N_A(x_0) \cap C$. Now, $u_0x_0y_0u_0$ is a triangle in G as desired.

If $A = \{x_0, y_0\}$, then $1 = d_A(x_0) = d_A(y_0) = a(x_0) = a(y_0)$. Recall that $A_0 \cup \{u_0\}$ is $(a+1)$-satisfactory. Thus, $2 = e_G(u_0, A) \geq a(u_0) + 1$ and hence $a(u_0) = 1$. Note that $B \setminus \{u_0\} \neq \emptyset$ by (2.2). Since G is $(K_4 - e)$-free, every vertex of $B \setminus \{u_0\}$ has at most one neighbor in $\{u_0, x_0, y_0\}$, and thus $(\{u_0, x_0, y_0\}, V(G) \setminus \{u_0, x_0, y_0\})$ is an (a, b)-feasible partition of $V(G)$, a contradiction. Therefore, $A \neq \{x_0, y_0\}$.

If $N_A(x_0) \cap (C \setminus \{y_0\})$ contains a vertex, say w, then $w \in N(u_0)$ which means that $G[\{u_0, w, x_0, y_0\}]$ contains a $K_4 - e$, a contradiction. The same contradiction occurs if $N_A(y_0) \cap C \neq \{x_0\}$. Therefore, $(N_A(x_0) \cup N_A(y_0)) \setminus \{x_0, y_0\} \subseteq A \setminus C$, i.e., $d_A(w) \geq a(w) + 1$ for each vertex w in $(N_A(x_0) \cup N_A(y_0)) \setminus \{x_0, y_0\}$.

Now, $A \setminus \{x_0, y_0\}$ is also a-satisfactory. Let $A' = A \setminus \{x_0, y_0\}$ and $B' = B \cup \{x_0, y_0\}$. Recall that G has no (a, b)-feasible pair by our assumption. Then, B' must be $(b-1)$-degenerate, and hence (A', B') is an $(a, b-1)$-degenerate partition of $V(G)$. Since $e_G(x_0, B) \geq b(x_0)$ and $e_G(y_0, B) \geq b(y_0)$,

$$\omega(A', B') - \omega(A, B) = e_G(x_0, B) + e_G(y_0, B) - (a(x_0) - 1) - (a(y_0) - 1) - b(x_0) - b(y_0) + a(x_0) + a(y_0) \geq 2$$

contradicting the choice of (A, B). This contradiction ends the proof of Theorem 1.3. ■

Let us now turn to the proof of Theorem 1.6. The proof is more complicated than that of Theorem 1.3. For convenience, we use $\mathcal{G}$ to denote the family of triangle-free graphs in which no two quadrilaterals share edges. We begin with a graph G of $\mathcal{G}$ which has $d(x) \geq a(x) + b(x) - 1$ for each vertex x and which contains no (a, b)-feasible pair, and show that G has an $(a-1, b-1)$-degenerate partition. Then, we will find a particular $(a-1, b-1)$-degenerate partition with some additional properties, and construct an (a, b)-feasible pair from this particular partition, and thus complete the proof.

Proof of Theorem 1.6. Let G be a graph in $\mathcal{G}$ with $d(x) \geq a(x) + b(x) - 1$ for each vertex x of G. Suppose that G has no (a, b)-feasible pair, and subject to this, G has minimum number of edges. We may assume that for every edge $xy \in E(G)$,

$$\text{either } d(x) = a(x) + b(x) - 1 \text{ or } d(y) = a(y) + b(y) - 1, \tag{2.3}$$

for otherwise, we consider the graph $G - xy$, and each (a, b)-feasible partition of $G - xy$ is also one of G.

Since $G \in \mathcal{G}$, for any two distinct vertices u and v of G,

$$N(u) \cap N(v) = \emptyset \text{ if } uv \in E(G), \text{ and } |N(u) \cap N(v)| \leq 2 \text{ if } uv \notin E(G).$$

This observation will be used frequently during the proof.

Recall that, for functions $p, q : V(G) \longmapsto \mathbb{N}$, a (p, q)-degenerate partition is a partition (U, W) such that U is p-degenerate and W is q-degenerate. We claim that G admits an $(a-1, b-1)$-degenerate partition. To see this, let S be an a-satisfactory subset of $V(G)$ of minimum size, and let $T = V(G) \setminus S$. Then, $T \neq \emptyset$ as $b(w) \geq 2$ for each vertex w, and T must be $(b-1)$-degenerate as otherwise we would have an (a, b)-feasible pair. By the minimality of $|S|$, each proper subset of S is $(a-1)$-degenerate, there must be a vertex, say x, in S such that $d_S(x) = a(x)$, and a vertex, say y, in $N_S(x)$ such that $d_S(y) = a(y)$ (since $S \setminus \{x\}$ is $(a-1)$-degenerate). We may suppose, by symmetry, that $d(x) = a(x) + b(x) - 1$ by (2.3). Now, $(S \setminus \{x\}, T \cup \{x\})$ is an $(a-1, b-1)$-degenerate partition in G since $e_G(x, T) = b(x) - 1$.

For convenience, we call an $(a-1, b-1)$-degenerate partition (A, B) a *maximum* $(a-1, b-1)$-*degenerate partition* if $\omega(A, B)$ reaches maximum among all $(a-1, b-1)$-degenerate partitions. From now on, we always assume that (A, B) is a maximum $(a-1, b-1)$-degenerate partition.

Let $A^- = \{x | x \in A, d_A(x) \leq a(x) - 1\}$, $A^= = \{x | x \in A, d_A(x) = a(x)\}$, and let $A^+ = A \setminus (A^- \cup A^=)$. Analogously, we define B^-, $B^=$ and B^+.

Since (A, B) is an $(a-1, b-1)$-degenerate partition, $A^- \neq \emptyset \neq B^-$. Let $u \in A^-$ and $v \in B^-$. Then, $e_G(u, B) \geq b(u)$ and $e_G(v, A) \geq a(v)$, and thus $|A| \geq 2$ and $|B| \geq 2$. It follows from (1.1) and (1.2) that

$$\omega(A \setminus \{u\}, B \cup \{u\}) - \omega(A, B) \geq b(u) - (a(u) - 1) - b(u) + a(u) = 1, \tag{2.4}$$

and

$$\omega(A \cup \{v\}, B \setminus \{v\}) - \omega(A, B) \geq a(v) - (b(v) - 1) - a(v) + b(v) = 1. \tag{2.5}$$

So, $A \cup \{v\}$ cannot be $(a-1)$-degenerate, and $B \cup \{u\}$ cannot be $(b-1)$-degenerate, and thus there exist an a-satisfactory subset A' of $A \cup \{v\}$ and a b-satisfactory subset B' of $B \cup \{u\}$. If $u \notin A'$ and $v \notin B'$, then (A', B') is an (a, b)-feasible pair. Therefore, we have Claim 1.

Claim 1. *For each pair of vertices $u \in A^-$ and $v \in B^-$, either every a-satisfactory subset of $A \cup \{v\}$ must include u, or every b-satisfactory subset of $B \cup \{u\}$ must include v.* ■

Furthermore, since $uv \notin E(G)$ implies that $u \notin A'$ and $v \notin B'$, and since $G \in \mathcal{G}$, it follows directly from Claim 1 that

$$A^- \cup B^- \text{ induces a complete bipartite subgraph of } G. \tag{2.6}$$

From Claim 1, we can also prove the following claim.

Claim 2. *Let (A, B) be a maximum $(a-1, b-1)$-degenerate partition with $u \in A^-$ and $v \in B^-$. If $u_1 \in N_A(u) \cap A^=$ and $v_1 \in N_B(v) \cap B^=$, then $u_1v_1 \in E(G)$.*

Proof. On contrary, assume that $u_1v_1 \notin E(G)$. By Claim 1, and by the symmetry between $(A \setminus \{u\}, B \cup \{u\})$ and $(A \cup \{v\}, B \setminus \{v\})$, we may suppose that every b-satisfactory subset of $B \cup \{u\}$ must contain v. Since $d_B(v) \leq b(v) - 1$, and since every b-satisfactory subset of $B \cup \{u\}$ must contain v, we can conclude that $d_B(v) = b(v) - 1$ and $uv \in E(G)$, both $(B \cup \{u\}) \setminus \{v\}$ and $(B \cup \{u\}) \setminus \{v_1\}$ are $(b-1)$-degenerate, and either $d(v) = a(v) + b(v) - 1$ or $d(v_1) = a(v_1) + b(v_1) - 1$ by (2.3).

If $d(v) = a(v) + b(v) - 1$, then $e_G(v, A \setminus \{u\}) = a(v) - 1$ by (2.6), and so $(A \cup \{v\}) \setminus \{u\}$ is $(a-1)$-degenerate. Let $A_1 = (A \cup \{v\}) \setminus \{u\}$ and $B_1 = (B \cup \{u\}) \setminus \{v\}$. Since $\omega(A_1, B_1) - \omega(A, B) \geq (a(v) - 1) + (b(u) - 1) + a(u) + b(v) - (b(v) - 1 + a(u) - 1 + a(v) + b(u)) = 0$, it follows that (A_1, B_1) is also a maximum $(a-1, b-1)$-degenerate partition. Since $u_1v \notin E(G)$ and $uv_1 \notin E(G)$ (otherwise, G may contain triangle), $u_1 \in A_1^-$ and $v_1 \in B_1^-$, and thus $u_1v_1 \in E(G)$ by (2.6), a contradiction. Therefore, $d(v) \geq a(v) + b(v)$, and so $d(v_1) = a(v_1) + b(v_1) - 1$ and $e_G(v_1, A) = a(v_1) - 1$. Let $A_2 = (A \cup \{v_1\}) \setminus \{u\}$ and $B_2 = (B \cup \{u\}) \setminus \{v_1\}$. Then, A_2 is $(a-1)$-degenerate. Furthermore, since every b-satisfactory subset of $B \cup \{u\}$ must contain v and $d_B(v) = b(v) - 1$, every b-satisfactory subset of $B \cup \{u\}$ must also contain every neighbor of v in B, and hence B_2 is $(b-1)$-degenerate. Thus, (A_2, B_2) is a maximum $(a-1, b-1)$-degenerate partition as $\omega(A_2, B_2) - \omega(A, B) \geq b(u) + a(v_1) - 1 + a(u) + b(v_1) - (a(u) - 1 + b(v_1) + b(u) + a(v_1)) = 0$. Since $u_1v_1 \notin E(G)$, $u_1 \in A_2^-$ and $v \in B_2^-$, and this implies that $G[\{u_1, u, v\}]$ induces a triangle by (2.6), a contradiction. Therefore, Claim 2 holds. ■

Recall that (A, B) is an arbitrary maximum $(a-1, b-1)$-degenerate partition. Since $A \cup \{v\}$ is not $(a-1)$-degenerate by (2.5), if $A^- = A$, then A is an independent set by (2.6), and so $A \cup \{v\}$ has an a-satisfactory subset, say X, giving $1 = d_X(x) \geq a(x) \geq 2$ for $x \in X \setminus \{v\}$. The same happens if $B^- = B$. Therefore,

$$A^- \neq A \text{ and } B^- \neq B \text{ for each maximum } (a-1, b-1)\text{-degenerate partition } (A, B). \tag{2.7}$$

Below Claim 3 demonstrates a local structure around some vertices in $A^- \cup B^-$, that is very useful in the remaining proof.

Claim 3. *Let (A, B) be a maximum $(a-1, b-1)$-degenerate partition, and let $x \in A^-$, $v \in B^-$, $v_1 \in N_B(v) \cap B^=$. If $d(v) = a(v) + b(v) - 1$, then $(B \cup \{x\}) \setminus \{v, v_1\}$ is $(b-1)$-degenerate.*

Proof. If it is not the case, let B_0 be a b-satisfactory subset of $(B \cup \{x\}) \setminus \{v, v_1\}$.

Let $S = \{w : w \in A \text{ and } d_A(w) \leq a(w) - 2\}$. If $S \neq \emptyset$, let $x' \in S$ and let A' be an a-satisfactory subset of $A \cup \{v\}$ (by (2.5), such an A' exists), then $A' \cap S = \emptyset$. By Claim 1 and (2.4), $B \cup \{x'\}$ contains a b-satisfactory subset B' with $v \in B'$. Thus, $d_B(v) = b(v) - 1$ and so $e_G(v, A) = a(v)$. Now, $S \subseteq A'$ (as $S \subseteq A^- \subseteq N(v)$ by (2.6)). This contradicts $A' \cap S = \emptyset$, and so $S = \emptyset$.

Let $A_0 = (A \cup \{v, v_1\}) \setminus \{x\}$. Since $xv_1 \notin E(G)$ (otherwise, G contains a triangle, as $xv \in E(G)$ by (2.6)), $d_{A_0}(v_1) \geq a(v_1)$ and $d_{A_0}(v) = a(v)$. For any vertex $z \in A^- \setminus \{x\}$, since $S = \emptyset$ and since $vz \in E(G)$ by (2.6), $d_{A_0}(z) = a(z)$. For each vertex $x_1 \in N_A(x) \cap A^=$, since $x_1v_1 \in E(G)$ by Claim 2, $d_{A_0}(x_1) = a(x_1)$. Now, we can conclude that A_0 is an a-satisfactory subset, giving an (a, b)-feasible pair (A_0, B_0). This contradiction completes the proof of Claim 3. ■

For a nonempty subset X of $V(G)$, we denote $N(X) = \cup_{x \in X} N(x)$. By (2.6) and since $G \in \mathcal{G}$, either $\min\{|A^-|, |B^-|\} = 1$, or $|A^-| = |B^-| = 2$. If $|A^-| = |B^-| = 2$, let $A^- = \{u, u'\}$ and $B^- = \{v, v'\}$. Then, $G[\{u, v, u', v'\}]$ is a quadrilateral by (2.6), and thus every other vertex has at most one neighbor on $G[\{u, v, u', v'\}]$ as $G \in \mathcal{G}$. Now the degeneracy of A and B guarantees that $A^= \cap N(A^-) \neq \emptyset \neq B^= \cap N(B^-)$. Without loss of generality, we may assume that $u_1 \in A^= \cap N(A^-)$ and $v_1 \in B^= \cap N(B^-)$. In this case, Claim 2 implies that $u_1v_1 \in E(G)$, and hence uv is in two quadrilaterals of $G[\{u, u', u_1, v, v', v_1\}]$, a contradiction. Thus,

$$\min\{|A^-|, |B^-|\} = 1. \tag{2.8}$$

Let (A, B) be a maximum $(a-1, b-1)$-degenerate partition, and suppose by symmetry that $|A^-| \geq |B^-|$. Then, $|B^-| = 1$ by (2.8). Let $B^- = \{v\}$. Since $B^- \neq B$ by (2.7), we may choose a vertex, say v_1, in $N_B(v) \cap B^=$. Since $G \in \mathcal{G}$, $B \setminus N_B[v] \neq \emptyset$

as $d_B(v_1) = b(v_1) \geq 2$, and every vertex but v has at most two neighbors in $N(v)$. If $N_B(w) \setminus \{v\} \subseteq B^+$ for each vertex $w \in N(v) \cap B^=$, then the $(b-1)$-degeneracy of B guarantees the existence of two vertices, say $v_2 \in N_B(v_1)$ and $v_3 \in N(v) \cap B^=$, such that $d_B(v_2) = b(v_2) + 1$ and $N_B(v_1) \cap N_B(v_3) = \{v, v_2\}$. Therefore, either

$$\text{there exists a vertex } v_2 \in N_B(v_1) \cap B^=, \tag{2.9}$$

or there exist $v_2 \in N_B(v_1)$ and $v_3 \in N_B(v) \cap B^=$ such that

$$d_B(v_2) = b(v_2) + 1 \text{ and } N_B(v_1) \cap N_B(v_3) = \{v, v_2\}. \tag{2.10}$$

To complete the proof, we will show that, for some vertex $w \in N(A^-)$, $(B \cup \{w\}) \setminus \{v, v_1\}$ has a b-satisfactory subset, and then apply Claim 3 to deduce a contradiction. For this purpose, we need to show

$$(B \cup \{w\}) \setminus \{v\} \text{ has a } b\text{-satisfactory subset for some } w \in A^- \tag{2.11}$$

since v_1 is not contained in any b-satisfactory subset of $(B \cup \{w\}) \setminus \{v\}$ (as $v_1 \in N(v) \setminus N(A^-)$ by (2.6) and $G \in \mathcal{G}$).

We distinguish two cases following $N(A^-) \cap A^= \neq \emptyset$ or not.

Case 1. First, we suppose that there is a vertex $u \in A^-$ and a vertex $u_1 \in N(u) \cap A^=$. We may choose $|A^-| + |B^-|$ as maximum as possible. We will check that $(B \cup \{u\}) \setminus \{v\}$ has a b-satisfactory subset. If it is not the case, then $d_B(v) = b(v) - 1$ and $N_B[v]$ is contained in every b-satisfactory subset of $B \cup \{u\}$, and so both $(B \cup \{u\}) \setminus \{v\}$ and $(B \cup \{u\}) \setminus \{v_1\}$ are $(b-1)$-degenerate.

If $d(v) = a(v) + b(v) - 1$, then $e_G(v, A \setminus \{u\}) = a(v) - 1$, and so $(A \cup \{v\}) \setminus \{u\}$ is $(a-1)$-degenerate. Remember that $A_1 = (A \cup \{v\}) \setminus \{u\}$ and $B_1 = (B \cup \{u\}) \setminus \{v\}$. Since $\omega(A_1, B_1) - \omega(A, B) \geq 0$, (A_1, B_1) is a maximum $(a-1, b-1)$-degenerate partition, and $d_{B_1}(u) = b(u) - 1$ (otherwise, $\omega(A_1, B_1) > \omega(A, B)$). Since $u_1 v, uv_1 \notin E(G)$, $u_1 \in A_1^-$ and $v_1 \in B_1^-$. Now, $\min\{|A_1^-|, |B_1^-|\} > 1$ as $v \in A_1^-$ and $u \in B_1^-$, contradicting (2.8).

So, $d(v) \geq a(v) + b(v)$, and hence $d(u) = a(u) + b(u) - 1$ and $d(v_1) = a(v_1) + b(v_1) - 1$ by (2.3). Recall that $A_2 = (A \cup \{v_1\}) \setminus \{u\}$ and $B_2 = (B \cup \{u\}) \setminus \{v_1\}$. Since $\omega(A_2, B_2) - \omega(A, B) \geq 0$, (A_2, B_2) is also a maximum $(a-1, b-1)$-degenerate partition, and $d_{B_2}(u) = b(u)$ (otherwise, $\omega(A_2, B_2) > \omega(A, B)$). Since $u_1 v_1 \in E(G)$ by Claim 2, $G[\{u, u_1, v_1, v\}]$ is a quadrilateral of G, and hence (2.10) cannot happen by $G \in \mathcal{G}$. Now, (2.9) guarantees the existence of a vertex v_2 such that $v_2 \in N_B(v_1) \cap B^=$. Again by considering the quadrilateral $G[\{u, u_1, v_1, v\}]$ and (2.6), $xv_2 \notin E(G)$ for every vertex $x \in A^-$. Now, $v_1 \in A_2^-$ and $\{v, v_2\} \subseteq B_2^-$. If $|A^-| \geq 2$, then $\min\{|A_2^-|, |B_2^-|\} \geq 2$, contradicting (2.8). Thus, $|A^-| = 1$, and hence $|A_2^-| + |B_2^-| \geq 3 > 2 = |A^-| + |B^-|$. On the other hand, $u_1 \in N_{A_2}(v_1) \cap A_2^=$ and $u \in N_{B_2}(v) \cap B_2^=$, which contradicts the maximum of $|A^-| + |B^-|$.

Let B_0 be a b-satisfactory subset of $(B \cup \{u\}) \setminus \{v\}$. Since G has no (a, b)-feasible pair, each a-satisfactory subset of $A \cup \{v\}$ must contain u by Claim 1, and so $d_A(u) = a(u) - 1$.

Since $v \notin B_0$, $e_G(u, B) \geq b(u) + 1$ and thus $d(u) \geq a(u) + b(u)$. Now, $d(v) = a(v) + b(v) - 1$ by (2.3), which contradicts Claim 3.

Case 2. In this case, we suppose $A \cap N(A^-) \subset A^+$, as $v_1 \in N(B^-) \cap B^=$. Since $A^- \neq A$ by (2.7), $|A^-| \geq 2$ by the degeneracy of A. Note that each vertex but v has at most two neighbors in A^- by (2.6) and $G \in \mathcal{G}$. The $(a-1)$-degeneracy of $A \setminus A^-$ guarantees the existence of two vertices, say x and y, in A^-, and a vertex, say z, with $N_A(x) \cap N_A(y) = \{z\}$ and $d_A(z) = a(z) + 1$. So, we have a quadrilateral $G[\{v, x, z, y\}]$.

Let w be a vertex in $\{x, y\}$. If (2.11) is not true, then

$$d_B(v) = b(v) - 1, \ (B \cup \{w\}) \setminus \{v\} \text{ is } (b-1)\text{-degenerate}, \tag{2.12}$$

and

$$(B \cup \{w\}) \setminus \{v'\} \text{ is } (b-1)\text{-degenerate for each } v' \in N_B(v). \tag{2.13}$$

Particularly, $(B \cup \{w\}) \setminus \{v_1\}$ is $(b-1)$-degenerate.

If $d(v) \geq a(v) + b(v)$, then $d(v') = a(v') + b(v') - 1$ for each vertex in $N(v)$ by (2.3). Let $A_3 = (A \cup \{v_1\}) \setminus \{w\}$ and $B_3 = (B \cup \{w\}) \setminus \{v_1\}$. Since $e_G(v_1, A) = a(v_1) - 1$, A_3 is $(a-1)$-degenerate, and so (A_3, B_3) is also a maximum $(a-1, b-1)$-degenerate partition as $\omega(A_3, B_3) - \omega(A, B) \geq (a(v_1) - 1) + b(w) + a(w) + b(v_1) - (a(w) - 1 + b(v_1) + b(w) + a(v_1)) = 0$. If $(N(v) \setminus \{v_1\}) \cap B^=$ has a vertex, say v', then $\{x, y\} \setminus \{w\} \subseteq A_3^-$, $z \in A_3^=$ (as $v_1 z \notin E(G)$ by $G \in \mathcal{G}$), $v \in B_3^-$ and $v' \in B_3^=$, giving $zv' \in E(G)$ by Claim 2, and then G contains $K_{2,3}$, a contradiction. So, $N(v) \cap B^= = \{v_1\}$. Now the $(b-1)$-degeneracy of B guarantees that $N(v_1) \cap B^= \neq \emptyset$, i.e., (2.9) holds. Since $|N(v_2) \cap N(v)| \leq 2$, we suppose that $xv_2 \notin E(G)$, and choose $w = x$. Now, (A_3, B_3) is a maximum $(a-1, b-1)$-degenerate partition such that $A_3^- = (A^- \cup \{v_1\}) \setminus \{x\}$ and $\{v, v_2\} \subseteq B_3^-$, contradicting (2.8).

So, we suppose that $d(v) = a(v) + b(v) - 1$. Now, $e_G(v, A) = a(v)$ by (2.12). Since $A \cup \{v\}$ has a-satisfactory subsets by (2.5), and since $e_G(v, A \setminus \{w\}) = a(v) - 1$, $(A \cup \{v\}) \setminus \{w\}$ is $(a-1)$-degenerate.

Let $A_4 = (A \cup \{v\}) \setminus \{w\}$ and $B_4 = (B \cup \{w\}) \setminus \{v\}$. Since $\omega(A_4, B_4) - \omega(A, B) \geq (a(v) - 1) + (b(w) - 1) + a(w) + b(v) - (b(v) - 1 + a(w) - 1 + a(v) + b(w)) = 0$, the maximality of $\omega(A, B)$ guarantees that (A_4, B_4) is also a maximum $(a-1, b-1)$-degenerate partition, $e_G(w, B) = b(w)$, $d_A(x) = a(x) - 1$ and $d_A(y) = a(y) - 1$.

If (2.9) holds, i.e., $d_B(v_2) = b(v_2)$, since $xv_2 \notin E(G)$ (as $G \in \mathcal{G}$), we choose $w = x$. Thus, $v_1 \in B_4^-$ and $v_2 \in N_{B_4}(v_1) \cap B_4^=$, and $v \in A_4^-$ and $y \in N_{A_4}(v) \cap A_4^=$, and so $yv_2 \in E(G)$ by Claim 2, contradicting $G \in \mathcal{G}$.

Suppose so that (2.10) holds. We may further assume that if $v' \in N_B(v) \cap B^{=}$, then $N_B(v') \setminus \{v\} \subseteq B^{+}$. Remember that $A_3 = (A \cup \{v_1\}) \setminus \{w\}$ and $B_3 = (B \cup \{w\}) \setminus \{v_1\}$. If A_3 is not $(a-1)$-degenerate, let A' be an a-satisfactory subset of A_3, since $N(v_1) \cap \{x, y, z\} = \emptyset$ (as $G \in \mathcal{G}$) and $d_A(z) = a(z) + 1$, $A' \subseteq (A \cup \{v_1\}) \setminus \{x, y, z\}$, and then $(A', (B \cup \{x, y, z\}) \setminus \{v_1\})$ is an (a, b)-feasible pair. So, A_3 is $(a-1)$-degenerate. By (2.13), (A_3, B_3) is also a maximum $(a-1, b-1)$-degenerate partition as $\omega(A_3, B_3) - \omega(A, B) \geq 0$. Now, we choose $w = x$. Since $N(v_1) \cap \{y, z\} = \emptyset$ and $xv_3 \notin E(G)$ as $G \in \mathcal{G}$, $y \in A_3^{-}$ and $z \in N(y) \cap A_3^{=}$, and $v \in B_3^{-}$ and $v_3 \in N(v) \cap B_3^{=}$, and so $v_3 z \in E(G)$ by Claim 2, and then G contains $K_{2,3}$, a contradiction. Therefore, (2.11) holds.

By symmetry, let B_0 be a b-satisfactory subset of $(B \cup \{x\}) \setminus \{v, v_1\}$. Let A' be an a-satisfactory subset of $A \cup \{v\}$ (such an A' exists by (2.5)). Since G has no (a, b)-feasible pair, $x \in A'$ by Claim 1, and so $d_A(x) = a(x) - 1$. Since $v \notin B_0$ and $x \in B_0$, $e_G(x, B) \geq b(x) + 1$, and thus $d(x) \geq a(x) + b(x)$. So, $d(v) = a(v) + b(v) - 1$ by (2.3), which contradicts Claim 3. This contradiction completes the proof of Theorem 1.6. ■

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图的 k 部划分的一个注记

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摘 要 设 $k \geq 2$ 是一个整数. 本文证明了任意有 m 条边的图都存在一个顶点的划分 $V_1, V_2, \ldots, V_k$, 使得 $e(V_1, V_2, \ldots, V_k) \geq \frac{k-1}{k}m + \frac{k-1}{2k}(\sqrt{2m+\frac{1}{4}} - \frac{1}{2}) - \frac{(k-2)^2}{8k}$, 且 $\max\{e(V_i) : 1 \leq i \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}(\sqrt{2m+\frac{1}{4}} - \frac{1}{2}) + \frac{3}{8} - \frac{7k-4}{8k^2}$. 我们的结果改进了 [Fan G., Hou J., Zeng Q., A bound for judicious k-partitions of graphs, *Discrete Appl. Math.*, 2014, **179**: 86–99] 的主要结论.

关键词 图的划分; 界; 图
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A Note on k-Partitions of Graphs

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Abstract Suppose that $k \geq 2$ is an integer. In this note, we prove that every graph with m edges admits a partition V_1, $V_2, \ldots, V_k$ such that $e(V_1, V_2, \ldots, V_k) \geq \frac{k-1}{k}m + \frac{k-1}{2k}(\sqrt{2m+\frac{1}{4}} - \frac{1}{2}) - \frac{(k-2)^2}{8k}$, and $\max\{e(V_i) : 1 \leq i \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}(\sqrt{2m+\frac{1}{4}} - \frac{1}{2}) + \frac{3}{8} - \frac{7k-4}{8k^2}$. This improves the main result of [Fan G., Hou J., Zeng Q., A bound for judicious k-partitions of graphs, *Discrete Appl. Math.*, 2014, **179**: 86–99].

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1 引言

设 G 是一个图, 而 $V_1, V_2, \ldots, V_k$ 是 $V(G)$ 的一个 k 部划分. 令 $e(V_i)$ 表示两个端点都在 V_i 的边的数目, 且令 $e(V_1, V_2, \ldots, V_k)$ 表示连接 $V_1, V_2, \ldots, V_k$ 之间的边的数目. 根据定义可知

$$e(V_1, V_2, \ldots, V_k) = |E(G)| - \sum_{i=1}^{k} e(V_i).$$

设 S 为 $V(G)$ 的一个子集, 我们用符号 $\bar{S}$ 表示 S 在 $V(G)$ 的补集, 即 $\bar{S} = V(G) \setminus S$.

记 $h(m) = \sqrt{2m + \frac{1}{4}} - \frac{1}{2}$. 1999 年, Bollobás 等 [1] 推广了 Edwards [4, 5] 的结果, 证明了:

定理 1.1 [1] 若 G 是一个有 m 条边的图, 则 $V(G)$ 存在一个二部划分 V_1, V_2, 使得

$$e(V_1, V_2) \geq \frac{m}{2} + \frac{1}{4}h(m) \quad \text{且} \quad \max\{e(V_i) : 1 \leq i \leq 2\} \leq \frac{m}{4} + \frac{1}{8}h(m).$$

后来, Bollobás 和 Scott [3] 证明了任意包含 m 条边的图都存在一个 k 部划分 $V_1, V_2, \ldots, V_k$, 使得

$$e(V_1, V_2, \ldots, V_k) \geq \frac{k-1}{k}m + \frac{k-1}{2k}h(m) - \frac{(k-2)^2}{8k}, \tag{1.1}$$

且文 [1] 还证明了任意包含 m 条边的图都存在一个 k 部划分 $V_1, V_2, \ldots, V_k$, 使得

$$\max\{e(V_i) : 1 \leq i \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}h(m). \tag{1.2}$$

受到定理 1.1, (1.1) 和 (1.2) 式的启发, Bollobás 和 Scott [2] 提出了以下有趣的问题.

问题 1.1 [2] 是否任意包含 m 条边的图都存在一个 k 部划分 V_1, $V_2, \ldots, V_k$, 使得 (1.1) 和 (1.2) 式同时成立?

根据定理 1.1, $k = 2$ 时问题 1.1 的答案是肯定的, 但对于 $k \geq 3$ 的情况而言问题 1.1 的答案至今仍然还是一个谜. 在此方向上, Xu 和 Yu [8, 9] 证明了, 任意包含 m 条边的图都存在一个接近 (1.1) 式且满足 (1.2) 式的 k 部划分, 即

定理 1.2 [8, 9] 若 G 是一个有 m 条边的图且 $k \geq 2$ 是一个整数, 则 $V(G)$ 存在一个 k 部划分 V_1, $V_2, \ldots, V_k$, 使得

$$e(V_1, V_2, \ldots, V_k) \geq \frac{k-1}{k}m + \frac{k-1}{2k}h(m) - \frac{17k}{8},$$

且 (1.2) 式成立.

后来, Fan 等人 [6] 证明了任意包含 m 条边的图都存在一个满足 (1.1) 式且接近 (1.2) 式的 k 部划分, 即

定理 1.3 [6] 若 G 是一个有 m 条边的图且 $k \geq 2$ 是一个整数, 则 $V(G)$ 存在一个 k 部划分 $V_1, V_2, \ldots, V_k$, 使得 (1.1) 式且

$$\max\{e(V_i) : 1 \leq i \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}h(m) + \frac{2}{3}$$

成立.

最近, 本文的作者 [7] 改进了定理 1.2 的结果, 证明了:

定理 1.4 [7] 若 G 是一个有 m 条边的图且 $k \geq 2$ 是一个整数, 则 $V(G)$ 存在一个 k 部划分 $V_1, V_2, \ldots, V_k$, 使得

$$e(V_1, V_2, \ldots, V_k) \geq \frac{k-1}{k}m + \frac{k-1}{2k}h(m) - \frac{(k-2)^2}{2(k-1)},$$

且 (1.2) 式成立.

进一步, 在文 [7] 中还证明了以下的结论:

定理 1.5 [7] 设 G 是一个有 m 条边的图且 $k \geq 2$ 是一个整数. 若 $m \geq \frac{9}{128}k^4(k-2)^2$ 且 G 最多包含 $\frac{1}{k}h(m) - \frac{1}{8}(3k^2 - 6k - 11)$ 个度为 k 的倍数的顶点, 则 $V(G)$ 存在一个 k 部划分 V_1, $V_2, \ldots, V_k$, 使得 (1.1) 和 (1.2) 式同时成立.

本文的主要结果是下面的定理, 该结果改进了定理 1.3 的结论:

定理 1.6 若 G 是一个有 m 条边的图且 $k \geq 2$ 是一个整数, 则 $V(G)$ 存在一个 k 部划分 $V_1, V_2, \ldots, V_k$, 使得 (1.1) 式且

$$\max\{e(V_i) : 1 \leq i \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}h(m) + \frac{3}{8} - \frac{7k-4}{8k^2}$$

成立.

2 定理 1.6 的证明

定理 1.6 的证明方法与文 [6–9] 中的证明方法类似, 只是加进了更精细的分析. 先介绍以下三个引理.

引理 2.1 [8] 若 $m' \leq \frac{(k-1)^2}{k^2}m + \frac{k-1}{2k^2}h(m)$, 则

$$\frac{m'}{(k-1)^2} + \frac{k-2}{2(k-1)^2}h(m') \leq \frac{m}{k^2} + \frac{k-1}{2k^2}h(m).$$

引理 2.2 [7] 若 G 是一个有 m 条边的图, 且 V_1, V_2, …, V_k 是 $V(G)$ 的一个使得 $e(V_1, V_2, \ldots, V_k)$ 达到极大的 k 部划分, 则

$$\max\{e(V_j) : 1 \leq j \leq k\} \leq \max\left\{0, \frac{8m - (k-1)(k-2)}{2(k^2+5k-2)}\right\}, \tag{2.1}$$

且若 $m < k(k+1)$, 则

$$\max\{e(V_j) : 1 \leq j \leq k\} \leq \frac{m}{k^2} + \frac{k-1}{2k^2}h(m). \tag{2.2}$$

引理 2.3 [7] 设 δ, k, m 是三个使得 $k \geq 3$ 和 $m \geq k(k+1)$ 成立的正整数, 而 α 是一个满足条件

$$0 < \alpha \leq \frac{(3k-2)(k-1)}{k^2(k^2+5k-2)}m - \frac{(k-1)(k-2)}{2(k^2+5k-2)}$$

的实数. 令

$$f(x) = \frac{x - (k-2)(\alpha-\delta)}{k-1} + \frac{k-2}{2(k-1)}\sqrt{\frac{2(k^2-1)}{k^2}m - 2x - 2(\alpha-\delta) + \frac{1}{4}}$$
$$- \frac{2m}{k^2} - \frac{k-1}{2k}\sqrt{2m + \frac{1}{4}} + \frac{(k+1)(k-2)}{8k(k-1)},$$

则当 $x \le \frac{k^2-1}{k^2}m-\alpha-(k-2)\delta$ 时, $f(x)$ 是一个凸函数, $\varphi(\alpha)=f(2(k-1)(\frac{m}{k^2}+\alpha)-(k-2)\delta)$ 是一个 α 的严格增函数, 且 $f(\frac{k^2-1}{k^2}m-\alpha-(k-2)\delta)\ge 0$.

定理 1.6 的证明 我们将对 k 使用数学归纳法来证. 由定理 1.1 可知 $k=2$ 时结论成立. 下文中假设 $k\ge 3$, 且根据 (2.2) 式假设 $m\ge k(k+1)$. 令 $V_1,V_2,\dots,V_k$ 是一个满足 (1.1) 式和

$$|N(v)\cap\overline{V_1}|\ge(k-1)|N(v)\cap V_1| \tag{2.3}$$

对于任意 $v\in V_1$ 都成立的条件下, 使得 $e(V_1)=\max\{e(V_i):1\le i\le k\}$ 达到极小的 k 部划分.

令 $e(V_1)=\frac{m}{k^2}+\alpha$, 则根据 (2.1) 式可设

$$\frac{k-1}{2k^2}\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)+\frac{3}{8}-\frac{7k-4}{8k^2}<\alpha\le\frac{(3k-2)(k-1)}{k^2(k^2+5k-2)}m-\frac{(k-1)(k-2)}{2(k^2+5k-2)}. \tag{2.4}$$

令 $H=G[V_1]$. 记 δ 为 H 中最小的非零度, 且设 v 是 H 中度等于 δ 的顶点. 令 $W_1=V_1-v$, 于是 $\overline{W_1}=\overline{V_1}+v$. 此时,

$$e(W_1)=e(V_1)-\delta=\frac{m}{k^2}+\alpha-\delta, \tag{2.5}$$

$$e(W_1,\overline{W_1})\ge 2(k-1)e(V_1)-(k-2)\delta, \tag{2.6}$$

且对于任意的 $w\in W_1$, 都有

$$|N(w)\cap\overline{W_1}|\ge|N(w)\cap\overline{V_1}|\ge(k-1)|N(w)\cap V_1|\ge(k-1)|N(w)\cap W_1|. \tag{2.7}$$

令 $m'=m-e(W_1)-e(W_1,\overline{W_1})$. 由 (2.5) 和 (2.6) 式可知

$$m'\le\frac{(k-1)^2}{k^2}m-(2k-1)\alpha+(k-1)\delta. \tag{2.8}$$

由归纳假设前提, $\overline{W_1}$ 存在一个 $k-1$ 部划分 $W_2,\dots,W_k$, 使得

$$\max\{e(W_i):2\le i\le k\}\le\frac{m'}{(k-1)^2}+\frac{k-2}{2(k-1)^2}h(m')+\frac{3}{8}-\frac{7k-11}{8(k-1)^2}, \tag{2.9}$$

$$e(W_2,W_3,\dots,W_k)\ge\frac{k-2}{(k-1)}m'+\frac{k-2}{2(k-1)}h(m')-\frac{(k-3)^2}{8(k-1)}. \tag{2.10}$$

令 $x=e(W_1,\overline{W_1})$. 因为 $m'=m-e(W_1)-x=\frac{k^2-1}{k^2}m-\alpha+\delta-x$, 所以由 (2.10) 式可得

$$\begin{aligned}e(W_1,W_2,\dots,W_k)&=e(W_1,\overline{W_1})+e(W_2,\dots,W_k)\\&\ge x+\frac{k-2}{(k-1)}m'+\frac{k-2}{2(k-1)}h(m')-\frac{(k-3)^2}{8(k-1)}\\&=\frac{k-1}{k}m+\frac{k-1}{2k}h(m)-\frac{(k-2)^2}{8k}+f(x),\end{aligned} \tag{2.11}$$

其中 $f(x)$ 恰好就是引理 2.3 中所定义的函数.

因为 $e(\overline{W_1})=e(\overline{V_1})+|N(v)\cap\overline{V_1}|\ge(k-1)\delta$, 所以

$$x=e(W_1,\overline{W_1})=m-e(W_1)-e(\overline{W_1})\le\frac{k^2-1}{k^2}m-\alpha-(k-2)\delta.$$

结合 (2.6) 式可得

$$a\le x\le b,$$

其中 $a=2(k-1)(\frac{m}{k^2}+\alpha)-(k-2)\delta$, 且 $b=\frac{k^2-1}{k^2}m-\alpha-(k-2)\delta$.

下面将证明 W_1, W_2, $W_3,\ldots,W_k$ 满足 (1.1) 式. 根据引理 2.3 可知 $f(x)$ 是一个凸函数, $f(\frac{k^2-1}{k^2}m-\alpha-(k-2)\delta)\geq 0$, 且 $\varphi(\alpha):=f(a)$ 是一个 α 的严格增函数.

由 $\varphi(\alpha):=f(a)$ 可知

$$\begin{aligned}\varphi(\alpha)=&\frac{k}{k-1}\alpha+\frac{k-2}{2(k-1)}\sqrt{\frac{2(k-1)^2}{k^2}m-(4k-2)\alpha+2(k-1)\delta+\frac{1}{4}}\\&-\frac{k-1}{2k}\sqrt{2m+\frac{1}{4}}+\frac{(k+1)(k-2)}{8k(k-1)}.\end{aligned}$$

根据 (2.4) 式, 有

$$\begin{aligned}\alpha>&\frac{k-1}{2k^2}\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)+\frac{3}{8}-\frac{7k-4}{8k^2}\\\geq&\frac{k-1}{2k^2}\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)+\frac{5}{36},\end{aligned}$$

所以

$$\begin{aligned}\varphi(\alpha)>&\frac{k-2}{2(k-1)}\sqrt{\frac{2(k-1)^2}{k^2}m-(4k-2)\left(\frac{k-1}{4k^2}\left(\sqrt{8m+1}-1\right)+\frac{5}{36}\right)+2(k-1)+\frac{1}{4}}\\&+\frac{1}{4k}\left(\sqrt{8m+1}-1\right)+\frac{3k-4}{8k}-\frac{k-1}{4k}\sqrt{8m+1}+\frac{(k+1)(k-2)}{8k(k-1)}\\=&\frac{k-2}{4k(k-1)}\sqrt{8(k-1)^2m-2(2k-1)(k-1)\sqrt{8m+1}+\frac{52k^3-17k^2-54k+18}{9}}\\&-\frac{k-2}{4k}\sqrt{8m+1}+\frac{(2k-1)(k-2)}{4k(k-1)}\\=&\frac{k-2}{4k(k-1)}\sqrt{\left((k-1)\sqrt{8m+1}-(2k-1)\right)^2+\frac{2k^2(26k-31)}{9}}\\&-\frac{k-2}{4k}\sqrt{8m+1}+\frac{(2k-1)(k-2)}{4k(k-1)}\\>&\frac{(k-2)\left((k-1)\sqrt{8m+1}-(2k-1)\right)}{4k(k-1)}-\frac{k-2}{4k}\sqrt{8m+1}+\frac{(2k-1)(k-2)}{4k(k-1)}\\=&0.\end{aligned}$$

再由 (2.11) 式可知 $W_1,W_2,W_3,\ldots,W_k$ 满足 (1.1) 式. 又因为 $W_1,W_2,W_3,\ldots,W_k$ 也满足 (2.7) 式, 且 $e(W_1)=e(V_1)-\delta<e(V_1)$, 所以

$$\max\{e(W_i):1\leq i\leq k\}\neq e(W_1).$$

若 $\delta\leq\frac{2k-1}{k-1}\alpha+\frac{1}{2k^2}h(m)$, 则根据 (2.8) 式可知

$$m'\leq\frac{(k-1)^2}{k^2}m+\frac{k-1}{2k^2}h(m).$$

再根据引理 2.1 和 (2.9) 式, 可得

$$\max\{e(W_i):1\leq i\leq k\}\leq\frac{m}{k^2}+\frac{k-1}{2k^2}h(m)+\frac{3}{8}-\frac{7k-4}{8k^2}.$$

若 $\delta > \frac{2k-1}{k-1}\alpha + \frac{1}{2k^2}h(m)$, 则根据 (2.4) 式可得 $\delta > \frac{h(m)}{k}$. 因为 V_1 至少包含 $\delta+1$ 个度至少为 δ 的顶点, 所以根据 (2.3) 式可知

$$e(W_1, \overline{W_1}) \geq \delta + (k-1)\delta^2.$$

注意到

$$e(W_1) = e(V_1) - \delta \geq \frac{\delta(\delta-1)}{2} \quad \text{且} \quad 2m = (h(m))^2 + h(m).$$

所以

$$\begin{aligned} m' &= m - e(W_1) - e(W_1, \overline{W_1}) \\ &\leq m - \frac{1}{2}\delta(\delta+1) - (k-1)\delta^2 \\ &< \frac{(k-1)^2}{k^2}m + \frac{k-1}{2k^2}h(m). \end{aligned}$$

现在, 根据引理 2.1 和 (2.9) 式可知

$$\max\{e(W_i) : 1 \leq i \leq k\} < \frac{m}{k^2} + \frac{k-1}{2k^2}h(m) + \frac{3}{8} - \frac{7k-4}{8k^2}.$$

于是, $W_1, W_2, W_3, \ldots, W_k$ 就是满足定理 1.6 的一个 k 部划分. 证毕.

注 2.4 似乎沿用文 [6–9] 和本文所用到的处理方法或者对现有方法进行更精细的分析都很难得到问题 1.1 的解答. 那么, 我们能否先对最小度满足 $\delta(G) = O(|V(G)|)$ 的图类进行研究, 来探索问题 1.1 的解答? 兴许该问题的答案恰恰就是要解决问题 1.1 的症结所在.

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Ordering (signless) Laplacian spectral radii with maximum degrees of graphs☆

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Ordering

ABSTRACT

Let $\lambda(G)$ and $\mu(G)$ be the Laplacian and signless Laplacian spectral radius of a graph G, respectively, and let $\Delta(G)$ be the maximum degree of G. We call a graph G an (n, m) graph if G contains n vertices and m edges. In this paper, we prove that for two connected (n, m) graphs G and G', if $\Delta(G) \geq m - \frac{n-3}{2}$ and $\Delta(G) > \Delta(G')$, then $\lambda(G) > \lambda(G')$ and $\mu(G) > \mu(G')$, and the bound "$m - \frac{n-3}{2}$" is optimal for the case of signless Laplacian spectral radius. Moreover, we use an example to illustrate that, as a consequence of our new result, when $m \leq \lfloor \frac{3n-5}{2} \rfloor$, the ordering of connected (n, m) graphs according to their largest (signless) Laplacian spectral radii can be transfer to the ordering of connected (n, m) graphs with large maximum degree and hence we can conclude that it is not a difficult problem to ordering connected (n, m) graphs via their largest (signless) Laplacian spectral radii.
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1. Introduction

Throughout the paper, $G = (V, E)$ is an undirected simple graph with $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. Sometimes, G is also referred to be an (n, m) graph. Let $N(v)$ be the neighbor vertex set of v. Then, $d(v) = |N(v)|$ is called the degree of v. A pendant vertex of G is a vertex of degree 1, and we use the notation $\Delta(G)$ to denote the maximum degree of G. Let $D(G)$ be the diagonal matrix of vertex degrees, and $A(G)$ be the adjacency matrix of G. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$. It is well known that $L(G)$ is positive semidefinite [7] so that its eigenvalues can be arranged as follows:

$$\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0.$$

The maximum eigenvalue of $L(G)$, namely $\lambda_1(G)$, is called the Laplacian spectral radius of G and denoted by $\lambda(G)$.

The *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. It is proved that $Q(G)$ is also positive semidefinite, and, when G is connected, it is irreducible [5]. Thus, its eigenvalues can be arranged as:

$$\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) \geq 0.$$

The maximum eigenvalue of $Q(G)$ is called the signless Laplacian spectral radius of G, and denoted by $\mu(G)$, i.e., $\mu(G) = \mu_1(G)$.

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Recall that a connected graph G of order n is called a tree, unicyclic and bicyclic graph if G has $n-1$, n and $n+1$ edges, respectively. The investigation on the spectra of graphs is an important topic in the graph theory. As early as 1980, several graph spectra, namely, spectra of $A(G)$, $L(G)$ and $Q(G)$, had been systematically studied in [2]. In 1981, Cvetković [1] indicated 12 directions in further investigations of graph spectra, one of which is classifying and ordering graphs. Hence, ordering graphs with various properties by their spectra, becomes an attractive topic (see [4–6,9–11]). Up to now, a simple and generality method to ordering graphs according to their spectra has not yet been obtained. An interesting problem would be whether we can transfer the comparison of spectra of two graphs to the comparison of some parameters of them. If this problem is solved, then (as we show in the following) the comparison of spectra of two graphs will become much easier. In this line, Yuan, Shan and Liu [11] proved that "Let T and T' be two trees on n vertices ($n \geq 6$). If $\Delta(T) \geq \lceil \frac{n}{2} \rceil + 1$ and $\Delta(T) > \Delta(T')$, then $\lambda(T) > \lambda(T')$". Two years later, Yuan, Liu and Han [10] improved the bound "$\lceil \frac{n}{2} \rceil + 1$" to "$\lceil \frac{11n}{30} \rceil + 1$", and they also showed that the later bound is the best possible.

By Yuan's result, if the maximum degrees of two trees on n vertices are at least $\lceil \frac{11n}{30} \rceil + 1$, then the comparison of the Laplacian spectral radii of two trees can be transfer to the comparison of the maximum degrees of them. Precisely, the tree with larger maximum degree also has larger Laplacian spectral radius. Moreover, among trees on n vertices, the Laplacian spectral radius of a tree with maximum degree not larger than $\lceil \frac{11n}{30} \rceil$ is always smaller than that of the tree with maximum degree at least $\lceil \frac{11n}{30} \rceil + 1$. So, the ordering of trees according to their largest Laplacian spectral radii can be transferred to the ordering of trees with large maximum degree, and hence we can conclude that, as illustrated for the Laplacian spectral radii of bicyclic graphs in the sequel, it is not a difficult problem to ordering trees via their largest Laplacian spectral radii. In this paper, we obtain a similar result for the (signless) Laplacian spectral radius of the generality connected (n, m) graph, and our main result is as follows.

Theorem 1.1. *Let G and G' be two connected (n, m) graphs. If $\Delta(G) \geq m - \frac{n-3}{2}$ and $\Delta(G) > \Delta(G')$, then $\lambda(G) > \lambda(G')$ and $\mu(G) > \mu(G')$.*

In Theorem 1.1, by setting $m = n$ and $m = n + 1$, respectively, we have

Corollary 1.1. (1) *Let G and G' be two unicyclic graphs on n vertices. If $\Delta(G) \geq \frac{n+3}{2}$ and $\Delta(G) > \Delta(G')$, then $\lambda(G) > \lambda(G')$ and $\mu(G) > \mu(G')$;* (2) *Let G and G' be two bicyclic graphs on n vertices. If $\Delta(G) \geq \frac{n+5}{2}$ and $\Delta(G) > \Delta(G')$, then $\lambda(G) > \lambda(G')$ and $\mu(G) > \mu(G')$.*

Remark 1.1. For the case of signless Laplacian spectral radius, the bound "$m - \frac{n-3}{2}$" of Theorem 1.1 (or Corollary 1.1) is optimal. To see this, let G_1 and G_1' be the unicyclic graphs on seven vertices as shown in Fig. 1, and let G_2 and G_2' be the bicyclic graphs on nine vertices as shown in Fig. 1. Note that $\Delta(G_1) = 4 > 3 = \Delta(G_1')$ and $\Delta(G_2) = 6 > 5 = \Delta(G_2')$. But $\mu(G_1) < 5.21 < 5.26 < \mu(G_1')$, and $\mu(G_2) < 7.2015 < 7.2019 < \mu(G_2')$.

Let $B_1, \ldots, B_{11}$ denote the bicyclic graphs on n vertices as shown in Fig. 2. Let $\mathcal{B}_n$ be the class of connected bicyclic graphs on n vertices. It is easily checked that B_1 and B_2 are all the bicyclic graphs with $\Delta = n - 1$, and $B_3, B_4, \ldots, B_{11}$ are all the bicyclic graphs with $\Delta = n-2$. By Corollary 1.1 (or Theorem 1.1), if $n \geq 9$, since $n-2 \geq \frac{n+5}{2}$, $\lambda(B_{11}) > \lambda(B)$ for every bicyclic graph B with $\Delta(B) \leq n - 3$. By applying the characteristic polynomials method, it is readily proved that $\lambda(B) < \lambda(B_{11}) = \lambda(B_{10}) < \lambda(B_9) < \lambda(B_8) < \lambda(B_7) < \lambda(B_6) = \lambda(B_5) < \lambda(B_4) < \lambda(B_3) < \lambda(B_2) = \lambda(B_1)$ for any $B \in \mathcal{B}_n$. This orderings had been proved in [4,9], while with much more difficult methods. Actually, with the similar reason, one can easily see that the possible candidates of bicyclic graphs, which have the ninth largest Laplacian spectral radii among $\mathcal{B}_n$, where $n \geq 11$, are the bicyclic graphs with maximum degree $\Delta = n - 3$. Moreover, by Corollary 1.1 (or Theorem 1.1), we can also employ the analogous method to deal with the ordering of bicyclic graphs according to their largest signless Laplacian spectral radii.

Fortunately, when $m \leq \lfloor \frac{3n-5}{2} \rfloor$, this approach can be extended to the general connected (n, m) graphs by Theorem 1.1. Thus, when $m \leq \lfloor \frac{3n-5}{2} \rfloor$, the ordering of connected (n, m) graphs according to their largest (signless) Laplacian spectral radii can be transfer to the ordering of connected (n, m) graphs with large maximum degree and hence we can conclude that it is not a difficult problem to ordering connected (n, m) graphs via their largest (signless) Laplacian spectral radii.

For the relation between $\mu(G)$ and $\lambda(G)$, it is well-known that

Theorem 1.2 *([7]). If G is connected, then $\lambda(G) \leq \mu(G)$, where the equality holds if and only if G is bipartite.*

By Theorem 1.2, the signless Laplacian spectral radius is not less than the Laplacian spectral radius of the same graph, and the equality can be achieved uniquely by the bipartite graphs. Generally, when $G \neq G'$, the size relationship between $\lambda(G)$ and $\mu(G')$ is uncertain. However, when $\Delta(G) \geq m - \frac{n-3}{2}$ and $\Delta(G) > \Delta(G')$, we have

Theorem 1.3. *Let G and G' be two connected (n, m) graphs. If $\Delta(G) \geq m - \frac{n-3}{2}$ and $\Delta(G) > \Delta(G')$, then $\lambda(G) > \mu(G')$.*

Now, one can easily see that Theorem 1.1 follows from Theorems 1.2 and 1.3. Thus, the remaining task of this work is to show Theorem 1.3.

Remark 1.2. The bound "$m - \frac{n-3}{2}$" of Theorem 1.3 is optimal. To see this, let G_2 and G_2' be the bicyclic graphs on nine vertices as shown in Fig. 1. By Remark 1.1 and Theorem 1.2, though $\Delta(G_2) = 6 > 5 = \Delta(G_2')$, $\lambda(G_2) < \mu(G_2')$.

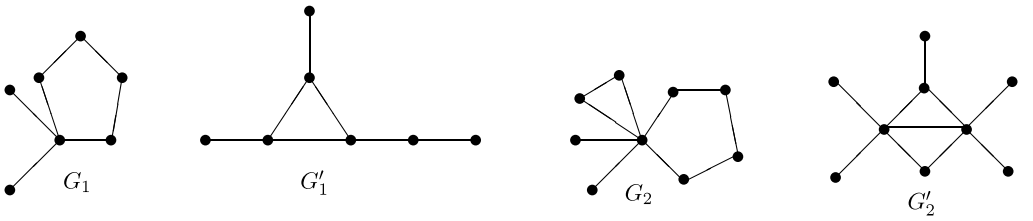


Fig. 1. The graphs G_1, G_1', G_2 and G_2'.

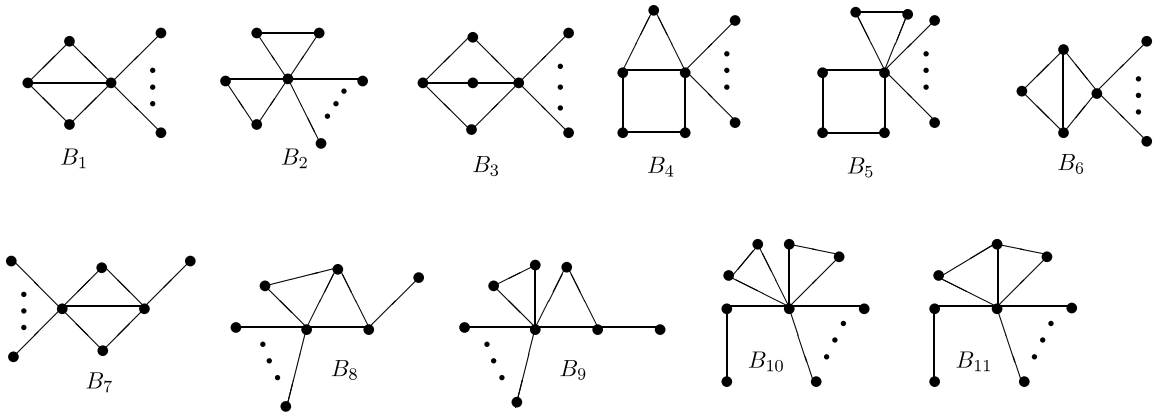


Fig. 2. The bicyclic graphs $B_1, B_2, \ldots, B_{11}$.

Remark 1.3. Remark 1.1 implies that the bound "$m - \frac{n-3}{2}$" is the best possible for the case of signless Laplacian spectral radius, but we do not know whether it is also optimal for the case of Laplacian spectral radius. Since the proof of Theorem 1.1 depends on Theorems 1.2 and 1.3. By Remark 1.2, it cannot improve the bound "$m - \frac{n-3}{2}$" in Theorem 1.1 by using our approach.

2. The proof of Theorem 1.3

The following is a well known lower bound for the Laplacian spectral radius.

Lemma 2.1 ([7]). *Let G be a graph with at least one edge, then $\lambda(G) \geq \Delta(G) + 1$. Moreover, if G is connected, then equality holds if and only if $\Delta(G) = n - 1$.*

Let $m(u)$ denote the average of the degrees of the vertices adjacent to vertex u of a connected graph, namely, $m(u) = \sum_{v \in N(u)} d(v)/d(u)$. A semiregular bipartite graph $G = (V, E)$ is a bipartite graph with bipartition (V_1, V_2) of V such that all vertices in V_i have the same degree k_i for $i = 1, 2$. In 2004, Das proved the next bound, which was shown to be an upper bound for $\lambda(G)$ by Merris [8] in 1998, was also suitable for $\mu(G)$.

Lemma 2.2 ([3]). *If G is a connected graph, then $\mu(G) \leq \max\{d(v) + m(v) : v \in V\}$, and equality holds if and only if G is either a regular graph or a semiregular bipartite graph.*

Actually, Lemma 2.2 can be slightly improved to be

Proposition 2.1. *Suppose G is a connected graph with $n \geq 3$ vertices. Then, $\mu(G) \leq \max\{d(v) + m(v) : v \in V$ and $d(v) > 1\}$, and equality holds if and only if G is either a regular graph or a semiregular bipartite graph.*

Proof. Suppose $\mu(G) > \max\{d(v) + m(v) : v \in V$ and $d(v) > 1\}$. By Lemma 2.2, we may let u be a pendent vertex of G such that $d(u) + m(u) = \max\{d(v) + m(v) : v \in V\}$. By Lemmas 2.1–2.2, $1 + \Delta(G) \leq \lambda(G) \leq \mu(G) \leq 1 + m(u) \leq 1 + \Delta(G)$, and hence $\mu(G) = \lambda(G) = 1 + \Delta(G)$. Now, Lemma 2.1 and Theorem 1.2 imply that G is bipartite with $\Delta(G) = n - 1$. So, $G \cong K_{1,n-1}$, and then $n = \mu(G) > \max\{d(v) + m(v) : v \in V$ and $d(v) > 1\} = n$, a contradiction. Thus, $\mu(G) \leq \max\{d(v) + m(v) : v \in V$ and $d(v) > 1\}$, and the result follows from Lemma 2.2. ■

Lemma 2.3. *Let G be a connected (n, m) graph. If $u \in V(G)$, then*

$$m(u) \leq \frac{2m - (n-1)}{d(u)},$$

where the equality holds if and only if for every vertex $w \neq u$, if $w \notin N(u)$, then w is a pendant vertex and adjacent to some vertex of $N(u)$.

Proof. Note that $2m = \sum_{v\in N(u)} d(v)+\sum_{v\notin N(u)} d(v) \geq \sum_{v\in N(u)} d(v)+d(u)+(n-d(u)-1)$. Thus, $m(u) = \sum_{v\in N(u)} d(v)/d(u) \leq \frac{2m-(n-1)}{d(u)}$.

It is easy to see that the equality holds if and only if for every vertex w, if $w \notin N(u)$, then w is a pendant vertex and adjacent to some vertex of $N(u)$. ■

Proposition 2.2. *Let G be a connected graph with $n \geq 4$ vertices and m edges. Then,*

$$\lambda(G) \leq \mu(G) < \max\left\{\Delta(G), m - \frac{n-1}{2}\right\} + 2.$$

Proof. Set $k = \max\left\{\Delta(G), m - \frac{n-1}{2}\right\}$.

Fact 1. $\mu(G) \leq k + 2$.

Let u be a vertex of G such that $d(u) > 1$ and $d(u)+m(u) = \max\{d(v)+m(v) : v \in V(G) \text{ and } d(v) > 1\}$. By Proposition 2.1 and Lemma 2.3, it suffices to show that

$$d(u) + m(u) \leq d(u) + \frac{2m-(n-1)}{d(u)} \leq k + 2.$$

Let $f(x) = x + \frac{(2m-n+1)}{x}$, where $2 \leq x \leq \Delta$. Then, $f(x)$ is a concave function for $x \geq 2$, and so

$$f(x) \leq \max\left\{2 + \frac{2m-(n-1)}{2}, \Delta + \frac{2m-(n-1)}{\Delta}\right\} \leq \max\left\{2 + \frac{2m-(n-1)}{2}, \Delta + 2\right\}.$$

So, Fact 1 is true.

Fact 2. $\mu(G) \neq k + 2$.

Assume, by contradiction, that $\mu(G) = k + 2$. By the proof of Fact 1, we have

$$\mu(G) = d(u) + m(u) = d(u) + \frac{2m-(n-1)}{d(u)} = k + 2.$$

Then, Proposition 2.1 implies that G is either a regular graph or a semiregular bipartite graph. We consider the next two cases.

Case 1. G is a regular graph.

Then, $\mu(G) = 2\Delta(G)$ follows from Proposition 2.1.

If $\Delta(G) \geq m - \frac{n-1}{2}$, then $2\Delta(G) = \mu(G) = k + 2 = \Delta(G) + 2$. Thus, $\Delta(G) = 2$, and hence $G = C_n$. On the other hand, we have $2 = \Delta(G) \geq m - \frac{n-1}{2} = n - \frac{n-1}{2}$, which implies that $n \leq 3$. It is a contradiction to the hypothesis $n \geq 4$.

If $\Delta(G) \leq m - \frac{n-1}{2}$, then $2\Delta(G) = \mu(G) = k + 2 = m - \frac{n-1}{2} + 2$, namely, we have

$$4\Delta(G) = n\Delta(G) - 2\left(\frac{n-1}{2}\right) + 4,$$

which implies that $\Delta(G) = \frac{n-5}{n-4} < 1$, a contradiction.

Case 2. G is a semiregular bipartite graph.

Recall that $d(u)+m(u) = d(u)+\frac{2m-(n-1)}{d(u)}$. By Lemma 2.3, for every vertex $w \neq u$, if $w \notin N(u)$, then w is a pendant vertex and adjacent to some vertex of $N(u)$. Moreover, since G is a semiregular bipartite graph, we can conclude that $wu \in E(G)$ holds for every vertex $w \neq u$, and hence $G \cong K_{1,n-1}$. Thus, $m = n - 1$. Note that $\Delta(K_{1,n-1}) = n - 1 > \frac{n-1}{2} = m - \frac{n-1}{2}$. Then, $k = \Delta(K_{1,n-1})$, and hence $n = \mu(K_{1,n-1}) = k + 2 = \Delta(K_{1,n-1}) + 2 = n + 1$, a contradiction.

By combining Facts 1, 2, and Theorem 1.2, the result holds. ■

Proof of Theorem 1.3. If $n \leq 3$, it is easy to check that the result follows. Thus, we may suppose that $n \geq 4$ in the following. If $\Delta(G') \leq m - \frac{n-1}{2}$, by Proposition 2.2 and Lemma 2.1, it follows that $\lambda(G) \geq \Delta(G) + 1 \geq m - \frac{n-3}{2} + 1 > \mu(G')$. If $\Delta(G') \geq m - \frac{n-1}{2}$, by Proposition 2.2 and Lemma 2.1, we have $\lambda(G) \geq \Delta(G) + 1 \geq \Delta(G') + 2 > \mu(G')$. ■

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SCIENCE CHINA
Mathematics

• ARTICLES •

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Bipartition of graph under degree constraints

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Abstract Let G be a graph, let s be a positive integer, and let X be a subset of $V(G)$. Denote $\delta(X)$ to be the minimum degree of the subgraph $G[X]$ induced by X. A partition (X, Y) of $V(G)$ is called s-good if $\min\{\delta(X), \delta(Y)\} \geqslant s$. In this paper, we strengthen a result of Maurer and a result of Arkin and Hassin, and prove that for any positive integer k with $2 \leqslant k \leqslant |V(G)| - 2$, every connected graph G with $\delta(G) \geqslant 2$ admits a 1-good partition (X, Y) such that $|X| = k$ and $|Y| = |V(G)| - k$, and $\delta(X) + \delta(Y) \geqslant \delta(G) - 1$.

Keywords partition of graph, degree constraint, minimum degree

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1 Introduction

All graphs considered in this paper are finite and simple. Let G be a graph, let X be a subset of $V(G)$. We use $G[X]$ to denote the subgraph of G induced by X, and simply write $\delta(G[X])$ as $\delta(X)$, where $\delta(G[X])$ denotes the minimum degree of $G[X]$. Let $E(X) = E(G[X])$ and $e(X) = |E(X)|$. For a vertex u of G, we use $N_X(u)$ to denote the set of neighbors of u in X and simply write $N_G(u)$ as $N(u)$ if there is no danger of confusion. Let $d_X(u) = |N_X(u)|$ whenever $u \in X$, and simply write $d(x)$ instead of $d_G(x)$ if $X = V(G)$. For two subsets X and Y of $V(G)$, we use $e(X, Y)$ to denote the number of edges with one end in X and the other in Y. Let r be a real number. As usual, we use $\lfloor r \rfloor$ to denote the biggest integer that is less than or equal to r, and use $\lceil r \rceil$ to denote the smallest integer not less than r.

A partition (X, Y) of G is a splitting of $V(G)$ into two disjoint subsets X and Y. Let s and t be two nonnegative integers, and let $g(s, t)$ be the smallest integer such that every graph of minimum degree at least $g(s, t)$ admits a partition (X, Y) such that $\delta(X) \geqslant s$ and $\delta(Y) \geqslant t$. Thomassen [17], and Szegedy independently (see [7]) proved the existence of $g(s, t)$, and Hajnal [7] improved the bound to $g(s, t) \leqslant t + 2s - 3$ while $s \geqslant 4$. Confirming a conjecture of Thomassen [17], Stiebitz [16] proved, with an elegant argument, that $g(s, t) \leqslant s + t + 1$. Stiebitz also asked if $g(s, t) \leqslant s + t$ on triangle-free graphs when $s \geqslant 1$ and $t \geqslant 1$ (it is natural to ask such kind of questions since many parameters can be greatly strengthened on subfamily of graphs, see, e.g., [4, 11, 18]).

Kaneko [8] answered Stiebitz's question in the affirmative. Diwan [5], and Gerber and Kobler [6] in its function form, showed that $g(s, t) \leqslant s + t - 1$ on graphs with neither triangles nor quadrilaterals when $s \geqslant 2$ and $t \geqslant 2$. Recently, the current authors [12] further generalized Kaneko's result to graphs without

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$K_4 - e$, and generalized Diwan's result to triangle-free graphs in which no two quadrilaterals share edges. Stiebitz's idea plays a key role in all of the proofs of [5, 6, 8, 12, 16].

A partition (X, Y) is called a bisection if $-1 \leqslant |X| - |Y| \leqslant 1$. Motivated by a conjecture of Bollobás and Scott [2] (every graph with m edges and minimum degree at least 2 admits a bisection (X, Y) such that $\max\{e(X), e(Y)\} \leqslant m/3$), there are quite a few papers on graph bisections with constraints on the edge density [3, 9, 19–21] in the recent years. Bollobás and Scott [3] proved that for large m, regular graphs with m edges admit bisections (X, Y) such that $\max\{e(X), e(Y)\} < m/4$. Xu et al. [19, 20] partially confirmed Bollobás and Scott's conjecture on graphs with the minimum degrees at least 5, and on graphs such that $\Delta(G) \leqslant 7\delta(G)/5$, where $\Delta(G)$ denotes the maximum degree of G. Lee et al. [9] asymptotically answered a question of Bollobás and Scott [2], and proved that for each integer k, every graph with m edges and the minimum degree either $2k$ or $2k+1$ admits a bisection (X, Y) such that $\max\{e(X), e(Y)\} \leqslant (\frac{k+1}{4k+2} + o(1))m$. Employing the idea of free vertex from [9], Xu and Yu [21] confirmed the conjecture of Bollobás and Scott and showed that the triangle is the only extremal graph.

Let s and t be two positive integers. Is there an integer l such that every graph with the minimum degree at least l has a bisection (X, Y) with $\delta(X) \geqslant s$ and $\delta(Y) \geqslant t$? If such a constant does exist, we use $g_b(s, t)$ to denote the smallest one.

In [2], Bollobás and Scott proposed the following conjecture.

Conjecture 1.1 (See [2]). *Every graph G admits a bisection (X, Y) such that*

$$|N_Y(x)| \geqslant d_X(x) - 1 \quad \textit{for each vertex } x \in X,$$

and

$$|N_X(y)| \geqslant d_Y(y) - 1 \quad \textit{for each vertex } y \in Y.$$

This conjecture is still open. In [10], Li and Xu confirmed it on d-regular graphs of order n when $d \in \{3, n-4, n-3, n-2\}$. Even a constant c has not been found such that every graph has a bisection (X, Y) such that $|N_Y(x)| \geqslant d_X(x) - c$ for each vertex $x \in X$, and $|N_X(y)| \geqslant d_Y(y) - c$ for each vertex $y \in Y$.

There is a close connection between Conjecture 1.1 and the existence of $g_b(s, s)$. The validity of Conjecture 1.1 on graphs of even orders is equivalent to say that every graph with even order admits a bisection (X, Y) such that $d_X(x) \geqslant \lceil \frac{d(x)}{2} \rceil - 1$ for each $x \in X$ and $d_Y(y) \geqslant \lceil \frac{d(y)}{2} \rceil - 1$ for each $y \in Y$. To see this, let G be a graph on $2k$ vertices. Suppose that Conjecture 1.1 does hold. Let (X, Y) be a bisection of the complement G^c of G that satisfies the requirements of Conjecture 1.1. Then, following the inequalities of Conjecture 1.1, $d_{G^c[X]}(x) \leqslant k - \lceil \frac{d(x)}{2} \rceil$ for each vertex x of X, and $d_{G^c[Y]}(y) \leqslant k - \lceil \frac{d(y)}{2} \rceil$ for each y of Y. So, the degree $d_X(x)$ of x in $G[X]$ equals $k - 1 - d_{G^c[X]}(x)$ which is at least $\lceil \frac{d(x)}{2} \rceil - 1$, and $d_Y(y) \geqslant \lceil \frac{d(y)}{2} \rceil - 1$ for each $y \in Y$. Conversely, let (X, Y) be a bisection of G^c such that $d_{G^c[X]}(x) \geqslant \lceil \frac{2k-1-d(x)}{2} \rceil - 1$ for each $x \in X$ and $d_{G^c[Y]}(y) \geqslant \lceil \frac{2k-1-d(y)}{2} \rceil - 1$ for each $y \in Y$, one can easily check that (X, Y) is a bisection of G satisfying the two inequalities of Conjecture 1.1.

With the same arguments as above, it is easy to see that if Conjecture 1.1 does hold, then every d-regular graph admits a bisection (X, Y) such that $\min\{\delta(X), \delta(Y)\} \geqslant \lceil \frac{d}{2} \rceil - 1$, and every graph with odd order admits a bisection (X, Y) such that $d_X(x) \geqslant \lceil \frac{d(x)}{2} \rceil - 2$ for each $x \in X$ and $d_Y(y) \geqslant \lceil \frac{d(y)}{2} \rceil - 2$ for each $y \in Y$. In the light of the connection to Conjecture 1.1, we propose the following, perhaps easier, question on $g_b(s, s)$.

Problem 1.1. *Let s be a positive integer. Is it true that every graph with minimum degree at least $2s+1$ admits a bisection (X, Y) such that $\min\{\delta(X), \delta(Y)\} \geqslant s$?*

If the answer is yes then the bound is best possible as evidenced by the complete graph K_{2s+1}. In the following, we say that a partition (X, Y) is s-good if $\min\{\delta(X), \delta(Y)\} \geqslant s$.

In [15], Sheehan showed that for each connected graph G with n vertices such that $2 \leqslant \delta(G) \leqslant n-2$, there is an integer $i \in [0, \lfloor \frac{\delta(G)}{2} \rfloor - 1]$ and a partition (X, Y) of G such that $|X| = \lceil \frac{n}{2} \rceil + i$, $|Y| = \lfloor \frac{n}{2} \rfloor - i$, $\delta(X) \geqslant \lceil \frac{\delta(G)}{2} \rceil + i$, and $\delta(Y) \geqslant \lfloor \frac{\delta(G)}{2} \rfloor - i$. In [1], Arkin and Hassin proved that every graph G has a bisection (X, Y) such that $\delta(X) + \delta(Y) \geqslant \delta(G) - 1$. While studying graph colorings with some particular

properties, Maurer proved an interesting result [13] (also see [14]) from which it is easy to see that $g_b(1,1)=3$.

Theorem 1.1 (See [13]). *Let G be a connected graph with n vertices and $\delta(G)\geqslant 2$. Then, for any positive integer k with $2\leqslant k\leqslant n-2$, G admits a 1-good partition (X,Y) such that $|X|=k$ and $|Y|=n-k$.*

The requirement of connectedness of graphs is necessary as evidenced by the disjoint union of odd number of triangles. The main result of this paper is the following theorem, which strengthens Theorem 1.1 and the above conclusion of Arkin and Hassin.

Theorem 1.2. *Let G be a connected graph with n vertices and $\delta(G)\geqslant 2$. Then, for any positive integer k with $2\leqslant k\leqslant n-2$, G admits a 1-good partition (X,Y) such that $|X|=k$ and $|Y|=n-k$, and $\delta(X)+\delta(Y)\geqslant\delta(G)-1$.*

The graph K_n ($n\geqslant 4$) shows that the bound $\delta(X)+\delta(Y)\geqslant\delta(G)-1$ in Theorem 1.2 is optimal. Arkin and Hassin [1] pointed out that the graphs G without cycles of length less than k do not admit 2-good partitions (X,Y) such that $|X|=k$ and $|Y|=|V(G)|-k$. So, one cannot expect to further improve the bound $\min\{\delta(X),\delta(Y)\}\geqslant 1$ under the same circumstances as those of Theorem 1.2. It should be also mentioned that a conjecture of Arkin and Hassin [1], which claims that each graph G with $\delta(G)\geqslant 4$ admits a 2-good partition (X,Y) such that $\lfloor\frac{1}{2}|V(G)|\rfloor-2\leqslant|X|\leqslant|Y|\leqslant\lceil\frac{1}{2}|V(G)|\rceil+2$, is not always true since in any partition (X,Y) of K_5, $\min\{\delta(X),\delta(Y)\}\leqslant 1$. It would be interesting if someone can find other family of counterexamples to this conjecture, or confirm the conjecture on some nontrivial family of graphs.

2 Proof of Theorem 1.2

Let (X,Y) be a partition of $V(G)$. For convenience, we use X_i to denote the subset of X of which each vertex has degree i in $G[X]$. Y_i is defined analogously.

Proof of Theorem 1.2. Suppose to the contrary that Theorem 1.2 does not hold, and let G be a counterexample with minimum number $e(G)$ of edges. For simplicity, let $\delta(G)=\delta$. By Theorem 1.1, we may choose (X,Y) to be a 1-good partition of $V(G)$ such that

(i) $|X|=k$ and $|Y|=n-k$, and

(ii) $e(X,Y)$ is minimum subject to (i).

It is clear that $\delta\geqslant 4$ by Theorem 1.1,

$$\delta(X)+\delta(Y)\leqslant\delta-2, \tag{2.1}$$

and

$$d(u)=\delta \quad \text{or} \quad d(v)=\delta \quad \text{for every edge } uv\in E(G) \tag{2.2}$$

by the minimality of $e(G)$.

Let $\delta(X)=p$ and $\delta(Y)=q$, and suppose by symmetry that $p\leqslant q$. Then, $\delta-2\geqslant p+q\geqslant 2p$ by (2.1).

If $p\geqslant 2$, choose $x\in X_p$ and $y\in Y_q$, and let $X'=(X\setminus\{x\})\cup\{y\}$ and $Y'=(Y\setminus\{y\})\cup\{x\}$. Then,

$$\begin{aligned} e(X',Y')-e(X,Y) &\leqslant d_X(x)+d_Y(y)-(|N_Y(x)|+|N_X(y)|-2)\\ &=2(p+q)-(d(x)+d(y)-2)\\ &\leqslant 2(\delta-2)-(2\delta-2)\\ &<0. \end{aligned}$$

Since $d_{X'}(y)\geqslant\delta-(\delta-2-p)-1=p+1\geqslant 3$, and $d_{Y'}(x)\geqslant\delta-p-1\geqslant p+1\geqslant 3$ as $\delta\geqslant 2p+2$, $\min\{\delta(X'),\delta(Y')\}\geqslant 1$. This contradicts the minimality of $e(X,Y)$. Therefore, $\min\{p,q\}=1$, i.e.,

$$p=1 \quad \text{and} \quad 1\leqslant q\leqslant\delta-3. \tag{2.3}$$

If $G[X_1]$ has an isolated vertex, say x, let y be a vertex in Y_q that maximizes $\max\{d_Y(z) : z \in N_Y(y)\}$, and let $X' = (X \setminus \{x\}) \cup \{y\}$ and $Y' = (Y \setminus \{y\}) \cup \{x\}$. Then, $e(X', Y') - e(X, Y) \leqslant 1 + q - (2\delta - q - 3) = 2q - 2(\delta - 2) < 0$ by (2.3). Since y has at least 2 neighbors in X', $\delta(X') \geqslant 1$, and hence $\delta(Y') = 0$ by the choice of (X, Y). Now, $q = 1$ as x has at least $\delta - 2$ neighbors in Y', and the only possibility is that $G[Y_1]$ consists of a matching. Since we have the symmetry between X and Y when $q = 1$, we may assume that

$$G[X_1] \text{ consists of a matching.} \tag{2.4}$$

Let x_1x_2 be an edge in $E(X_1)$. We consider two cases depending on $|Y_q|$.

Case 1. First we suppose that $|Y_q| \geqslant 2$.

If $e(Y_q) \neq 0$, let y_1y_2 be an edge in $E(Y_q)$ and let $h = 1$. Otherwise, let y_1 and y_2 be two vertices in Y_q and let $h = 0$. We will show that $q = h + 1$, and y_1 and y_2 have a common neighbor in Y.

Let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, y_2\}$ and $Y' = (Y \setminus \{y_1, y_2\}) \cup \{x_1, x_2\}$. Then,

$$\begin{aligned} e(X', Y') - e(X, Y) &= (d_X(x_1) + d_X(x_2) - 2) + (d_Y(y_1) + d_Y(y_2) - 2h) \\ &\quad - (e(\{x_1, x_2\}, Y) + e(\{y_1, y_2\}, X) - 2e(\{x_1, x_2\}, \{y_1, y_2\})) \\ &\leqslant 2(q - h) - (4\delta - 2 - 2q - 2e(\{x_1, x_2\}, \{y_1, y_2\})) \\ &\leqslant -2h - 4(\delta - q) + 10 \\ &< 0. \end{aligned}$$

Since $d_Y(y_1) \leqslant \delta - 3$ and $d_Y(y_2) \leqslant \delta - 3$ by (2.3), $d_{X'}(y_1) \geqslant \delta - (\delta - 3) - 2 + h \geqslant 1$ and $d_{X'}(y_2) \geqslant \delta - (\delta - 3) - 2 + h \geqslant 1$. Thus, $\delta(X') \geqslant 1$ which implies that $\delta(Y') = 0$ by the choice of (X, Y). Since $d_{Y'}(x_1) \geqslant \delta - 2 \geqslant 2$ and $d_{Y'}(x_2) \geqslant \delta - 2 \geqslant 2$, y_1 and y_2 must have a common neighbor, say y_3, in Y such that

$$d_{Y'}(y_3) = 0. \tag{2.5}$$

So, $N_Y(y_3) = \{y_1, y_2\}$, and thus $1 \leqslant q \leqslant 2$. If $q = 2$, then $d_Y(y_1) = d_Y(y_2) = d_Y(y_3) = q = 2$, and $y_1y_2 \in E(G)$ by the choice of y_1 and y_2. Otherwise, $q = 1$, and $y_1y_2 \notin E(G)$. In either case, $\{y_1, y_2, y_3\}$ induces a component in $G[Y]$.

By (2.5), $N_X(y_3) \cap \{x_1, x_2\} = \emptyset$. If $y_1x_1 \in E(G)$, let $X' = (X \setminus \{x_2\}) \cup \{y_1\}$ and $Y' = (Y \setminus \{y_1\}) \cup \{x_2\}$, then $\min\{\delta(X'), \delta(Y')\} \geqslant 1$ and $e(X', Y') - e(X, Y) \leqslant (1+q) - (2\delta - q - 3) = 4 + 2q - 2\delta < 0$, contradicting the choice of (X, Y). Therefore, there exists no edge between $\{x_1, x_2\}$ and $\{y_1, y_2\}$ by symmetry.

Since $G[X_1]$ is a matching by (2.4), we can conclude that

$$N_X(y) \cap X_1 = \emptyset \quad \text{for every } y \in \{y_1, y_2, y_3\}. \tag{2.6}$$

Since G is connected, there must be an edge w_1w_2 such that $w_1 \in X \setminus X_1$ and $w_2 \in Y \setminus \{y_1, y_2, y_3\}$. Then, either $d(w_1) = \delta$ or $d(w_2) = \delta$ by (2.2).

If $d(w_1) = \delta$, let $X' = (X \setminus \{x_1, x_2, w_1\}) \cup \{y_1, y_2, y_3\}$ and $Y' = (Y \setminus \{y_1, y_2, y_3\}) \cup \{x_1, x_2, w_1\}$, then $\min\{\delta(X'), \delta(Y')\} \geqslant 1$, and by (2.6),

$$\begin{aligned} e(X', Y') - e(X, Y) &= d_X(w_1) - (|N_Y(w_1)| + d(x_1) + d(x_2) - 2) \\ &\quad - (|N_X(y_1)| + |N_X(y_2)| + |N_X(y_3)| - 2e(\{x_1, x_2, w_1\}, \{y_1, y_2, y_3\})) \\ &\leqslant (\delta - 1) - (5\delta - 3 - 2q - 2e(\{x_1, x_2, w_1\}, \{y_1, y_2, y_3\})) \\ &\leqslant -4\delta + 8 + 2q \quad \text{(by (2.6))} \\ &< 0. \end{aligned}$$

If $d(w_2) = \delta$, let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, w_2\}$ and $Y' = (Y \setminus \{y_1, w_2\}) \cup \{x_1, x_2\}$, then $\min\{\delta(X'), \delta(Y')\} \geqslant 1$ and $e(X', Y') - e(X, Y) \leqslant -2(\delta - q) + 4 < 0$ by (2.6). Both contradict the choice of (X, Y). This completes the proof of Case 1.

Case 2. Now, we suppose that Y_q consists of a single vertex, say y_1.

If $y_1x_1 \in E(G)$, let $X' = (X \setminus \{x_2\}) \cup \{y_1\}$ and $Y' = (Y \setminus \{y_1\}) \cup \{x_2\}$, then $\min\{\delta(X'), \delta(Y')\} \geqslant 1$ since $|Y_q| = 1$, and $e(X', Y') - e(X, Y) \leqslant -(\delta - 3) - (\delta - 1) + 2(\delta - 3) < 0$, contradicting the choice of (X, Y). Therefore, we may suppose that

$$N(y_1) \cap X_1 = \emptyset, \tag{2.7}$$

since $G[X_1]$ consists of a matching by (2.4).

If $N_Y(y_1)$ has a vertex, say z, such that $d_Y(z) \leqslant \delta + 2$, let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, z\}$ and $Y' = (Y \setminus \{y_1, z\}) \cup \{x_1, x_2\}$. Since $q \leqslant \delta - 3$, $\min\{\delta(X'), \delta(Y')\} \geqslant 1$, and $e(X', Y') - e(X, Y) \leqslant -2(\delta - 1) - |N_X(y_1)| - |N_X(z)| + 2e(\{x_1, x_2\}, z) + (d_Y(y_1) + d_Y(z) - 2) \leqslant 4 + 2(q - \delta) < 0$ by (2.3) and (2.7), a contradiction to the choice of (X, Y). Therefore,

$$d_Y(z) \geqslant \delta + 3 > \delta \quad \text{for each } z \in N_Y(y_1), \tag{2.8}$$

and so by (2.2),

$$d(w) = \delta \quad \text{for every } z \in N_Y(y_1) \text{ and every } w \in N(z).$$

Let $V' = \{w : w \in Y \text{ and } d(w) = \delta\}$. It is clear that $y_1 \in V'$ by (2.8). Since $Y_q = \{y_1\}$ and $q \geqslant 1$, $Y \setminus (N_Y(y_1) \cup \{y_1\}) \neq \emptyset$, and thus $|V'| \geqslant 2$.

We will show that

$$d_Y(w) \geqslant \delta - |N_X(w) \cap \{x_1, x_2\}| \geqslant \delta - 2 \quad \text{for every } w \in Y \setminus \{y_1\}. \tag{2.9}$$

It is certain that (2.9) holds for every vertex in $N_Y(y_1)$ by (2.8). Let w be a vertex in $V' \setminus \{y_1\}$. If $N_X(w) \setminus \{x_1, x_2\} \neq \emptyset$, let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, w\}$ and $Y' = (Y \setminus \{y_1, w\}) \cup \{x_1, x_2\}$, then $e(X', Y') - e(X, Y) \leqslant -(2(\delta - 1) + |N_X(y_1)| + |N_X(w)| - 2e(\{x_1, x_2\}, \{w\})) + d_Y(y_1) + d_Y(w) \leqslant 4 + 2(q - \delta) < 0$ by (2.3) and (2.7). Since $d_Y(z) \geqslant \delta + 3$ for each $z \in N_Y(y_1)$ by (2.8), and since $Y_q = \{y_1\}$, $\min\{\delta(X'), \delta(Y')\} \geqslant 1$, contradicting the choice of (X, Y). Therefore, $N_X(w) \setminus \{x_1, x_2\} = \emptyset$, i.e., (2.9) holds for every vertex in $V' \setminus \{y_1\}$.

If $Y = V' \cup N_Y(y_1)$, we are done. Without loss of generality, let w be a vertex in $Y \setminus \{V' \cup N_Y(y_1)\}$ such that $N_X(w) \not\subseteq \{x_1, x_2\}$ and $d_Y(w) < \delta + 3$. Let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, w\}$ and $Y' = (Y \setminus \{y_1, w\}) \cup \{x_1, x_2\}$. Then $\min\{\delta(X'), \delta(Y')\} \geqslant 1$ since $Y_q = \{y_1\}$ and $N_Y(w) \subseteq V'$, and $e(X', Y') - e(X, Y) \leqslant -2(\delta - 1) - |N_X(y_1)| - |N_X(w)| + 2e(\{x_1, x_2\}, \{w\}) + d_Y(y_1) + d_Y(w) \leqslant d_Y(w) - \delta - 3 < 0$ by (2.7), contradicting the choice of (X, Y). This contradiction proves (2.9).

Let z be a vertex in $N_Y(y_1)$, and let $X' = (X \setminus \{x_1, x_2\}) \cup \{y_1, z\}$ and $Y' = (Y \setminus \{y_1, z\}) \cup \{x_1, x_2\}$. Then, $\min\{\delta(X'), \delta(Y')\} \geqslant 1$ and $\delta(Y') \geqslant \delta - 2$, and we get a partition of G as required. This contradiction to the choice of G completes the proof. □

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On the signless Laplacian spectra of bicyclic and tricyclic graphs *

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Abstract

In this paper, the first two (resp. four) largest signless Laplacian spectral radii together with the corresponding graphs in the class of bicyclic (resp. tricyclic) graphs of order n are determined, and the first two (resp. four) largest signless Laplacian spreads together with the corresponding graphs in the class of bicyclic (resp. tricyclic) graphs of order n are identified.

1 Introduction

Throughout the paper, $G = (V, E)$ is a connected undirected simple graph with $|V| = n$ and $|E| = m$. If $m = n+c-1$, then G is called a *c-cyclic graph*. Especially, if $c = 1, 2, 3$, then G is called a unicyclic, bicyclic, or tricyclic graph, respectively. The neighbors of a vertex v is denoted by $N(v)$. Write $d(v)$ for the degree of vertex v. Specially, $\Delta = \Delta(G)$ denotes the maximum degree of G.

Let $A(G)$ denote the *adjacency matrix* of G. Let $D(G)$ be the diagonal matrix whose (i, i)-entry is $d(v_i)$. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$, and the *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. The largest eigenvalues of $A(G)$, $L(G)$ and $Q(G)$ are called the *adjacency, Laplacian, and signless Laplacian spectral radii*, respectively. It is well-known that graph spectrum has great important applications in many fields. Several graph spectra, i.e., spectra of $A(G)$, $L(G)$ and $Q(G)$,

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had been defined in [1]. The spectra of $A(G)$, $L(G)$ are well studied (for instance see [2-10]), but the spectrum of $Q(G)$ seems to be less well known. It is not until recent years, some researchers found that the spectrum of $Q(G)$ has a strong connection with the structures of graph (see [11, 12]). For the new results on the signless Laplacian spectrum, one can refer to [11-14].

The largest adjacency spectral radius in the class of unicyclic graphs of given order was firstly determined in [2]. Following this, Guo [3] determined the first six largest adjacency spectral radii in the class of unicyclic graphs of given order. After then, the first three largest adjacency spectral radii in the class of bicyclic graphs of given order were given in [4]. Similarly, the researchers had investigated the Laplacian spectral radius in the class of unicyclic, bicyclic and tricyclic graphs. Up to now, the first to thirteenth largest Laplacian spectral radii were given in the class of unicyclic graphs of given order in [5, 6, 7]. After then, the first eight largest Laplacian spectral radii in the class of bicyclic graphs of given order were given in [8, 9]. Recently, the first nineteen largest Laplacian spectral radii in the class of tricyclic graphs of given order were determined in [10]. Motivated by the above results on $A(G)$ and $L(G)$, we shift our goals to the investigation of signless Laplacian spectral radius. Recently, we had identified the first four largest signless Laplacian spectral radii in the class of unicyclic graphs of given order in [15]. This paper will present the first two (resp. four) largest signless Laplacian spectral radii together with the corresponding graphs in the class of bicyclic (resp. tricyclic) graphs of given order.

Since $A(G)$ is symmetric, the eigenvalues of $A(G)$ can be arranged as follows: $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$. The *adjacency spread* of the graph G, denoted by $SA(G)$, is defined as (see [16]):

$$SA(G) = \rho_1(G) - \rho_n(G).$$

It is well known that $L(G)$ is positive semidefinite so that its eigenvalues can be arranged as follows: $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0$, where $\lambda_{n-1}(G) > 0$ if and only if G is connected and is called the *algebraic connectivity* of the graph G. Because $\lambda_n(G) = 0$, the *Laplacian spread* of the graph G, denoted by $SL(G)$, is defined as [17]

$$SL(G) = \lambda_1(G) - \lambda_{n-1}(G).$$

Note that $Q(G)$ is also positive semidefinite [14] and its eigenvalues can be arranged as: $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) \geq 0$. Thus, the *signless Laplacian spread* of the graph G, denoted by $SQ(G)$, is defined as

$$SQ(G) = \mu_1(G) - \mu_n(G).$$

This definition firstly appeared in the conjecture 25 of the literature [12], but well studied in [13] by the name of Q-spread. In [14], it is called signless

Laplacian spread to distinguish the known notations adjacency spread and Laplacian spread.

The adjacency spread of a graph had received much attention. In [18], Petrović determined all connected graphs with adjacency spread at most 4. In [16, 19], some lower and upper bounds for the adjacency spread of a graph were given. After then, the maximum adjacency spreads among all unicyclic graphs and all bicyclic graphs of given order were determined in [20] and [21], respectively. Similarly, the maximum and minimum Laplacian spreads among all trees of given order were identified in [17], the maximum and minimum Laplacian spreads among all unicyclic graphs of given order were determined in [22] and [23], respectively, the maximum Laplacian spread among tricyclic graphs of given order was identified in [24]. However, the signless Laplacian spread seems less well-known because it was introduced somewhat later [13, 14]. Up to now, there are only very limited results on the signless Laplacian spread. Some lower and upper bounds for the signless Laplacian spread of a graph were given in [13, 14], and the largest signless Laplacian spread in the class of unicyclic graphs of given order was determined in [14]. In this paper, by using different method from [13, 14], we determine the first two (resp. four) largest signless Laplacian spreads together with the corresponding graphs in the class of bicyclic (resp. tricyclic) graphs of given order.

This paper is organized as follows: The first two (resp. four) largest signless Laplacian spectral radii among the class of bicyclic (resp. tricyclic) graphs of given order are presented in Section 2. In Section 3, we determine the first two (resp. four) largest signless Laplacian spreads among the class of bicyclic (resp. tricyclic) graphs of given order.

2 The first two (resp. four) largest signless Laplacian spectral radii of bicyclic (resp. tricyclic) graphs

In the sequel, the notations $\mathcal{B}_n$, $\mathcal{T}_n$ are used to denote the class of bicyclic graphs and tricyclic graphs of order n, respectively.

Lemma 2.1 [25] $\mu_1(G) \leq max\{d(v) + m(v) : v \in V\}$, *where* $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.

Lemma 2.2 [26, 27] *If G is a graph with at least one edge, then $\mu_1(G) \geq \lambda_1(G) \geq \Delta + 1$. If G is connected, the first equality holds if and only if G is bipartite.*

Proposition 2.3 *Suppose $c \geq 0$ and G is a c-cyclic graph on n vertices with $\Delta \leq n-2$. If $n \geq max\{c+5, 2c+3\}$, then $\mu_1(G) \leq n$.*

Proof. By Lemma 2.1, we only need to prove that $max\{d(v)+m(v) : v \in V\} \leq n$.

Suppose $max\{d(v)+m(v) : v \in V\}$ occurs at the vertex u. Three cases arise $d(u)=1$, $d(u)=2$, or $3 \leq d(u) \leq n-2$.

Case 1. $d(u)=1$. Suppose $v \in N(u)$. Since $m(u)=d(v) \leq \Delta \leq n-2$, thus $d(u)+m(u) \leq n-1 < n$.

Case 2. $d(u)=2$. Suppose that v,$w \in N(u)$. Note that G is a c-cyclic graph, then $|N(v) \cap N(w)| \leq c+1$ and $|N(v) \cup N(w)| \leq n$. Therefore, $d(u)+m(u) = 2+\frac{d(v)+d(w)}{2} \leq 2+\frac{n+c+1}{2} \leq n$.

Case 3. $3 \leq d(u) \leq n-2$. Suppose G has m edges. Note that $3 \leq d(u) \leq n-2$, then $d(u)+m(u) \leq d(u)+\frac{2m-d(u)-1}{d(u)} = d(u)-1+\frac{2m-1}{d(u)}$. Next we shall prove that $d(u)-1+\frac{2m-1}{d(u)} \leq n$, equivalently, $d(u)(n+1-d(u)) \geq 2m-1$. Once this is proved, we are done. Let $f(x)=(n+1-x)x$.

When $x \in [3, \frac{n+1}{2}]$, since $f'(x)=n+1-2x \geq 0$, then $f(x) \geq f(3) = 3(n-2) \geq 2(n+c-1)-1 = 2m-1$.

When $x \in [\frac{n+1}{2}, n-2]$, since $f'(x)=n+1-2x \leq 0$, then $f(x) \geq f(n-2) = 3(n-2) \geq 2(n+c-1)-1 = 2m-1$.

By combining the above arguments, the assertion follows. ∎

Corollary 2.4 (1) *Suppose $G \in \mathcal{B}_n$. If $n \geq 7$ and $\Delta \leq n-2$, then $\mu_1(G) \leq n$.* (2) *Suppose $G \in \mathcal{T}_n$. If $n \geq 9$ and $\Delta \leq n-2$, then $\mu_1(G) \leq n$.*

It is well-known that $\lambda_1(G) \leq n$ (for example see [26]). For $\mu_1(G)$, we have

Corollary 2.5 *Suppose $c \geq 0$ and G is a c-cyclic graph with order $n > max\{c+5, 2c+3\}$, then* (1) *$\mu_1(G) > n$ if and only if $\Delta = n-1$ and G contains cycle of length odd.* (2) *$\mu_1(G) = n$ if and only if $\Delta = n-1$ and G is bipartite.*

Proof. It can be proved similarly with Proposition 2.3 that if $\Delta \leq n-2$, then $\mu_1(G) < n$ because $n > max\{c+5, 2c+3\}$. Next we only need to consider the case of $\Delta = n-1$. If $\Delta = n-1$ and G is bipartite, then $\mu_1(G) = n$ follows from Lemma 2.2. If $\Delta = n-1$ and G contains cycle of length odd, by Lemma 2.2 $n = \lambda_1(G) < \mu_1(G)$. ∎

In the following, $V \backslash \{u\}$ is written as $V-u$ for convenience. Let H_1, H_2 be the bicyclic graphs on $n \geq 7$ vertices as shown in Fig. 1.

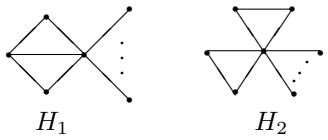


Fig. 1

Theorem 2.6 *Suppose $G \in \mathcal{B}_n$ and $n \geq 7$. Then, (1) $\mu_1(G) \leq \mu_1(H_1)$, the equality holds if and only if $G \cong H_1$, where $\mu_1(H_1)$ is the maximum root of the equation $\lambda^3 - (n+4)\lambda^2 + 4n\lambda - 8 = 0$. (2) If $G \ncong H_1$, then $\mu_1(G) \leq \mu_1(H_2)$, the equality holds if and only if $G \cong H_2$, where $\mu_1(H_2)$ is the maximum root of the equation $\lambda^3 - (n+3)\lambda^2 + 3n\lambda - 8 = 0$.*

Proof. Let $\Phi(G, \lambda)$=det$(\lambda I - Q(G))$ denote the signless Laplacian characteristic polynomial of G. By a straightforward computation, we have

$$\Phi(H_1, \lambda) = (\lambda - 1)^{n-4}(\lambda - 2)(\lambda^3 - (n+4)\lambda^2 + 4n\lambda - 8). \quad (1)$$

$$\Phi(H_2, \lambda) = (\lambda - 1)^{n-4}(\lambda - 3)(\lambda^3 - (n+3)\lambda^2 + 3n\lambda - 8). \quad (2)$$

Since $\Phi(H_1, n) = (n-1)^{n-4}(16-8n) < 0$ and $\lim\limits_{\lambda \longrightarrow +\infty} \Phi(H_1, \lambda) = +\infty$, thus $\mu_1(H_1) > n$. With the same reason, $\mu_1(H_2) > n$. Suppose that $G \in \mathcal{B}_n$ and $\mu_1(G) > n$, Corollary 2.4 implies that $\Delta = n - 1$. Next we shall show that $G \cong H_1$ or $G \cong H_2$.

Assume that $u \in V(G)$ such that $d(u) = n - 1$. It is easy to see that $uv \in E(G)$ holds for every $v \in V - u$. Since $G \in \mathcal{B}_n$, then $1 \leq max\{|N(u) \cap N(v)| : v \in V - u\} \leq 2$. Thus, two cases should be considered.

Case 1. $max\{|N(u) \cap N(v)| : v \in V - u\} = 2$. It is easy to see that $G \cong H_1$.

Case 2. $max\{|N(u) \cap N(v)| : v \in V - u\} = 1$. It is easy to see that $G \cong H_2$.

When $\lambda \geq n \geq 7$, since $\Phi(H_2, \lambda) - \Phi(H_1, \lambda) = (\lambda-1)^{n-4}((\lambda-n)\lambda+8) > 0$, thus $\mu_1(H_1) > \mu_1(H_2)$ because $\mu_1(H_1)$, $\mu_1(H_2) > n$.

By Eqs. (1)-(2) and the above arguments, the conclusion follows. ∎

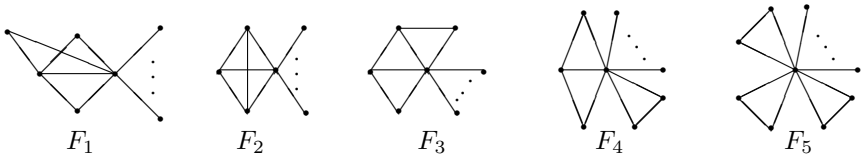


Fig. 2

Let F_1, F_2, F_3, F_4, F_5 be the tricyclic graphs on $n \geq 9$ vertices as shown in Fig. 2.

Lemma 2.7 *Suppose $G \in \mathcal{T}_n$ and $n \geq 9$. If $\mu_1(G) > n$, then G should be the graph F_1, F_2, F_3, F_4 or F_5.*

Proof. Since $G \in \mathcal{T}_n$ and $\mu_1(G) > n$, Corollary 2.4 implies that $\Delta = n-1$. Next we shall show that $G \cong F_i$, where $1 \leq i \leq 5$.

Assume that $u \in V(G)$ such that $d(u) = n-1$. It is easy to see that $uv \in E(G)$ holds for every $v \in V-u$. Since $G \in \mathcal{T}_n$, then $1 \leq max\{|N(u) \cap N(v)| : v \in V-u\} \leq 3$. Thus, three cases should be considered.

Case 1. $max\{|N(u) \cap N(v)| : v \in V-u\} = 3$. It is easy to see that $G \cong F_1$.

Case 2. $max\{|N(u) \cap N(v)| : v \in V-u\} = 2$. It is easy to see that $G \cong F_2$ or F_3 or F_4.

Case 3. $max\{|N(u) \cap N(v)| : v \in V-u\} = 1$. It is easy to see that $G \cong F_5$. ∎

Lemma 2.8 *If $n \geq 9$, then $\mu_1(F_1) = \mu_1(F_2) > \mu_1(F_3) > \mu_1(F_4) > \mu_1(F_5) > n$.*

Proof. By an elementary calculation, we have

$$\Phi(F_1, \lambda) = (\lambda-1)^{n-5}(\lambda-2)^2(\lambda^3 - (n+5)\lambda^2 + 5n\lambda - 12). \quad (3)$$

$$\Phi(F_2, \lambda) = (\lambda-1)^{n-5}(\lambda-2)^2(\lambda^3 - (n+5)\lambda^2 + 5n\lambda - 12). \quad (4)$$

$$\Phi(F_3, \lambda) = (\lambda-1)^{n-5}(\lambda-3)(\lambda^4 - (n+6)\lambda^3 + (6n+7)\lambda^2$$

$$-(7n+12)\lambda + 20). \quad (5)$$

$$\Phi(F_4, \lambda) = (\lambda-1)^{n-5}(\lambda-2)(\lambda^4 - (n+7)\lambda^3 + (7n+12)\lambda^2$$

$$-(12n+12)\lambda + 40). \quad (6)$$

$$\Phi(F_5, \lambda) = (\lambda-1)^{n-5}(\lambda-3)^2(\lambda^3 - (n+3)\lambda^2 + 3n\lambda - 12). \quad (7)$$

By Eqs. (3) and (4), $\mu_1(F_1) = \mu_1(F_2)$. Since $n \geq 9$ and $\Phi(F_1, n) = -12(n-1)^{n-5}(n-2)^2 < 0$ and $\lim_{\lambda \longrightarrow +\infty} \Phi(F_1, \lambda) = +\infty$, thus $\mu_1(F_1) > n$. With the same reason, $\mu_1(F_i) > n$ also holds for $2 \leq i \leq 5$.

We divide the proof into the next three processes.

(1) $\mu_1(F_2) > \mu_1(F_3)$. Rewrite Eq. (4) as $\Phi(F_2, \lambda) = (\lambda-1)^{n-5} f_1(\lambda)$, where $f_1(\lambda) = \lambda^5 - (n+9)\lambda^4 + (9n+24)\lambda^3 - (24n+32)\lambda^2 + (20n+48)\lambda - 48$. Thus, $\mu_1(F_2)$ equals the maximum root of the equation $f_1(\lambda) = 0$. Rewrite Eq. (5) as $\Phi(F_3, \lambda) = (\lambda-1)^{n-5} f_2(\lambda)$, where $f_2(\lambda) = \lambda^5 - (n+9)\lambda^4 + (9n+25)\lambda^3 - (25n+33)\lambda^2 + (21n+56)\lambda - 60$. Thus, $\mu_1(F_3)$ equals the maximum root of the equation $f_2(\lambda) = 0$. Let $\psi_1(\lambda) = f_2(\lambda) - f_1(\lambda) =$

$\lambda^3-(n+1)\lambda^2+(n+8)\lambda-12$. When $\lambda \geq n \geq 9$, since $\psi_1'(\lambda)=3\lambda^2-2(n+1)\lambda+(n+8)=\lambda(3\lambda-2n-2)+n+8>0$, then $\psi_1(\lambda)\geq\psi_1(n)=8n-12>0$. Thus, when $\lambda \geq n \geq 9$, $f_2(\lambda)>f_1(\lambda)$. This implies that $\mu_1(F_2)>\mu_1(F_3)$ because $\mu_1(F_2)$, $\mu_1(F_3)>n$.

(2) $\mu_1(F_3)>\mu_1(F_4)$. Rewrite Eq. (6) as $\Phi(F_4,\lambda)=(\lambda-1)^{n-5}f_3(\lambda)$, where $f_3(\lambda)=\lambda^5-(n+9)\lambda^4+(9n+26)\lambda^3-(26n+36)\lambda^2+(24n+64)\lambda-80$. Thus, $\mu_1(F_4)$ equals the maximum root of the equation $f_3(\lambda)=0$. Let $\psi_2(\lambda)=f_3(\lambda)-f_2(\lambda)=\lambda^3-(n+3)\lambda^2+(3n+8)\lambda-20$. When $\lambda \geq n \geq 9$, since $\psi_2'(\lambda)=3\lambda^2-2(n+3)\lambda+(3n+8)=\lambda(3\lambda-2n-6)+3n+8>0$, thus $\psi_2(\lambda)\geq\psi_2(n)=8n-20>0$. Thus, when $\lambda \geq n \geq 9$, $f_3(\lambda)>f_2(\lambda)$. This implies that $\mu_1(F_3)>\mu_1(F_4)$ because $\mu_1(F_3)$, $\mu_1(F_4)>n$.

(3) $\mu_1(F_4)>\mu_1(F_5)$. Rewrite Eq. (7) as $\Phi(F_5,\lambda)=(\lambda-1)^{n-5}f_4(\lambda)$, where $f_4(\lambda)=\lambda^5-(n+9)\lambda^4+(9n+27)\lambda^3-(27n+39)\lambda^2+(27n+72)\lambda-108$. Thus, $\mu_1(F_5)$ equals the maximum root of the equation $f_4(\lambda)=0$. Let $\psi_3(\lambda)=f_4(\lambda)-f_3(\lambda)=\lambda^3-(n+3)\lambda^2+(3n+8)\lambda-28$. When $\lambda \geq n \geq 9$, since $\psi_3'(\lambda)=3\lambda^2-2(n+3)\lambda+(3n+8)=\lambda(3\lambda-2n-6)+3n+8>0$, thus $\psi_3(\lambda)\geq\psi_3(n)=8n-28>0$. Thus, when $\lambda \geq n \geq 9$, $f_4(\lambda)>f_3(\lambda)$. This implies that $\mu_1(F_4)>\mu_1(F_5)$ because $\mu_1(F_4)$, $\mu_1(F_5)>n$. ∎

By combining Corollary 2.4, Lemmas 2.7-2.8, and Eqs. (3)-(7), we have

Theorem 2.9 *Suppose $G \in \mathcal{T}_n$ and $n \geq 9$. Then, (1) $\mu_1(G)\leq\mu_1(F_1)$, the equality holds if and only if $G\cong F_1$ or $G\cong F_2$, where $\mu_1(F_1)$ is the maximum root of the equation $\lambda^3-(n+5)\lambda^2+5n\lambda-12=0$. (2) If $G\notin\{F_1,F_2\}$, then $\mu_1(G)\leq\mu_1(F_3)$, the equality holds if and only if $G\cong F_3$, where $\mu_1(F_3)$ is the maximum root of the equation $\lambda^4-(n+6)\lambda^3+(6n+7)\lambda^2-(7n+12)\lambda+20=0$. (3) If $G\notin\{F_1,F_2,F_3\}$, then $\mu_1(G)\leq\mu_1(F_4)$, the equality holds if and only if $G\cong F_4$, where $\mu_1(F_4)$ is the maximum root of the equation $\lambda^4-(n+7)\lambda^3+(7n+12)\lambda^2-(12n+12)\lambda+40=0$. (4) If $G\notin\{F_1,F_2,F_3,F_4\}$, then $\mu_1(G)\leq\mu_1(F_5)$, the equality holds if and only if $G\cong F_5$, where $\mu_1(F_5)$ is the maximum root of the equation $\lambda^3-(n+3)\lambda^2+3n\lambda-12=0$.*

3 The first two (resp. four) largest signless Laplacian spreads of bicyclic (resp. tricyclic) graphs

Lemma 3.1 *If G is a bicyclic graph on $n\geq 12$ vertices with $\Delta\leq n-2$, then $\mu_1(G)\leq n-0.5$.*

Proof. By Lemma 2.1, we only need to prove that $max\{d(v)+m(v): v\in V\}\leq n-0.5$.

Suppose $max\{d(v)+m(v) : v \in V\}$ occurs at the vertex u. Three cases arise $d(u) = 1$, $d(u) = 2$, or $3 \leq d(u) \leq n-2$.

Case 1. $d(u) = 1$. Suppose $v \in N(u)$. Since $m(u) = d(v) \leq \Delta \leq n-2$, thus $d(u)+m(u) \leq n-1 < n-0.5$.

Case 2. $d(u) = 2$. Suppose that v,$w \in N(u)$. Note that G is a bicyclic graph, then $|N(v) \cap N(w)| \leq 3$ and $|N(v) \cup N(w)| \leq n$. Therefore, $d(u)+m(u) = 2+\frac{d(v)+d(w)}{2} \leq 2+\frac{n+3}{2} \leq n-0.5$.

Case 3. $3 \leq d(u) \leq n-2$. Note that $3 \leq d(u) \leq n-2$ and G has $n+1$ edges, then $d(u)+m(u) \leq d(u)+\frac{2n+1-d(u)}{d(u)} = d(u)-1+\frac{2n+1}{d(u)}$. Next we shall prove that $d(u)-1+\frac{2n+1}{d(u)} \leq n-0.5$, equivalently, $d(u)(n+0.5-d(u)) \geq 2n+1$. Let $f(x) = (n+0.5-x)x$.

When $x \in [3, \frac{2n+1}{4}]$, since $f'(x) = n+0.5-2x \geq 0$, then $f(x) \geq f(3) = 3(n-2.5) \geq 2n+1$.

When $x \in [\frac{2n+1}{4}, n-2]$, since $f'(x) = n+0.5-2x \leq 0$, then $f(x) \geq f(n-2) = 2.5(n-2) \geq 2n+1$.

This completes the proof of this result. ∎

Theorem 3.2 *If G is a bicyclic graph on $n \geq 12$ vertices and $G \notin \{H_1, H_2\}$, then $SQ(H_1) > SQ(H_2) > SQ(G)$.*

Proof. Let $f_5(\lambda) = \lambda^3-(n+4)\lambda^2+4n\lambda-8$ and $f_6(\lambda) = \lambda^3-(n+3)\lambda^2+3n\lambda-8$. Since $f_5(0) = -8 < 0$, $f_5(1) = 3n-11 > 0$, $f_5(n) = -8 < 0$ and $f_5(n+1) = n^2-2n-11 > 0$, by Eq. (1) we can conclude that $0 < \mu_n(H_1) < 1$ and $n < \mu_1(H_1) < n+1$.

Similarly, since $f_6(0) = -8 < 0$, $f_6(0.5) = \frac{1}{8}(10n-69) > 0$, $f_6(n) = -8 < 0$ and $f_6(n+1) = n^2-n-10 > 0$, by Eq. (2) it follows that $0 < \mu_n(H_2) < 0.5$ and $n < \mu_1(H_2) < n+1$, this implies that $SQ(H_2) = \mu_1(H_2)-\mu_n(H_2) > n-0.5$.

When $0 < \lambda < 1$, $f_5(\lambda)-f_6(\lambda) = -(\lambda-n)\lambda > 0$, thus $\mu_n(H_1) < \mu_n(H_2)$ because $0 < \mu_n(H_1) < 1$ and $0 < \mu_n(H_2) < 0.5$. By Theorem 2.6, we have

$$SQ(H_1) = \mu_1(H_1)-\mu_n(H_1) > \mu_1(H_2)-\mu_n(H_2) = SQ(H_2) > n-0.5.$$

Moreover, note that $\mu_n(G) \geq 0$ and $G \notin \{H_1, H_2\}$, by Lemma 3.1 it follows that $SQ(G) = \mu_1(G)-\mu_n(G) \leq \mu_1(G) \leq n-0.5 < SQ(H_2)$.

By combining the above arguments, the result follows. ∎

Remark 1. By Theorems 2.6 and 3.2, the graphs which share the first two largest signless Laplacian spectral radii even share the first two largest signless Laplacian spreads in the class of bicyclic graphs on $n \geq 12$ vertices.

It can be proved similarly with Lemma 3.1 that

Lemma 3.3 *If G is a tricyclic graph on $n \geq 16$ vertices with $\Delta \leq n-2$, then $\mu_1(G) \leq n-0.5$.*

Lemma 3.4 *If $n \geq 16$, then $SQ(F_1) = SQ(F_2) > SQ(F_3) > SQ(F_4) > SQ(F_5) > n - 0.5$.*

Proof. By Eqs. (3) and (4), it follows that $SQ(F_1) = SQ(F_2)$. We divide the proof into the next three processes.

(1) $SQ(F_2) > SQ(F_3)$. If $16 \leq n \leq 30$, it can be checked readily that $SQ(F_2) > SQ(F_3)$ by Eqs. (4) and (5). Next we may suppose that $n \geq 31$. Note that $f_1(0) = -48 < 0$, $f_1(1) = 4n - 16 > 0$, $f_1(3) = 6n - 30 > 0$, $f_1(5) = -108 < 0$ and $f_1(n+5) = 5n^4+55n^3+183n^2+153n-108 > 0$, then $0 < \mu_n(F_2) < 1$, $\mu_{n-1}(F_2) = 1$ by Eq. (4). Note that $f_2(0) = -60 < 0$, $f_2(1) = 4n - 20 > 0$, $f_2(2) = 8 - 2n < 0$ and $f_2(4) = 4n - 44 > 0$, $f_2(8) = 6980-920n < 0$ and $f_2(n+5) = 5n^4+55n^3+188n^2+206n+20 > 0$, then $0 < \mu_n(F_3) < 1$, $\mu_{n-1}(F_3) = 1$ by Eq. (5).

Let α_1 be the minimum root of $\psi_1(\lambda) = 0$. Since $\psi_1(0) = -12 < 0$, $\psi_1(0.625) = \frac{1}{512}(120n - 3659) > 0$, $\psi_1(1) = -4 < 0$ and $\psi_1(n) = 8n - 12 > 0$, then $0 < \alpha_1 < 0.625$.

It is easy to see that

$$f_1(\lambda) = (\lambda^2 - 8\lambda + 8)\psi_1(\lambda) + \gamma_1(\lambda), \tag{8}$$

$$f_2(\lambda) = (\lambda^2 - 8\lambda + 9)\psi_1(\lambda) + \gamma_1(\lambda), \tag{9}$$

where $\gamma_1(\lambda) = -4(2n - 13)\lambda^2 + 4(3n - 28)\lambda + 48$.

When $0 < \lambda < 0.625$, since $\gamma_1'(\lambda) = -8(2n - 13)\lambda + 4(3n - 28) > 4(3n - 28) - 0.625 \times 8(2n - 13) = 2n - 47 > 0$, then $\gamma_1(\lambda) > \gamma_1(0) = 48 > 0$. Recall that $0 < \alpha_1 < 0.625$, by Eqs. (8) and (9) it follows that $f_1(\alpha_1) = f_2(\alpha_1) = \gamma_1(\alpha_1) > 0$. This implies that $\mu_n(F_2)$, $\mu_n(F_3) \in (0, \alpha_1)$. Moreover, when $0 < \lambda < \alpha_1$, since $f_2(\lambda) - f_1(\lambda) = \psi_1(\lambda) < 0$, then $\mu_n(F_2) < \mu_n(F_3)$. By Theorem 2.9, we have

$$SQ(F_2) = \mu_1(F_2) - \mu_n(F_2) > \mu_1(F_3) - \mu_n(F_3) = SQ(F_3).$$

(2) $SQ(F_3) > SQ(F_4)$. Note that $f_3(0) = -80 < 0$, $f_3(1) = 6n-34 > 0$, $f_3(2.5) = \frac{1}{32}(235 - 30n) < 0$, $f_3(3) = 4 > 0$, $f_3(5) = 90 - 30n < 0$ and $f_3(n + 5) = 5n^4 + 55n^3 + 193n^2 + 249n + 90 > 0$, then $0 < \mu_n(F_4) < 1$, $\mu_{n-1}(F_4) = 1$ by Eq. (6).

Let α_2 be the minimum root of $\psi_2(\lambda) = 0$. Since $\psi_2(\frac{6}{n}) = \frac{-2}{n^3}(n^3 - 6n^2 + 54n - 108) < 0$, $\psi_2(1) = 2n - 14 > 0$, $\psi_2(5) = 70 - 10n < 0$ and $\psi_2(n) = 8n - 20 > 0$, then $\frac{6}{n} < \alpha_2 < 1$.

It is easy to see that

$$f_2(\lambda) = (\lambda^2 - 6\lambda - 1)\psi_2(\lambda) + \gamma_2(\lambda), \tag{10}$$

$$f_3(\lambda) = (\lambda^2 - 6\lambda)\psi_2(\lambda) + \gamma_2(\lambda), \tag{11}$$

where $\gamma_2(\lambda) = -8(n - 4)\lambda^2 + 8(3n - 7)\lambda - 80$.

When $\frac{6}{n} < \lambda < 1$, since $\gamma_2'(\lambda) = -16(n-4)\lambda + 8(3n-7) > 8(3n-7) - 16(n-4) = 8n+8 > 0$, then $\gamma_2(\lambda) > \gamma_2(\frac{6}{n}) = \frac{16}{n^2}(4n^2-39n+72) > 0$. Recall that $\frac{6}{n} < \alpha_2 < 1$, by Eqs. (10) and (11) it follows that $f_2(\alpha_2) = f_3(\alpha_2) = \gamma_2(\alpha_2) > 0$. This implies that $\mu_n(F_3)$, $\mu_n(F_4) \in (0, \alpha_2)$. Moreover, when $0 < \lambda < \alpha_2$, since $f_3(\lambda) - f_2(\lambda) = \psi_2(\lambda) < 0$, then $\mu_n(F_3) < \mu_n(F_4)$. By Theorem 2.9, we have

$$SQ(F_3) = \mu_1(F_3) - \mu_n(F_3) > \mu_1(F_4) - \mu_n(F_4) = SQ(F_4).$$

(3) $SQ(F_4) > SQ(F_5)$. Note that $f_4(\lambda) = (\lambda-3)^2\varphi_1(\lambda)$, where $\varphi_1(\lambda) = \lambda^3-(n+3)\lambda^2+3n\lambda-12$. Since $\varphi_1(0) = -12 < 0$, $\varphi_1(0.5) = \frac{1}{8}(10n-101) > 0$, $\varphi_1(1) = 2n - 14 > 0$, $\varphi_1(3) = -12 < 0$ and $\varphi_1(n+1) = n^2 - n - 14 > 0$, then $0 < \mu_n(F_5) < 0.5$, $\mu_{n-1}(F_5) = 1$ by Eq. (7). By Lemma 2.4, it follows that $SQ(F_5) = \mu_1(F_5) - \mu_n(F_5) > n - 0.5$.

Let α_3 be the minimum root of $\psi_3(\lambda) = 0$. Since $\psi_3(\frac{8}{n}) = \frac{-4}{n^3}(n^3 + 48n - 128) < 0$, $\psi_3(1) = 2n - 22 > 0$, $\psi_3(5) = 62 - 10n < 0$ and $\psi_3(n) = 8n - 28 > 0$, then $\frac{8}{n} < \alpha_3 < 1$.

It is easy to see that

$$f_3(\lambda) = (\lambda^2 - 6\lambda)\psi_3(\lambda) + \gamma_3(\lambda), \tag{12}$$

$$f_4(\lambda) = (\lambda^2 - 6\lambda + 1)\psi_3(\lambda) + \gamma_3(\lambda), \tag{13}$$

where $\gamma_3(\lambda) = -8(n-5)\lambda^2 + 8(3n-13)\lambda - 80$.

When $\frac{8}{n} < \lambda < 1$, since $\gamma_3'(\lambda) = -16(n-5)\lambda + 8(3n-13) > 8(3n-13) - 16(n-5) = 8n - 24 > 0$, then $\gamma_3(\lambda) > \gamma_3(\frac{8}{n}) = \frac{16}{n^2}(7n^2 - 84n + 160) > 0$. Recall that $\frac{8}{n} < \alpha_3 < 1$, by Eqs. (12) and (13) it follows that $f_3(\alpha_3) = f_4(\alpha_3) = \gamma_3(\alpha_3) > 0$. This implies that $\mu_n(F_4)$, $\mu_n(F_5) \in (0, \alpha_3)$. Moreover, when $0 < \lambda < \alpha_3$, since $f_4(\lambda) - f_3(\lambda) = \psi_3(\lambda) < 0$, then $\mu_n(F_4) < \mu_n(F_5)$. By Theorem 2.9, we have

$$SQ(F_4) = \mu_1(F_4) - \mu_n(F_4) > \mu_1(F_5) - \mu_n(F_5) = SQ(F_5) > n - 0.5.$$

By combining the above arguments, the result follows. ∎

Note that $\mu_n(G) \geq 0$, by Lemmas 3.3-3.4 we can conclude that

Theorem 3.5 *If $G \in \mathcal{T}_n \setminus \{F_1, F_2, F_3, F_4, F_5\}$ and $n \geq 16$, then $SQ(F_1) = SQ(F_2) > SQ(F_3) > SQ(F_4) > SQ(F_5) > SQ(G)$.*

Remark 2. By Theorems 2.9 and 3.5, the graphs which share the first four largest signless Laplacian spectral radii even share the first four largest signless Laplacian spreads in the class of tricyclic graphs on $n \geq 16$ vertices.

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RECENT RESULTS ON THE MAJORIZATION THEORY OF GRAPH SPECTRUM AND TOPOLOGICAL INDEX THEORY - A SURVEY*

MUHUO LIU†, BOLIAN LIU‡, AND KINKAR CH. DAS§

Abstract. Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two positive non-increasing degree sequences, write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Let $\rho(G)$ and $\mu(G)$ be the spectral radius and signless Laplacian spectral radius of G, respectively. Also let G and G' be the extremal graphs with the maximal (signless Laplacian) spectral radii in the class of connected graphs with π and π' as their degree sequences, respectively. If $\pi \lhd \pi'$ can deduce that $\rho(G) < \rho(G')$ (respectively, $\mu(G) < \mu(G')$), then it is said that the spectral radii (respectively, signless Laplacian spectral radii) of G and G' satisfy the majorization theorem. This paper presents a survey to the recent results on the theory and application of the majorization theorem in graph spectrum and topological index theory.

Key words. (Signless Laplacian) Spectral radius, Degree sequence, Majorization.

AMS subject classifications. 05C35, 05C75, 05C05.

1. Introduction.

Throughout the paper, $G = (V, E)$ is a connected undirected (not necessarily simple) graph with $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. The degree of vertex v of G, denoted $d(v)$, is the number of edges of G incident with v, each loop counting as two edges. The degree sequence $(d_1, d_2, \ldots, d_n)$ of G is enumerated in a non-increasing ordering , i.e., $d_1 \geq d_2 \geq \cdots \geq d_n \geq 1$ (hereafter, we assume that $d(v_i) = d_i$ for $1 \leq i \leq n$). We use $\Gamma(\pi)$ to denote the class of connected graphs with degree sequence π, and we use $S(\pi)$ to denote the class of connected simple graphs with degree sequence π.

Denote the neighbor set of vertex v in G as $N(v)$. Let Υ_{uv} be the number of edges joining vertices u and v in G. In particular, Υ_{uu} indicates the number of loops incident with vertex u in G. The adjacency matrix of G is an $n \times n$ matrix $A(G) = (a_{ij})$,

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where a_{ij} is the number of edges joining vertices v_i and v_j, each loop counting as two edges.

Suppose $f = (f(v_1), f(v_2), \ldots, f(v_n))^T \neq 0$ is a column vector defined on $V(G)$. If there exists a real number q such that for each $u \in V(G)$,

$$qf(u) = (A(G)f)(u) = \sum_{v \in N(u)\setminus\{u\}} \Upsilon_{uv} f(v) + 2\Upsilon_{uu} f(u),$$

then q is called an *eigenvalue of* $A(G)$. The *spectral radius of* G, denoted $\rho(G)$, is the largest eigenvalue of $A(G)$.

The *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees of G. If there exists a real number p such that for each $u \in V(G)$,

$$pf(u) = (Q(G)f)(u) = \sum_{v \in N(u)\setminus\{u\}} \Upsilon_{uv}(f(u) + f(v)) + 4\Upsilon_{uu} f(u),$$

then p is called an *eigenvalue of* $Q(G)$. It is easy to see that $Q(G)$ is positive semidefinite [14], and hence, we use $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ to denote the eigenvalues of $Q(G)$ and use $\mu(G)$ to define the largest eigenvalue of $Q(G)$. That means $\mu(G) = \mu_1(G)$. The *signless Laplacian spectral radius* of G is $\mu(G)$.

Hereafter, unless specially indicated, we only concern with connected simple graph. In this case, $A(G) = (a_{ij})$ is an $(0,1)$-matrix, where $a_{ij} = 1$ if and only if v_i is adjacent with v_j. Furthermore, there is a unique positive unit eigenvector corresponding to $\rho(G)$ (respectively, $\mu(G)$), we use f to denote such a unit eigenvector corresponding to $\rho(G)$ or $\mu(G)$, and we call f the *Perron vector* of G.

The *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$. When G is a connected simple graph, it is well known that $L(G)$ is positive semidefinite [45] so that we can use $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ to denote the eigenvalues of $L(G)$ and we use $\lambda(G)$ to denote the largest eigenvalue of $L(G)$. From the definition, $\lambda(G) = \lambda_1(G)$, and we will call $\lambda(G)$ the *Laplacian spectral radius* of G.

As usual, if $m = n + c - 1$, then G is called a *c-cyclic graph*. When $c = 0$, 1, 2, or 3, G is always called a *tree, unicyclic graph, bicyclic graph* and *tricyclic graph*, respectively.

When G is a tree, let ∂V be the set of pendant vertices (vertices of degrees one) of G, and let $V_0 = V \setminus \partial V$. In [18], ∂V is called the *boundary vertices of* G, while V_0 is called the *interior vertices of* G. A *discrete Dirichlet operator* $L_0(G)$ (see [18]) is the Laplacian matrix restricted to interior vertices, i.e., $L_0(G) = D_0(G) - A_0(G)$, where $A_0(G)$ is the adjacency matrix of the graph induced by V_0, and where D_0 is the degree matrix D restricted to V_0. From the definition of $L_0(G)$ and $L(G)$, $L_0(G)$ is obtained

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from $L(G)$ by deleting all rows and columns that correspond to boundary vertices. The *first Dirichlet eigenvalue* of G, denote by $\lambda_0(G)$, is the smallest eigenvalue of $L_0(G)$ (see [18]).

Suppose $G \in \Gamma(\pi)$. If $\rho(G) \geq \rho(G')$ (respectively, $\mu(G) \geq \mu(G')$) for any other $G' \in \Gamma(\pi)$, then we say G has maximal (respectively, signless Laplacian) spectral radius in $\Gamma(\pi)$. Furthermore, we call G a *maximal extremal graph* of $\Gamma(\pi)$ if G has the maximal spectral radius or signless Laplacian spectral radius in $\Gamma(\pi)$.

Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two non-increasing sequences of real numbers, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is sometimes called *majorization* (see [23]).

This notion was introduced because of the following well-known theorem.

THEOREM 1.1. [44, p. 218] *The spectrum of a positive semidefinite Hermitian matrix majorizes its main diagonal* (*when both are rearranged in non-increasing order*).

From Theorem 1.1, it easily follows:

PROPOSITION 1.2. [33] *Let G be a graph with n vertices. Then, $(d_1, d_2, \ldots, d_n) \lhd (\mu_1, \mu_2, \ldots, \mu_n)$ and $(d_1, d_2, \ldots, d_n) \lhd (\lambda_1, \lambda_2, \ldots, \lambda_n)$.*

From Proposition 1.2, $\lambda_1 \geq d_1$. Indeed, when G has at least one edge, Grone and Merris proved that $\lambda_1 \geq d_1 + 1$ [19]and they also put forward the following conjecture.

CONJECTURE 1.3. [19] *Let G be a connected graph on $n \geq 2$ vertices. Then, $(d_1 + 1, d_2, \ldots, d_n - 1) \lhd (\lambda_1, \lambda_2, \ldots, \lambda_n)$.*

For a non-negative integral sequence $d = (d_1, d_2, \ldots, d_n)$, we define its conjugate degree sequence as the sequence $d^* = (d_1^*, d_2^*, \ldots, d_n^*)$, where

$$d_k^* = \#\{i : d_i \geq k\}.$$

In [19], Grone and Merris raised another question on the Laplacian spectrum sequence and the conjugate degree sequence, and they conjectured that

CONJECTURE 1.4. [19] *For any graph G with n vertices,*

$$(\lambda_1, \lambda_2, \ldots, \lambda_n) \lhd (d_1^*, d_2^*, \ldots, d_n^*).$$

It is surprised that Conjecture 1.3 was proved in 1995 by Grone [20], while the complete proof of Conjecture 1.4 was given in 2011 by Bai [4]. Furthermore, Liu and

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Liu [33] pointed out that the relation $(d_1+1, d_2, \ldots, d_n-1) \lhd (\mu_1, \mu_2, \ldots, \mu_n)$ does not hold.

Motivated by the above results on the relation between the Laplacian spectrum and the degree sequence of a graph, Bıyıkoğlu and Leydold [8] considered the relation between the minimal first Dirichlet eigenvalues in two classes of trees with given degree sequences, they proved:

THEOREM 1.5. [8] *Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Suppose T and T' are the trees with the minimal first Dirichlet eigenvalues in $S(\pi)$ and $S(\pi')$, respectively. Then, $\lambda_0(T) < \lambda_0(T')$.*

By Theorem 1.5, we can deduce the size of the relationship between the minimal first Dirichlet eigenvalues of $S(\pi)$ and $S(\pi')$ from the majorization relationship of two given degree sequences π and π'. Thus, such relation is called the *majorization theorem* by Jiang et al. [26] and Liu and Liu [37]. This method (i.e., the majorization theorem method) was discovered a long time ago, and was widely applied in different branches of Mathematics. For instance, the following famous "majorization theorem" of strictly Schur-convex function [23] was proved by Schur in 1923, and also discovered by Hardy, Littlewood and Pólya in 1929. Recall that a *strictly convex function* is a real valued function φ defined on a convex set B such that

$$\varphi(px + (1-p)y) < p\varphi(x) + (1-p)\varphi(y)$$

for all $0 < p < 1$ and all x, $y \in B$. A symmetric function ϕ: $D \to \mathbb{R}$, $D \subseteq \mathbb{R}^n$, is said to be *strictly Schur-convex* on D if $a \lhd b$ implies that $\phi(a) < \phi(b)$, where $(a) = (a_1, a_2, \ldots, a_n)$ and $(b) = (b_1, b_2, \ldots, b_n)$ are two non-increasing sequences of real numbers.

THEOREM 1.6. [23] *Given an interval $I \subseteq \mathbb{R}$, and a strictly convex function $\varphi : I \to \mathbb{R}$, the function $\phi(b) = \sum_{i=1}^{n} \varphi(b_i)$ is strictly Schur convex on I^n.*

The next result follows immediately from Theorem 1.6.

COROLLARY 1.7. [23] *If $(a) \lhd (b)$ and φ is a strictly convex function, then $\sum_{i=1}^{n} \varphi(a_i) < \sum_{i=1}^{n} \varphi(b_i)$.*

Therefore, it seems impossible to give a survey of all the majorization theorems appear in Mathematics, and hence, this survey mainly focuses on some recent results of the theory and application to the majorization theorem in graph spectrum and topological index theory.

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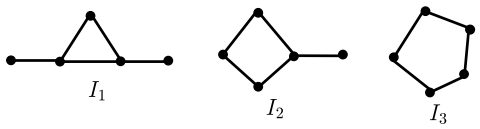


FIG. 2.1. *The unicyclic graphs I_1, I_2 and I_3.*

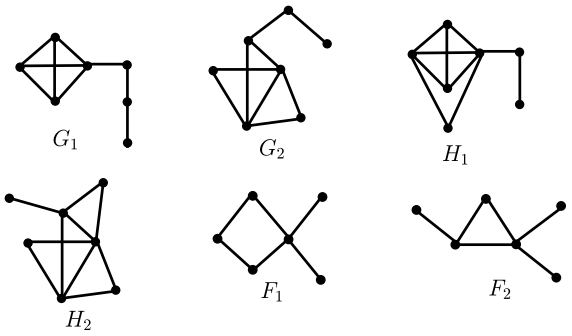


FIG. 2.2. *The graphs G_1, G_2, H_1, H_2, F_1, and F_2.*

2. The majorization theorem of graph spectrum.

2.1. Some known majorization theorems of graph spectrum. Motivated by Theorem 1.5, Bıyıkoğlu and Leydold [9] also considered the similar relation between the spectral radii of the maximal extremal graphs in two classes of trees with given degree sequences, and Zhang [54] considered the similar problem for the Laplacian spectral radii (i.e., the signless Laplacian spectral radii since $L(G)$ and $Q(G)$ share the same spectra [45] when G is a simple bipartite graph), and they showed that

THEOREM 2.1. *Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Suppose T and T' are the maximal extremal trees in $S(\pi)$ and $S(\pi')$, respectively. Then,* [9] $\rho(T) < \rho(T')$ *and* [54] $\lambda(T) < \lambda(T')$.

Furthermore, the majorization theorems for unicyclic and bicyclic graphs were also proved.

THEOREM 2.2. *Let π and π' be two different non-increasing degree sequences of unicyclic (respectively, bicyclic) graphs with $\pi \lhd \pi'$.*

(1) *Suppose U and U' are the maximal extremal unicyclic graphs in $S(\pi)$ and $S(\pi')$, respectively. Then,* [37] $\rho(U) < \rho(U')$ *and* [55] $\mu(U) < \mu(U')$.
(2) *Suppose B and B' are the maximal extremal bicyclic graphs in $S(\pi)$ and $S(\pi')$, respectively. Then,* [26] $\rho(B) < \rho(B')$ *and* [25] $\mu(B) < \mu(B')$.

As usual, $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$ denote the eigenvalues of $A(G)$. Let I_1,

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I_2 and I_3 be the unicyclic graphs as shown in Fig. 2.1, and also let G_1, G_2, H_1, H_2, F_1, and F_2 be the graphs as shown in Fig. 2.2.

In view of Theorems 1.5, 2.1 and 2.2, it is natural for us to consider the following problems:

PROBLEM 2.3. Whether Theorem 1.5 also holds for $\rho_n(G)$ $\lambda_n(G)$, and/or $\mu_n(G)$?

PROBLEM 2.4. Whether Theorems 2.1 and 2.2 also hold for any connected simple c-cyclic graphs?

The answer to Problem 2.3 is negative, since $\lambda_n(G) = 0$ holds for any graph and we have the following example.

EXAMPLE 2.5. Let $\pi_1 = (3, 3, 2, 1, 1)$, $\pi_2 = (3, 2, 2, 2, 1)$ and $\pi_3 = (2, 2, 2, 2, 2)$. By an elementary computation, I_1, I_2 and I_3 are the graphs with minimal smallest adjacency eigenvalues (respectively, minimal smallest signless Laplacian eigenvalues) in $S(\pi_1)$, $S(\pi_2)$ and $S(\pi_3)$, respectively. Clearly, $\pi_3 \lhd \pi_2 \lhd \pi_1$, but $\rho_n(I_1) = \rho_n(I_3) > \rho_n(I_2)$ and $\mu_n(I_1) = \mu_n(I_3) > \mu_n(I_2)$.

REMARK 2.6. Since the "symmetrical property" of the eigenvalues of $A(G)$ for a bipartite graph [12], Theorem 2.1 implies that "Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Suppose T and T' are the extremal trees with minimal smallest adjacency eigenvalues in $S(\pi)$ and $S(\pi')$, respectively. Then, $\rho_n(T) > \rho_n(T')$".

The answer to Problem 2.4 is also negative, since we have the following three examples.

EXAMPLE 2.7. [41] Let $\pi = (4, 3, 3, 3, 2, 2, 1)$ and $\pi' = (4, 4, 3, 2, 2, 2, 1)$. By the data of the spectra of connected graphs with seven vertices [12], G_1 and G_2 are the graphs with maximal spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \lhd \pi'$, but $\rho(G_1) > \rho(G_2)$.

EXAMPLE 2.8. [28] Let $\pi = (5, 4, 3, 3, 2, 2, 1)$ and $\pi' = (5, 4, 4, 2, 2, 2, 1)$. By the table of the connected graphs with seven vertices [12], H_1 and H_2 are the graphs with maximal signless Laplacian spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \lhd \pi'$, but $\mu(H_1) > \mu(H_2)$.

EXAMPLE 2.9. [28] Let $\pi = (4, 2, 2, 2, 1, 1)$ and $\pi' = (4, 3, 2, 1, 1, 1)$. By the table of the connected graphs with six vertices [13], F_1 and F_2 are the graphs with maximal Laplacian spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \lhd \pi'$, but $\lambda(F_1) > \lambda(F_2)$.

Though the answers to Problems 2.3 and 2.4 are negative, the majorization theorem also holds for the maximal (signless Laplacian) spectral radii between two degree

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sequences with special restriction, as we will see below. To this aim we introduce another important concept.

If $\pi \lhd \pi'$ are two degree sequences of simple c-cyclic graphs, and there exists some t $(1 \leq t \leq n)$ such that $d'_t \geq c+1$ and $d_i = d'_i$ holds for all $t+1 \leq i \leq n$, then the majorization $\pi \lhd \pi'$ is called a *normal majorization* [37].

Clearly, a normal majorization must also be a majorization, but not the Vice-Versa. For example, we have

EXAMPLE 2.10. [37] Let $\pi_1 = (4,4,3,2,1,1,1)$, $\pi_2 = (5,4,2,2,1,1,1)$ and $\pi_3 = (5,3,3,2,1,1,1)$. Then, π_1, π_2 and π_3 are three bicyclic degree sequences. One can easily see that $\pi_1 \lhd \pi_2$ is a majorization, but not a normal majorization, while $\pi_1 \lhd \pi_3$ is a normal majorization.

Actually, when $\pi \lhd \pi'$ are two degree sequences of trees, then $\pi \lhd \pi'$ must be also a normal majorization. Thus, Theorem 2.1 can be improved to

THEOREM 2.11. *Let π and π' be two different non-increasing c-cyclic $(c \geq 0)$ degree sequences, and let G and G' be the maximal extremal graphs in $S(\pi)$ and $S(\pi')$, respectively. If $\pi \lhd \pi'$ and it is a normal majorization, then* [37] *$\rho(G) < \rho(G')$, and* [28] *$\mu(G) < \mu(G')$.*

Furthermore, some other majorization theorems between two special degree sequences were given in Liu [30]. For instance, the following is one of them.

THEOREM 2.12. [30] *Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two different c-cyclic degree sequences, and let G and G' be the maximal extremal c-cyclic graphs of $S(\pi)$ and $S(\pi')$, respectively. Suppose $\pi \lhd \pi'$, $d_1 = d'_1$ and $c \geq 4$. If there exists some t such that $d'_t \geq c-1$ and $d_i = d'_i$ holds for all $1+t \leq i \leq n$, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.*

Astoundingly, when we relax the condition "simple connected graphs" to "general connected graphs", the result becomes more appealing. In Liu and Liu [40], the following result was proved.

THEOREM 2.13. [40] *Let π and π' be two different non-increasing degree sequences, and let G and G' be the maximal extremal graphs in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd \pi'$, then $\rho(G) < \rho(G')$, and $\mu(G) < \mu(G')$.*

As claimed in [40], if π is a degree sequence of trees, then $S(\pi) = \Gamma(\pi)$. So, Theorem 2.13 is another extension to Theorem 2.1.

Given a connected simple graph $G = (V, E)$, the *discrete p-Laplacian* $L_p(G)$ of a column vector $g = (g(v_1), g(v_2), \ldots, g(v_n))^T$ defined on $V(G)$ $(1 < p < \infty)$ is given

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by

$$L_p(G)g(v) = \sum_{u\in V, uv\in E} (g(v) - g(u))^{[p-1]},$$

where the symbol $t^{[q]}$ denotes a "power" function that preserves the sign of t, i.e., $t^{[q]} = \text{sign}(t)|t|^q$. In Bıyıkoğlu et al. [10], it is shown that $L_2(G) = L(G)$ and $L_2(G)$ is a non-linear operator. If there exists a column vector g ($\neq 0$) defined on $V(G)$ such that $L_p(G)g(v) = \lambda g(v)^{[p-1]}$, then the real number λ is called an *eigenvalue of* $L_p(G)$. Denote by $\lambda_p(G)$ the maximal eigenvalue of $L_p(G)$.

As another extension to Theorem 2.1, Bıyıkoğlu et al. [10] showed that

THEOREM 2.14. [10] *Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Let T and T' be the maximal extremal trees in $S(\pi)$ and $S(\pi')$, respectively. Then, $\lambda_p(T) < \lambda_p(T')$.*

Furthermore, Zhang and Zhang [53] extended Theorem 2.14 to p-Laplacian spectral radii of weighted trees with a positive weight set.

For any $k \geq 0$, the k-th *spectral moment* of G is defined by $Z_k(G) = \sum_{i=1}^n \rho_i^k(G)$. Very recently, Andriantiana and Wagner [1] showed that

THEOREM 2.15. [1] *Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Let T and T' be the trees with maximal k-th spectral moments in $S(\pi)$ and $S(\pi')$, respectively. Then, $Z_k(T) \leq Z_k(T')$. Furthermore, if $k \geq 4$ is even, then the inequality is strict.*

2.2. How to prove the majorization theorem of graph spectrum. The fundamental tool to prove Proposition 1.2, Conjecture 1.3 and Conjecture 1.4 depends on Theorem 1.1. Different from this, the proofs to majorization theorems of (signless Laplacian) spectral radii are based on the structure of maximal extremal graphs of $S(\pi)$. Thus, the investigation of majorization theorem is closely related with the maximal extremal graphs of $S(\pi)$. In this section, we shall introduce some results on the maximal extremal graphs of $S(\pi)$, and we first need the important concepts of BFS-ordering and BFS-graphs. The BFS-ordering was firstly introduced by Pruss in [46] and called the *spiral like ordering*. Bıyıkoğlu and Leydold [9] found that the extremal graphs with maximal spectral radii of $S(\pi)$ are BFS-graphs, and Zhang [55] discovered that the extremal graphs with maximal signless Laplacian spectral radii of $S(\pi)$ are also BFS-graphs. The following concept proposed by Liu [30] is originally from [9, 55].

DEFINITION 2.16. [9, 30, 55] Let G be a connected graph and f be the Perron vector of G. A well-ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ is called a *BFS-ordering* if the following hold for all vertices $u, v \in V(G)$:

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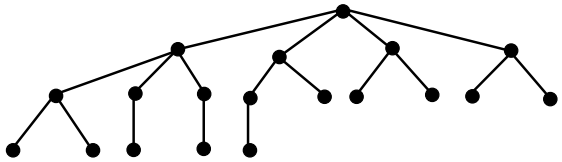


FIG. 2.3. *The BFS-tree T_π^*.*

(*i*) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$, $f(v_1) \geq f(v_2) \geq \cdots \geq f(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1.

(*ii*) If $v \in N(u)\backslash N(x)$, $y \in N(x)\backslash N(u)$ such that $h(u) = h(x) = h(v) - 1 = h(y) - 1$, then $f(u) > f(x)$ if and only if $f(v) > f(y)$, and $f(u) = f(x)$ if and only if $f(v) = f(y)$.

Furthermore, if $V(G)$ has a BFS-ordering, then G is called a *BFS-graph*.

A BFS-tree is also called a greedy tree in [47, 48]. For example, for a given tree degree sequence $\pi^* = (4, 4, 3, 3, 3, 3, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$, T_π^* is the BFS-tree of order 19 (see Fig. 2.3). Bıyıkoğlu and Leydold [9] and Zhang [55], independently, showed the following theorem.

THEOREM 2.17. [9, 55] *Let π be a tree degree sequence. Then, there is a unique BFS-tree, which is the maximal extremal tree of $S(\pi)$.*

Let U_π^* be the unique unicyclic graph in $S(\pi)$, where v_1, v_2 and v_3 are mutually adjacent to form C, the unique cycle of U_π^*, and the remaining vertices appear in BFS-ordering with respect to C starting from v_4 which is adjacent to v_1 [3, 55].

THEOREM 2.18. [3, 55] *Let π be a unicyclic degree sequence. Then, U_π^* is the unique maximal extremal unicyclic graph of $S(\pi)$.*

Denote by $\mathcal{R}(G)$ the reduced graph obtained from G by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. If G is a connected c-cyclic graph, it is easy to see that $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a connected c-cyclic graph.

Let $\theta(p_1, p_2, \ldots, p_r)$ denote the graph, which is obtained from r vertex-disjoint paths (of orders $p_1 + 1$, $p_2 + 1$, $\ldots$, $p_r + 1$, respectively) by identifying the r initial (respectively, terminal) vertices of them. Specially, let $B_D = \theta(2, 1, 2)$ be the bicyclic graph such that $V(B_D) = \{v_1, v_2, v_3, v_4\}$ and $E(B_D) = \{v_1v_2, v_1v_3, v_1v_4, v_2v_3, v_2v_4\}$.

Let $C(q_1, q_2, \ldots, q_r)$ denote the graph obtained from r cycles C_{q_1}, C_{q_2}, $\ldots$, C_{q_r} by identifying a vertex of them. If $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence, π should be one of the following four cases since $\sum_{i=1}^n d_i = 2n + 2$ (recently, Bianchi et al. [6] presented the characterization of integers $n - 1 \geq d_1 \geq d_2 \geq \cdots \geq d_n$ to be the

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degree sequence of a c-cyclic graph for $0 \leq c \leq 6$). Moreover, we construct a special bicyclic graph B_π^* with degree sequence π as follows (For more detail, see [25, 42]).

(1) $\pi = (4, 2, \ldots, 2)$. Let $B_\pi^* = C(3, n-2)$.

(2) $\pi = (3, 3, 2, \ldots, 2)$. Let $B_\pi^* = \theta(1, 2, n-2)$.

(3) $d_n = 1$ and $d_2 = 2$. Then we have $d_1 > 4$, $d_i = 2$ $(i = 3, 4, 5)$, and $d_j \leq 2$ $(6 \leq j \leq n-1)$. Denote by B_π^* the bicyclic graph of order n obtained from $C(3,3)$ by attaching $d_1 - 4$ paths of almost equal lengths (i.e., their lengths differ by at most one) to v_1 of $C(3,3)$.

(4) $d_n = 1$ and $d_1 \geq d_2 \geq 3$. Let B_π^* be the bicyclic graph with $\mathcal{R}(B_\pi^*) = B_D$, and the remaining vertices appear in BFS-ordering with respect to B_D starting from v_5 that is adjacent to v_1.

THEOREM 2.19. [25, 42] *Let π be a bicyclic degree sequence. Then, B_π^* is the unique maximal extremal bicyclic graph of $S(\pi)$.*

For the case of tricyclic graphs, the maximal extremal graphs become much more complicated.

THEOREM 2.20. [30] *Let π be a tricyclic degree sequence, and let J_π^* be a maximal extremal tricyclic graph of $S(\pi)$. Suppose $P_{n-4} = w_1 w_2 \ldots w_{n-4}$.*

(1) *If $d_1 = 6$ and $d_2 = \cdots = d_n = 2$, then $J_\pi^* = C(3, 3, n-6)$;*
(2) *If $d_1 = 5$, $d_2 = 3$ and $d_3 = \cdots = d_n = 2$, then J_π^* is obtained from B_D and P_{n-4} by adding two edges v_1w_1 and v_1w_{n-4};*
(3) *If $d_1 = d_2 = 4$ and $d_3 = \cdots = d_n = 2$, then $J_\pi^* = \theta(2, 1, 2, n-3)$;*
(4) *If $d_1 = 4$, $d_2 = d_3 = 3$ and $d_4 = \cdots = d_n = 2$, then J_π^* is obtained from B_D and P_{n-4} by adding two edges v_1w_1 and v_3w_{n-4};*
(5) *If $d_1 = d_2 = d_3 = d_4 = 3$ and $d_5 = \cdots = d_n = 2$, then J_π^* is obtained from B_D and P_{n-4} by adding two edges v_3w_1 and v_4w_{n-4}.*

In the following, let J_1, J_2, …, J_6 be the tricyclic graphs as shown in Fig. 2.4. Let W_1 (respectively, W_2, W_5, W_6) be the unique tricyclic graph with $\mathcal{R}(W_1) = J_1$ (respectively, $\mathcal{R}(W_2) = J_2$, $\mathcal{R}(W_5) = J_5$, $\mathcal{R}(W_6) = J_6$), and the remaining vertices appear in BFS-ordering with respect to J_1 (respectively, J_2, J_5, J_6) starting from v_5 (respectively, v_6 , v_7, v_6) that is adjacent to v_1. Denote W_3 the unique tricyclic graph with $\mathcal{R}(W_3) = J_3$ so that the remaining vertices appear in BFS-ordering with respect to J_3 starting from v_6 that is adjacent to v_5. Let W_4 be the unique tricyclic graph obtained from J_4 by attaching k paths of almost equal lengths to v_1 of J_4.

THEOREM 2.21. [30] *Let π be a tricyclic degree sequence and let J_π^* be a maximal extremal tricyclic graph of $S(\pi)$ with $d_n = 1$.*

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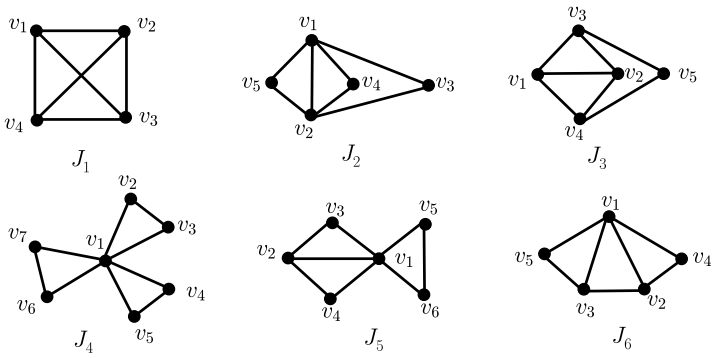


FIG. 2.4. *The tricyclic graphs J_1, J_2, ..., J_6.*

(1) *If $d_1 \geq 4$ and $d_4 \geq 3$, then $J_\pi^* = W_1$ or $J_\pi^* = W_2$;*
(2) *If $d_1 = 3$ and $d_4 = 3$, then $J_\pi^* = W_3$;*
(3) *If $d_2 = d_3 = d_4 = 2$, then $J_\pi^* = W_4$;*
(4) *If $d_2 = 3$ and $d_3 = d_4 = 2$, then $J_\pi^* = W_5$;*
(5) *If $d_2 = d_3 = 3$ and $d_4 = 2$, then $J_\pi^* = W_6$;*
(6) *If $d_2 \geq 4$ and $d_4 = 2$, then $J_\pi^* = W_2$.*

For the general case, some properties were given to the maximal extremal graphs of $S(\pi)$ [9, 30, 55], and the main property of maximal extremal graphs of $S(\pi)$ is

THEOREM 2.22. [9, 30, 55] *Suppose π is a non-increasing degree sequence. If G is a maximal extremal graph of $S(\pi)$, then it is a BFS-graph.*

Recently, more extra properties of maximal extremal graphs of $S(\pi)$ were added by Liu in [30]. Furthermore, for the maximal extremal graphs of $\Gamma(\pi)$, similar results as those in Theorem 2.22 were obtained in Liu and Liu [40].

Theorem 2.22 shows that the maximal extremal graphs of $S(\pi)$ are BFS-graphs, but the BFS-graphs of $S(\pi)$ are not unique. Thus, from Theorems 2.17–2.20, it is natural for us to consider the following question: Whether the maximal extremal graph of $S(\pi)$ is unique for any c-cyclic degree sequence π? Actually, Belardo et al. [3] conjectured that the answer is positive.

CONJECTURE 2.23. [3] *Let π be a c-cyclic degree sequence. Then, the extremal graph with the maximal spectral radius of $S(\pi)$ is unique.*

It is rather interesting that the structure of maximal extremal graphs of $S(\pi)$ is not unique, as the size of the relationship between W_1 and W_2 in Theorem 2.21 is uncertain [30]. Actually, Belardo et al. [3] gave a routine to build the maximal extremal graph, but a counterexample to the routine was given by Liu [30] (see Example 24 of

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[30]).

At the end of this section, let us come back to deal with the proof of majorization theorems of (signless Laplacian) spectral radii. In addition to the maximal extremal graphs theo- rems, the following results hold.

PROPOSITION 2.24. [50, 54] *Let u, v be two vertices of the connected graph G, and $w_1, w_2, \ldots, w_k$ $(1 \leq k \leq d(v))$ be some vertices of $N(v) \setminus (N(u) \cup \{u\})$. Let G' be a new graph obtained from G by deleting the edges w_1v, ..., w_kv, and then adding the edges w_1u, ..., w_ku. Suppose f is the Perron vector of G. If $f(u) \geq f(v)$, then $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$.*

If $d = (d_1, d_2, \ldots, d_n)$ is a non-increasing integer sequence and $d_i \geq d_j + 2$, then the following operation is called a *unit transformation from i to j on d*: subtract 1 from d_i and add 1 to d_j. The following famous majorization of integer sequences, is due to Muirhead (see [44]).

PROPOSITION 2.25. [44] (*Muirhead's Lemma*) *If d and d' are two non-increasing integer sequences and $d \lhd d'$, then d can be obtained from d' by a finite sequence of unit transformations.*

Suppose $\pi \lhd \pi'$, G and G' are the maximal extremal graphs of $\Gamma(\pi)$ and $\Gamma(\pi')$ (or $S(\pi)$ and $S(\pi')$), respectively. In order to prove the majorization theorems of (signless Laplacian) spectral radii, by Proposition 2.25, we may always suppose that π and π' differ only in two positions where the difference is 1, that is, $d_i = d'_i$, $i \neq p, q$, $1 \leq p < q \leq n$, and $d'_p = d_p + 1$, $d'_q = d_q - 1$. In this case, $\pi \lhd \pi'$ is also called a *star majorization* and written as $\pi \lhd^* \pi'$ [26]. Let $P_{v_pv_q}$ be a shortest path from v_p to v_q. By the choice of G and $p < q$, $f(v_p) \geq f(v_q)$ follows from Theorem 2.22 and Definition 2.16. In the following, if w is a vertex of G such that $w \in N(v_q) \setminus (N(v_p) \cup \{v_p\})$ and $w \notin V(P_{v_pv_q})$, then we call w a *surprising vertex of G*. If G contains some surprising vertex, say w, let $G^* = G + v_pw - v_qw$. Then, $G^* \in \Gamma(\pi')$. Since $f(v_p) \geq f(v_q)$, by Proposition 2.24, $\rho(G) < \rho(G^*) \leq \rho(G')$ and $\mu(G) < \mu(G^*) \leq \mu(G')$. Therefore, if G contains a surprising vertex, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.

Generally speaking, a surprising vertex cannot always exist for $G \in S(\pi)$, as the case $N(v_p) = N(v_q)$ may occur. That is the reason "why majorization theorems cannot hold for any c-cyclic graphs". But from the structure of maximal extremal graph G as described in Theorems 2.17–2.19, we can deduce that G must contain a surprising vertex if G is a maximal extremal graph of $S(\pi)$ when $c \in \{0, 1, 2\}$. In the following, as an illustrated example, we will provide the proof of Theorem 2.2. Actually, the main idea of the proofs of Theorems 2.1, 2.2, 2.11–2.14 is similar.

Proof of Theorem 2.2. By Proposition 2.25, we may suppose that $\pi \lhd^* \pi'$. Theorem 2.18 implies that $U = U^*_\pi$. If $2 \leq q \leq 3$, then $d_q \geq 3$ and $v_q \in C_3$ since $U' \in S(\pi')$.

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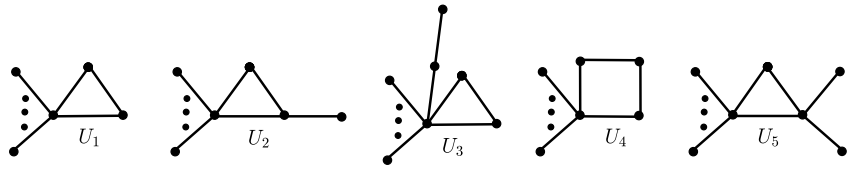


FIG. 2.5. *The unicyclic graphs U_1, U_2, U_3, U_4 and U_5.*

If $q \geq 4$, then $d_q \geq 2$ and v_q does not lie on any cycle. In both cases, there exists a vertex v_k $(k > q)$ such that $v_k \in N(v_q) \setminus (N(v_p) \cup \{v_p\})$ and $v_k \notin V(P_{v_p v_q})$, namely, v_k is a surprising vertex. Let U'' be the graph obtained from U by deleting the edge $v_q v_k$, and then adding the edge $v_p v_k$. Note that U'' is connected and $U'' \in S(\pi')$. By Proposition 2.24, $\rho(U) < \rho(U'') \leq \rho(U')$. □

2.3. The application of majorization theorem to graph spectrum. In 1981, Cvetković [11] indicated 12 directions for further investigations of graph spectra, one of which is classifying and ordering graphs. Hence, ordering graphs with various properties by their spectra, especially by their (Laplacian) spectral radii, became an attractive topic (see [24, 35, 43]). Up to now, more than 50 papers were published on this item, but a simple and general method has not yet been obtained. Not long before, we found that the majorization theorem is a good tool to deal with the above Cvetkovic's problem on the ordering of graphs according to their largest (signless Laplacian) spectral radii [35].

Next we will use an examples to illustrate the application of the majorization theorem to solve Cvetković's problem. Let $\mathbb{U}_n$ be the class of unicyclic graphs on n vertices, and $\mathbb{U}_{n,k}$ be the class of unicyclic graphs with n vertices and k pendant vertices.

EXAMPLE 2.26. Let $U_1, U_2, \ldots, U_5$ be the unicyclic graphs on n vertices as shown in Fig. 2.5. Clearly, U_1 is the unique unicyclic graph with $d_1 = n - 1$, U_2, U_3, U_4 are all the unicyclic graphs with $d_1 = n - 2$.

If $U \in \mathbb{U}_n \setminus \{U_1, U_2, \ldots, U_5\}$, then $d_1(U) \leq n-3$. Let $(b) = (n-3, 4, 2, 1, \ldots, 1)$. It is easily checked that U_5 is the unique unicyclic graph with (b) as its degree sequence. Suppose the degree sequence of U is $(a) = (d_1, d_2, d_3, \ldots, d_n)$. Then, $(a) \lhd (b)$, and hence, $\rho(U) < \rho(U_5)$ follows from Theorem 2.2.

Clearly, U_1 is the unique unilcyclic graph with $(c) = (n-1, 2, 2, 1, \ldots, 1)$ as its degree sequence, U_2 is the unique unilcyclic graph with $(d) = (n-2, 3, 2, 1, \ldots, 1)$ as its degree sequence and $S(e) = \{U_3, U_4\}$, where $(e) = (n-2, 2, 2, 2, 1, \ldots, 1)$. Since $(e) \lhd (d) \lhd (c)$, $\rho(U_3) < \rho(U_2) < \rho(U_1)$ according to Theorem 2.2. From Theorem 2.18, $\rho(U_4) < \rho(U_3)$.

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Let $\Phi(G,x)$ denote the characteristic polynomial of $A(G)$. By an elementary computation, it easily follows that

$$\Phi(U_4,x) = x^{n-4}\left(x^4 - nx^2 + 2n - 8\right), \tag{2.1}$$

$$\Phi(U_5,x) = x^{n-4}\left(x^4 - nx^2 - 2x + 3n - 13\right). \tag{2.2}$$

From Equation (2.1), it is easy to see that $\rho(U_4) = \sqrt{\frac{n+\sqrt{n^2-8n+32}}{2}} < \sqrt{n}$ when $n \geq 12$. When $x \geq \sqrt{n}$ and $n \geq 12$, by Equations (2.1) and (2.2), we have

$$\Phi(U_5,x) - \Phi(U_4,x) = x^{n-4}(n-5-2x) \geq n^{\frac{n-4}{2}}(n-5-2\sqrt{n}) > 0.$$

Thus, $\rho(U_5) < \rho(U_4)$, and hence $\rho(U) < \rho(U_5) < \rho(U_4) < \rho(U_3) < \rho(U_2) < \rho(U_1)$ when $n \geq 12$. Now, the five unicyclic graphs with the first five largest spectral radii in $\mathbb{U}_n$ are determined for $n \geq 12$.

As mentioned before, the majorization theorem holds for the maximal (signless Laplacian) spectral radii of the extremal graphs between two classes of trees, unicyclic and bicyclic graphs with given degree sequences. Thus, as claimed in Liu and Liu [35], it is not a difficult problem to order trees, unicyclic graphs and bicyclic graphs via their largest (signless Laplacian) spectral radii by applying the corresponding majorization theorem. But unfortunately, the majorization theorem can not holds for general c-cyclic graphs, and hence, this method cannot be applied to deal with Cvetković's problem in the general case.

The majorization theorem is also effective when we deal with the other extremal problems in some special graph categories. For instance,

Example 2.27. Suppose $U \in \mathbb{U}_{n,k}$, and suppose the degree sequence of U is $(a) = (d_1, d_2, \ldots, d_{n-k}, 1, \ldots, 1)$, where the multiplicity of 1 is k. Let $(b) = (k+2, 2, 2, \ldots, 2, 1, \ldots, 1)$, where the multiplicity of 1 is k. If $(a) \neq (b)$, then $(a) \lhd (b)$. By Theorems 2.2 and 2.18, $\rho(U) < \rho(U^*)$, where U^* is obtained from a triangle by attaching k paths of almost equal lengths to a vertex of the triangle.

More examples on the application of majorization theorem to the extremal problem of graph spectrum can be referred to [25, 54, 55].

3. The majorization theorem of topological index. In this section, we will explain how the theory of majorization can be applied to face other problems in different branches of graph theory; in particular we will focus on some theorems concerning topological indices.

The first and second Zagreb indices are, respectively, defined as

$$M_1(G) = \sum_{v \in V(G)} d^2(v), \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

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The first and second Zagreb indices are two important topological indices, which were first introduced by Gutman and Trinajstić in 1972 [22]. Before 2009, similar with the case of (signless Laplacian) spectral radii, many papers concerned with the ordering of $M_1(G)$ and $M_2(G)$ among some given graph categories were published [15, 51], but a simple and general method has not yet been obtained.

In 2009, Liu [29] proved that the majorization theorem holds for the first Zagreb index for any c-cyclic graphs. That is

THEOREM 3.1. [29] *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $M_1(G) < M_1(G')$.*

By applying Theorem 3.1, Liu extended [29] almost all known results before 2009 on the ordering of the first Zagreb index in some given graph categories like c-cyclic graphs. Note that the proof of Theorem 3.1 follows easily from Corollary 1.7, since the function $\varphi(x) = x^2$ is strictly convex. A similar approach allowed Liu and Liu to extend Theorem 3.1 in [32] to the first general Zagreb index $M_1^\alpha(G) = \sum_{v \in V} d(v)^\alpha$ [27], where α is a given real number not equal to 0 and 1.

THEOREM 3.2. [32] *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. Suppose $G \in S(\pi)$ and $G' \in S(\pi')$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G')$;*
(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G')$.*

Motivated from the definition of $M_1(G)$ and $M_2(G)$, Došlić [16] defined two new graphical invariants $\overline{M_1(G)}$ and $\overline{M_2(G)}$, where

$$\overline{M_1(G)} = \sum_{uv \notin E(G)} (d(u) + d(v)), \qquad \overline{M_2(G)} = \sum_{uv \notin E(G)} d(u)d(v).$$

Došlić called $\overline{M_1(G)}$ and $\overline{M_2(G)}$, the first and second Zagreb coindices of G, respectively. For the relationship between $M_1(G)$ and $\overline{M_1(G)}$, it is well-known that $\overline{M_1(G)} = 2m(n-1) - M_1(G)$ [2]. Thus, from Theorem 3.1, we have

THEOREM 3.3. [31] *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $\overline{M_1(G)} > \overline{M_1(G')}$.*

The first and second multiplicative Zagreb indices of a connected graph G, are defined as $\prod_1(G) = \prod_{v \in V(G)} d^2(v)$ and $\prod_2(G) = \prod_{uv \in E(G)} d(u)d(v)$, respectively [21]. Recently, by applying Corollary 1.7, Eliasi proved that

THEOREM 3.4. [17] *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $\prod_1(G) > \prod_1(G')$ and $\prod_2(G) < \prod_2(G')$.*

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While the proofs of Theorem 3.1–3.4 are essentially based on Corollary 1.7, it is not evident how $M_2(G)$ can be expressed as a suitable Schur-convex function in order to apply Corollary 1.7. To this point we can refer the reader to Bianchi et al. [5]. However, up to now, the following majorization theorem holds for $M_2(G)$.

THEOREM 3.5. [38, 39, 52] *Let π and π' be two different non-increasing tree (respectively, unicyclic, bicyclic) degree sequences with $\pi \lhd \pi'$. Let G and G' be the trees (respectively, unicyclic graphs, bicyclic graphs) with the maximal second Zagreb indices in $S(\pi)$ and $S(\pi')$, respectively. Then, $M_2(G) < M_2(G')$.*

In Ashrafi et al. [2], it was proved that $\overline{M_2(G)} = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$, and hence, by Theorem 3.5, we have:

THEOREM 3.6. [31] *Let π and π' be two different non-increasing tree (respectively, unicyclic, bicyclic) degree sequences with $\pi \lhd \pi'$. Suppose G and G' have the minimal second Zagreb coindices in $S(\pi)$ and $S(\pi')$, respectively. If $\pi \lhd \pi'$, then $\overline{M_2(G)} > \overline{M_2(G')}$.*

Similar to the proofs of the majorization theorems for (signless Laplacian) spectral radii, the proof of Theorem 3.5 also mainly depends on the structure of the extremal graphs with maximal second Zagreb indices in $S(\pi)$. In 2008, Zhang and Xiang [56] used this method (as to our best knowledge, [56] is the first literature applying the majorization theorem to topological index theory) to prove the majorization theorem for the Wiener index $W(G)$, where $W(G)$ is the sum of topological distances between all pairs of vertices in G [49]. If we use $d(u, v)$ to denote the distance of u and v, then $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v)$.

THEOREM 3.7. [56] *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Suppose T and T' have the minimal Wiener indices in $S(\pi)$ and $S(\pi')$, respectively. Then, $W(T) > W(T')$, and T and T' are the unique BFS-trees of $S(\pi)$ and $S(\pi')$ respectively.*

Let $P_r(T)$ be the number of pairs (u, v) of vertices such that $d(u, v) \leq r$. Recently, as an extension of Theorem 3.7, Wagner et al. [47] showed that

THEOREM 3.8. [47] *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Suppose T and T' have the maximal number of pairs (u, v) of vertices such that $d(u, v) \leq r$ in $S(\pi)$ and $S(\pi')$, respectively, where r is an arbitrary positive integer. Then, $P_r(T) < P_r(T')$, and T and T' are the unique BFS-trees of $S(\pi)$ and $S(\pi')$, respectively.*

Let $\gamma(T)$ denote the number of subtrees of T. The following majorization theorem for $\gamma(T)$ was proved by Zhang et al. [57].

THEOREM 3.9. [57] *Let π and π' be two different non-increasing tree degree*

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sequences with $\pi \lhd \pi'$. Suppose T and T' have the maximal number of subtrees in $S(\pi)$ and $S(\pi')$, respectively. Then, $\gamma(T) < \gamma(T')$, and T and T' are the unique BFS-trees of $S(\pi)$ and $S(\pi')$, respectively.

As shown in Example 2.26, by Theorem 2.2, we can easily determine the first five largest spectral radii in $\mathbb{U}_n$, but it become much more complicated to deal with the smallest case. The crucial problem is that it is a difficult problem to determine the exact value of spectral radius of a given graph. Analogous with the spectral theory, the majorization theorem of topological index can be applied to deal with the ordering or extremal problems of the corresponding topological indices in some given graph categories. Moreover, since the exact values of many topological indices of a given graph can be determined easily, we can obtain a better result when we employ the majorization theorem to deal with the ordering problem of topological indices. For instance,

EXAMPLE 3.10. Let $\pi_1 = (2, 2, 2, \ldots, 2)$, $\pi_2 = (3, 2, 2, \ldots, 2, 1)$ and $\pi_3 = (3, 3, 2, \ldots, 2, 1, 1)$. Suppose $U \in \mathbb{U}_n$. If $\pi(U) \notin \{\pi_1, \pi_2, \pi_3\}$, then $\pi_1 \lhd \pi_2 \lhd \pi_3 \lhd \pi(U)$.

By Theorem 3.1, the cycle has the smallest first Zagreb index in $\mathbb{U}_n$, the unicyclic graphs of $S(\pi_2)$ have the second smallest first Zagreb index in $\mathbb{U}_n$, and the unicyclic graphs of $S(\pi_3)$ have the third smallest first Zagreb index in $\mathbb{U}_n$.

By applying Corollary 1.7, we can obtain good bounds for some topological indices. For instance, by Corollary 1.7, bounds for the sum of the α-th power of the non-zero Laplacian eigenvalues of G were given in [34, 58], for the sum of the α-th power of the non-zero signless Laplacian eigenvalues of G were given in Liu and Liu [36], and for the sum of power of Laplacian Estrada index of G were given in Zhou [59].

Recently, Bianchi et al. [5] presented a unified approach for localizing some relevant graph topological indices via majorization techniques. Furthermore, via characterizing c-cyclic graphs ($0 \leq c \leq 6$) as those whose degree sequence belongs to particular subsets of $\mathbb{R}^n$, Bianchi et al. [6] identified the maximal and minimal vectors of these subsets with respect to the majorization order. They also employed a majorization technique for a suitable class of graphs to derive upper and lower bounds for some topological indices depending on the degree sequence over all vertices. Through this method, old and new bounds can be easily reobtained and improved [5, 6]. If the reader is interested in this topic, he can refer to [5, 6, 7] and the references therein.

4. Further discussion. As referred in the former sections, the majorization theorem has important application in graph spectrum and topological index theory. Actually, lots of open problems were solved by this tool [1, 31, 47, 57]. Thus, we hope

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that more scholars can pay their attention to this interesting research field.

Though several majorization theorems have been proved, a number of questions have been left unsolved. Here, we present two problems for further study.

PROBLEM 4.1. Does there exist some other majorization theorem for graph spectrum (of the orientated or unorientated graph, the hypergraph and so on) or for other topological indices?

PROBLEM 4.2. Give more accurate description of the maximal extremal graphs of $S(\pi)$ or $\Gamma(\pi)$. Furthermore, prove or disprove Conjecture 2.23.

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The strong pseudoachromatic number of a graph*

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Abstract

Given a graph G, partition $V(G)$ into k disjoint subsets $V_1, \ldots, V_k$ such that (a) there is at least one edge in G connecting V_i and V_j $(i \neq j)$, and (b) each $G[V_i]$ (the subgraph of G induced by V_i) contains at least one edge for any $i, j \in \{1, 2, ..., k\}$. The maximum number k for which such a partition exists is called the *strong pseudoachromatic number* of G, and is denoted by $\psi^*(G)$. In this paper, we determine the strong pseudoachromatic number of some special

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family of graphs. We also investigate the relationship between the strong pseudoachromatic number of G and its subgraphs obtained by deleting an edge or a vertex of G, and find some bounds for $\psi^*(G)$. Moreover, we characterize the class of all graphs $\mathcal{G}$ that $\psi^*(G \vee H) = \psi^*(G) + \psi^*(H)$ for any $G, H \in \mathcal{G}$, where $G \vee H$ denotes the join of G and H.

1 Introduction

All graphs considered in this paper are finite, undirected and simple. Let $[k] = \{1, ..., k\}$. A k-coloring of a graph $G = (V, E)$ is a mapping $c : V \to [k]$; thus, a k-coloring is an assignment of k colors to the vertices of G. A k-coloring may be viewed as a partition $\{V_1, V_2, ..., V_k\}$ of V, where each V_i is the color class that contains all the vertices assigned color i in G, $i \in [k]$. A coloring is called a proper coloring if no two adjacent vertices are assigned the same color. A graph is k-colorable if it has a proper k-coloring. The minimum k for which a graph G is k-colorable is called the chromatic number, and is denoted by $\chi(G)$.

A *complete k-coloring* of a graph $G = (V, E)$ is a k-coloring c of G such that, for any two distinct $i, j \in [k]$, there is at least one edge $e = uv \in E(G)$ such that $c(u) = i$ and $c(v) = j$. The maximum k in a complete-coloring of G is called the *pseudoachromatic number* of G, and is denoted by $\Psi(G)$. It was first introduced by Gupta [5]. Obviously, if G has at least one vertex, then $\Psi(G) \geq 1$, where the equality holds if and only if G is an empty graph.

A complete coloring is also called an *achromatic coloring*. The maximum number of colors used in an achromatic coloring of G is called the *achromatic number* of G, and is denoted by $\alpha(G)$.

These colorings were studied extensively. For example, see [4, 8]. The readers are referred to [4–6, 9] for further details of these colorings.

As usual, K_n, P_n and C_n denote the complete graph, the path and the cycle of order n, respectively. Let $K_{n_1,n_2,...,n_s}$ be the complete s-partite

graph. Let c be a k-coloring of G, then G has k color classes, say V_1, ..., V_k. The *partition graph*, denoted by H_G, of G is a simple graph such that $V(H_G) = \{V_1, V_2, ..., V_k\}$, and $i, j \in E(H_G)$ if and only if there is at least one edge between V_i and V_j. Actually, $\chi(G)$ (respectively, $\alpha(G)$) is the minimum (respectively, maximum) number k such that H_G is K_k, and in a chromatic or achromatic coloring a partite set V_i is always an independent set, but, in a pseuduochromatic coloring it is not so. That is, a partite set V_i may be or may not be an independent set in a pseudochromatic coloring. Hence it is easy to see that

$$\chi(G) \leq \alpha(G) \leq \Psi(G). \tag{1}$$

It is interesting for us to consider the following problem.

Problem 1.1 *For any given graph $G = (V, E)$, what is the maximum number k such that the partition graph $H_G \cong K_k$ where the subgraph induced by each element of H_G, denoted $G[V_i]$, contains at least one edge?*

Motivated by Problem 1.1, we establish the following definition.

Definition 1.1 *Let c be a complete k-coloring of a graph $G = (V, E)$ with partite sets $\{V_1, ..., V_k\}$. c is called a strong-k-coloring of G if the subgraph induced by each V_i contains at least one edge. The maximum k used in a strong-k-coloring is called the strong pseudoachromatic number of G, denoted as above by $\psi^*(G)$.*

Even though $\psi^*(G) \leq \Psi(G)$, an inequality of type (1.1) does not hold between χ, α and ψ^*, see Example 1.1.

Example 1.1 (1) $\psi^*(K_2) = 1 < 2 = \chi(K_2)$, $\psi^*(K_{2,2} - e) = 2 = \chi(K_{2,2} - e)$, *and* $\psi^*(K_{3,3}) = 3 > 2 = \chi(K_{3,3})$; (2) $\psi^*(K_{2,2} - e) = 2 < 3 = \alpha(K_{2,2} - e)$, $\psi^*(K_{2,2}) = 2 = \alpha(K_{2,2})$, *and* $\psi^*(K_{3,3}) = 3 > 2 = \alpha(K_{3,3})$.

Let G_1, G_2 be two vertex disjoint graphs. The *join graph* $G_1 \vee G_2$ is the graph with $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and $E(G_1 \vee G_2) = E(G_1) \cup$

$E(G_2) \cup \{(u,v) : u \in V(G_1), v \in V(G_2)\}$. Let W_n be the wheel graph on n vertices (i.e., $W_n = K_1 \vee C_{n-1}$), and F_n be the fan graph on n vertices (i.e., $F_n = K_1 \vee P_{n-1}$). Let $L(G)$ denote the line graph of G. In [7, 9], the pseudoachromatic number of C_n, P_n, K_n, W_n, $L(W_n)$, and $K_{n_1,n_2,\ldots,n_s}$ were determined. The relationship between the pseudoachromatic number of G and its subgraphs obtained by deleting an edge or a vertex were discussed in [3]. Moreover, Bhave also found some bounds for $\Psi(G)$ in [3]. In [1, 14], the relationship between $\Psi(G_1 \vee G_2)$ and $\Psi(G_1) + \Psi(G_2)$ were discussed. For more results related to this topic, one can refer to [2, 10–13].

In this paper, the strong pseudoachromatic numbers of C_n, P_n, K_n, W_n, $L(W_n)$, F_n, $L(F_n)$, and $K_{n_1,n_2,\ldots,n_s}$ are determined. We also discuss the relationship between the strong pseudoachromatic number of G and its subgraphs obtained by deleting an edge or a vertex, and find some bounds for $\psi^*(G)$ in term of the order or the number of edges or the maximum degree of G. Moreover, we characterize the class of all graphs $\mathcal{G}$ that $\psi^*(G \vee H) = \psi^*(G) + \psi^*(H)$ for any $G, H \in \mathcal{G}$.

2 Some properties, bounds and values of $\psi^*(G)$

Theorem 2.1 *Let G be a graph with n vertices, m (≥ 1) edges and maximum degree Δ. Then,*

$$(1)\quad \psi^*(G) \leq \min\left\{\frac{1}{2}\left(\sqrt{8m+1}-1\right), \frac{n}{2}\right\}; \quad (2)\quad \psi^*(G)\left\lceil\frac{\psi^*(G)+1}{\Delta}\right\rceil \leq n.$$

Proof. Suppose that V_i is a color class of a strong-ψ^*-coloring of G, $i \in [\psi^*]$. Since $H_G = K_{\psi^*}$, and each $G[V_i]$ contains at least one edge, $\psi^* + \frac{1}{2}\psi^*(\psi^*-1) \leq m$ and $2\psi^* \leq n$, which implies (1).

Let $|V_i| = x$. Since there are at least $\psi^* - 1$ edges between V_i and the other color classes, $\Delta(x-2) + 2(\Delta-1) \geq \psi^* - 1$. So, $x \geq \lceil\frac{\psi^*+1}{\Delta}\rceil$, and hence $n \geq \psi^*\lceil\frac{\psi^*+1}{\Delta}\rceil$. ∎

Corollary 2.1 $\psi^*(K_n) = \lfloor\frac{n}{2}\rfloor$.

Remark 2.1 Let $m(G)$ be the number of edges in G. By the proof of Theorem 2.1, $m(G) \geq \binom{\psi^*(G)+1}{2}$. Similarly, we have $m(G) \geq \binom{\Psi(G)}{2}$ and $n \geq \Psi(G)\left\lceil \frac{\Psi(G)-1}{\Delta} \right\rceil$, where $\Delta \geq 1$.

The next result presents a relation between $\psi^*(G)$ and $\Psi(G)$.

Theorem 2.2 *For any graph G, $\lfloor \frac{\Psi(G)}{2} \rfloor \leq \psi^*(G) \leq \Psi(G)$.*

Proof. It suffices to show the lower bound. Let $\Psi(G) = t$, and V_1, ..., V_t be the color classes of a complete-t-coloring of G. If $0 \leq t \leq 1$, the lower bound follows naturally. Thus, we may suppose that $t \geq 2$ in the following.

If t is even, we color V_1 and V_t with color 1, V_2 and V_{t-1} with color 2, ..., $V_{\frac{t}{2}}$ and $V_{\frac{t}{2}+1}$ with color $\frac{t}{2}$. Then, we obtain a strong-$\frac{t}{2}$-coloring of G. If t is odd, we color V_1, $V_{\frac{t+1}{2}}$ and V_t with color 1, V_2 and V_{t-1} with color 2, ..., $V_{\frac{t-1}{2}}$ and $V_{\frac{t+3}{2}}$ with color $\frac{t-1}{2}$. Then, we obtain a strong-$\frac{t-1}{2}$-coloring of G. Thus, the lower bound follows. ∎

Corollary 2.2 *Let G be a graph of order n. Then $0 \leq \Psi(G) - \psi^*(G) \leq \lceil \frac{n}{2} \rceil$.*

Lemma 2.1 *Let H be the graph obtained from $K_{s,s}$ by deleting a perfect matching. If $s \geq 3$, then $\psi^*(H) = \Psi(H) = s$.*

Proof. Note that $\Psi(H) \geq s+1$ would imply that H has at least $2(s+1)$ vertices since $\Delta(H) = s-1$. So, $\Psi(H) \leq s$.

Let $V_i = \{v_{ij} : 1 \leq j \leq s\}$ be the i-th part of $K_{s,s}$ for $1 \leq i \leq 2$. Without loss of generality, let $v_{11}v_{21}$, $v_{12}v_{22}$, ..., $v_{1s}v_{2s}$ be the s edges being deleted from $K_{s,s}$. Let $c(v_{1j}) = j$ for $1 \leq j \leq s$, $c(v_{2j}) = j-1$ for $2 \leq j \leq s$ and $c(v_{21}) = s$. It is easy to see that c is a strong-s-coloring of H. Thus, $\psi^*(H) \geq s$, and hence the result follows from Theorem 2.2. ∎

Proposition 2.1 *Let s, t be two positive integers with $s \geq 3$ and $s \geq t \geq \lfloor \frac{s}{2} \rfloor$. Then there exists a graph G such that $\psi^*(G) = t$ and $\Psi(G) = s$.*

Proof. If $s = t$, then we can invoke Lemma 2.1 to prove the result. If $s > t = \lfloor \frac{s}{2} \rfloor$, let $G = K_s$, then the result follows from Corollary 2.1. So, we consider the case of $s > t > \lfloor \frac{s}{2} \rfloor$.

Let $G = K_s \cup (2t - s)K_2$. It suffices to show the following two Facts.

Fact 1. $\Psi(G) = s$.

Proof of Fact 1. Since K_s is a subgraph of G, $\Psi(G) \geq s$. If $\Psi(G) \geq s+1$, then $m(G) \geq \binom{s+1}{2}$ by Remark 2.1. But $m(G) = \binom{s}{2} + 2t - s < \binom{s}{2} + s = \binom{s+1}{2}$, a contradiction. Thus, $\Psi(G) = s$.

Fact 2. $\psi^*(G) = t$.

Proof of Fact 2. We color the i-th pair of vertices of K_s by the color i for $1 \leq i \leq s - t$, and color the i-th vertex of the left $2t - s$ vertices of K_s by the color $s - t + i$ for $1 \leq i \leq 2t - s$, and then color the i-th edge of $(2t - s)K_2$ by the color $s - t + i$ for $1 \leq i \leq 2t - s$. It is easy to check that c is a strong-t-coloring for G. Thus, $\psi^*(G) \geq t$.

Let $\psi^*(G) = k$. Then, G has a strong-k-coloring with color classes V_1, V_2, ..., V_k. Assume to the contrary, $k \geq t + 1$. If there exists some i $(1 \leq i \leq k)$ such that $V_i \cap K_s = \emptyset$, then by Definition 1.1, $2t - s = m(G \setminus K_s) \geq k \geq t + 1$, and hence $t \geq s + 1$, a contradiction. Thus, $V_i \cap K_s \neq \emptyset$ holds for $1 \leq i \leq k$. Suppose that there are x colors which color exactly one vertex of K_s. Since $G[V_i]$ contains at least one edge, $x \leq 2t - s$. Thus, $k \leq x + \frac{s-x}{2} = \frac{s+x}{2} \leq t$, a contradiction. ∎

Remark 2.2 If $\psi^*(G) = 2$, by Remark 2.1 $m(G) \geq 3$, and hence $\Psi(G) \geq 3$. So, there does not exist a graph G with $\Psi(G) = \psi^*(G) = 2$. Moreover, $\Psi(K_2) = 2$, and $\psi^*(K_2) = 1$.

In [3], Bhave proved that $\Psi(G) \geq \Psi(G - v) \geq \Psi(G) - 1$ and $\Psi(G) \geq \Psi(G - e) \geq \Psi(G) - 1$. In the following, we will give the analogous result for $\psi^*(G)$.

Proposition 2.2 *Let $v \in V$, $e \in E$ be a vertex and an edge of the graph $G = (V, E)$. Then, $\psi^*(G) \geq \psi^*(G - v) \geq \psi^*(G) - 1$ and $\psi^*(G) \geq \psi^*(G - e) \geq \psi^*(G) - 1$.*

Proof. Clearly, a strong-$\psi^*(G-v)$-coloring of $G-v$ yields a strong-$\psi^*(G-v)$-coloring of G, and so does strong-$\psi^*(G-e)$-coloring. Thus, $\psi^*(G) \geq \psi^*(G-v)$ and $\psi^*(G) \geq \psi^*(G-e)$.

Suppose that $\psi^*(G) = t$ and V_1, ..., V_t are the color classes of a strong-t-coloring of G. Without loss of generality, suppose that $v \in V_t$. We can obtain a strong-$(t-1)$-coloring of $G-v$ by coloring $V_t - v$ with the color $t-1$, and V_i with the color i for $1 \leq i \leq t-1$. Thus, $\psi^*(G-v) \geq \psi^*(G)-1$.

Suppose $e = uv$. Then, either u and v belong to the same color class, say V_t, or different color classes, say $u \in V_t$ and $v \in V_{t-1}$. We can obtain a strong-$(t-1)$-coloring of $G-e$ by coloring V_t with the color $t-1$, and V_i with the color i for $1 \leq i \leq t-1$. Thus, $\psi^*(G-e) \geq \psi^*(G)-1$. ∎

Theorem 2.3 *For any $n \geq 3$,*

$$\psi^*(C_n) = \begin{cases} 2k-1 & if \quad k(2k-1) \leq n \leq 2k(k+1)-1, \\ 2k & if \quad 2k(k+1) \leq n \leq (2k+1)(k+1)-1. \end{cases}$$

Proof. Note that there is a unique k such that $k(2k-1) \leq n \leq (2k+1)(k+1)-1$ for $n \geq 3$. We consider two cases as follows.

Case 1. $k(2k-1) \leq n \leq 2k(k+1)-1$.

By (2) of Theorem 2.1, $\psi^*(C_n) \leq 2k-1$. Next we shall show that C_n has a strong-$(2k-1)$-coloring. For this, consider K_{2k-1} and label its vertices by v_1, ..., v_{2k-1}. Let H be the graph obtained from K_{2k-1} by subdividing the $2k-1$ edges of the cycle C_{2k-1}, where $C_{2k-1} = v_1 ... v_{2k-1} v_1$, and then label the new $2k-1$ vertices by v_1, ..., v_{2k-1} such that H has a cycle C_{4k-2} with $C_{4k-2} = v_1 v_1 v_2 v_2 ... v_{2k-1} v_{2k-1} v_1$. Note that H has an euler tour, say $EU(H)$. Then, we can obtain a strong-$(2k-1)$-coloring for $C_{k(2k-1)}$ such that if the i-th vertex of $EU(H)$ is v_t, then the i-th vertex of $C_{k(2k-1)}$ is colored t, where $1 \leq t \leq 2k-1$. This strong-$(2k-1)$-coloring of $C_{k(2k-1)}$ can be extended to a strong-$(2k-1)$-coloring of C_n by adding $n-k(2k-1)$ new vertices to the edge $v_1 v_2$ of $C_{k(2k-1)}$, and color these $n-k(2k-1)$ new vertices with $c(v_1)$. Thus, $\psi^*(C_n) = 2k-1$ follows.

Case 2. $2k(k+1) \leq n \leq (2k+1)(k+1)-1$.

By (2) of Theorem 2.1, $\psi^*(C_n) \leq 2k$. Next we shall show that C_n has a strong-$2k$-coloring. Now label the vertices of K_{2k} by v_1, ..., v_{2k}, and let $C_{2k} = v_1...v_{2k}v_1$. Let K^*_{2k} be the (not simple) graph obtained from K_{2k} by duplicating k edges, say v_1v_{2k}, v_2v_{2k-1}, ..., v_kv_{k+1}, which form a perfect matching of K_{2k}. We can construct a new graph H from K^*_{2k} by subdividing the $2k$ edges of C_{2k}, and then label the new $2k$ vertices by v_1, ..., v_{2k} such that H has a cycle C_{4k}, where $C_{4k} = v_1v_1v_2v_2...v_{2k}v_{2k}v_1$. Then, H also has an euler tour with $2k(k+1)$ edges. One can now proceed further analogously as in Case 1. ∎

Theorem 2.4 *For any $n \geq 3$,*

$$\psi^*(P_n) = \begin{cases} 2k-1 & if \quad k(2k-1)+1 \leq n \leq 2k(k+1)-1, \\ 2k & if \quad 2k(k+1) \leq n \leq (2k+1)(k+1). \end{cases}$$

Proof. By (2) of Theorem 2.1 and Remark 2.1, the result can be proved on similar lines as in Proposition 2.1 except for the case of $n = 2k(k+1)$. So, it suffices to deal with that case of exception. By (2) of Theorem 2.1, $\psi^*(P_{2k(k+1)}) \leq 2k$. Let $H_1 = H - v_1v_{2k}$, where H is as defined in Case 2 of Theorem 2.3. Then, H_1 has an euler trail with $2k(k+1)-1$ edges from v_1 to v_{2k}. It can be proved on similar lines as in Theorem 2.3 that $P_{2k(k+1)}$ has a strong-$2k$-coloring. Thus, $\psi^*(P_{2k(k+1)}) = 2k$. ∎

Note that $L(C_n) \cong C_n$ and $L(P_n) \cong P_{n-1}$. Thus, $\psi^*(L(C_n))$ and $\psi^*(L(P_n))$ are identified by Theorems 2.3 and 2.4. The next result determines the values of $\psi^*(L(W_n))$ and $\psi^*(L(F_n))$.

Theorem 2.5 *For any integer $n \geq 4$, $\psi^*(L(W_n)) = n-1$ and $\psi^*(L(F_n)) = n-2$.*

Proof. Note that the orders of $L(W_n)$ and $L(F_n)$ are $2n-2$ and $2n-3$, respectively. By (1) of Theorem 2.1, we have $\psi^*(L(W_n)) \leq n-1$ and $\psi^*(L(F_n)) \leq n-2$.

Let $V(L(W_n)) = \{v_1, v_2, ..., v_n\}$ where $d(v_n) = n-1$, and let e_{ij} $(1 \leq i \leq n, 1 \leq j \leq n)$ denote the edge which connected the vertices v_i and v_j. Let w_{ij} $(1 \leq i \leq n, 1 \leq j \leq n)$ be the vertex of $L(W_n)$, which represents the edge e_{ij}. Now, let $c(w_{12}) = 1$, $c(w_{23}) = 2$, ..., $c(w_{n-2,n-1}) = n-2$, $c(w_{n-1,1}) = n-1$ and $c(w_{ni}) = i$, where $1 \leq i \leq n-1$. It is easy to see that c is a strong-$(n-1)$-coloring of $L(W_n)$.

Let $V(L(F_n)) = \{v_1, v_2, ..., v_n\}$ where $d(v_n) = n-1$, and let e_{ij} $(1 \leq i \leq n, 1 \leq j \leq n)$ denote the edge which connected the vertices v_i and v_j. Let f_{ij} $(1 \leq i \leq n, 1 \leq j \leq n)$ be the vertex of $L(F_n)$, which represents the edge e_{ij}. Now, let $c(f_{12}) = 1$, $c(f_{23}) = 2$, ..., $c(f_{n-2,n-1}) = n-2$, $c(f_{n-1,n}) = 1$ and $c(f_{ni}) = i$, where $1 \leq i \leq n-2$. It is easy to see that c is a strong-$(n-2)$-coloring of $L(F_n)$.

Thus, $\psi^*(L(W_n)) = n-1$ and $\psi^*(L(F_n)) = n-2$. ∎

Theorem 2.6 *Let $n_1 \leq n_2 \leq \cdots \leq n_s$ be s positive integers and $n = \sum_{i=1}^{s} n_i$. If $s \geq 2$, then*

$$\psi^*(K_{n_1,n_2,...,n_s}) = \begin{cases} \lfloor \frac{n}{2} \rfloor & if \quad n_s \leq \lfloor \frac{n}{2} \rfloor, \\ n - n_s & if \quad n_s \geq \lceil \frac{n}{2} \rceil. \end{cases}$$

Proof. Let $G = K_{n_1,n_2,...,n_s}$, and let $V_i = \{v_{ij} : 1 \leq j \leq n_i\}$ be the i-th part of $V(G)$ for $i \in [s]$.

Case 1. $n_s \leq \lfloor \frac{n}{2} \rfloor$.

By (1) of Theorem 2.1, $\psi^*(G) \leq \lfloor \frac{n}{2} \rfloor$. Next we shall show that G has a strong-$\lfloor \frac{n}{2} \rfloor$-coloring. For this, we color the vertices of G with a lexicographical order corresponding to the consecutive colors of $1, 2, ..., \lfloor \frac{n}{2} \rfloor, 1, 2, ..., \lfloor \frac{n}{2} \rfloor$ if n is even, and $1, 2, ..., \lfloor \frac{n}{2} \rfloor, 1, 2, ..., \lfloor \frac{n}{2} \rfloor, 1$ if n is odd, namely, we first let $c(v_{1j}) = j$, where $1 \leq j \leq n_1$, and then let $c(v_{2j}) = n_1 + j \pmod{\lfloor \frac{n}{2} \rfloor}$. By repeating the above said procedure, we can obtain a coloring of G. To complete the proof, it suffices to show that every color cannot appear in the same partite set of the vertex partition of G. On the contrary, assume that there exists some color, say j, that appears only in V_i.

By the coloring method employed, one can notice that the following colors $j, j+1, ..., \lfloor \frac{n}{2} \rfloor, 1, 2, ..., j$ appear in V_i. But then, $n_i = |V_i| \geq \lfloor \frac{n}{2} \rfloor + 1$, contradicts $n_i \leq n_s \leq \lfloor \frac{n}{2} \rfloor$.

Case 2. $n_s \geq \lceil \frac{n}{2} \rceil$.

If $\psi^*(G) \geq n - n_s + 1$, then there is at least one color class belonging to V_s, which implies that this color class is an independent set, a contradiction. Thus, $\psi^*(G) \leq n - n_s$. Next we shall show that G has a strong-$(n - n_s)$-coloring. Let

$$c(v_{ij}) = \begin{cases} \sum_{t=1}^{i-1} n_t + j & if \quad 1 \leq i \leq s-1 \quad and \quad 1 \leq j \leq n_i, \\ j & if \quad i = s \quad and \quad 1 \leq j \leq \sum_{t=1}^{s-1} n_t, \\ 1 & if \quad i = s \quad and \quad \sum_{t=1}^{s-1} n_t + 1 \leq j \leq n_s. \end{cases} \tag{2}$$

Since $n_s \geq \lceil \frac{n}{2} \rceil \geq \frac{n}{2}$, we have $2n_s \geq n = \sum_{t=1}^{s} n_t$, and $\sum_{t=1}^{s-1} n_t \leq n_s$. Hence, the coloring c defined in (2) exists, and it is easy to see that c is a strong-$(n - n_s)$-coloring of G. ∎

Corollary 2.3 *If $K_{n_1,n_2} - e$ has at least one edge, then $\psi^*(K_{n_1,n_2}) = \psi^*(K_{n_1,n_2} - e) = \min\{n_1, n_2\}$.*

Proof. Without loss of generality, assume that $n_1 \leq n_2$. By Proposition 2.2 and Theorem 2.6, $\psi^*(K_{n_1,n_2} - e) \leq \psi^*(K_{n_1,n_2}) = n_1$. Let $V_i = \{v_{ij} : 1 \leq j \leq n_i\}$ be the i-th partite vertex set of $V(K_{n_1,n_2} - e)$ for $1 \leq i \leq 2$. We may suppose that $e = v_{1n_1}v_{2n_2}$. Let $c(v_{1j}) = j$ for $1 \leq j \leq n_1$, $c(v_{2j}) = j + 1$ for $1 \leq j \leq n_1 - 1$, and $c(v_{2j}) = 1$ for $n_1 \leq j \leq n_2$. Then, a strong-n_1-coloring for $K_{n_1,n_2} - e$ can be obtained. ∎

Remark 2.3 By Corollaries 2.1 and 2.3, if G is obtained from $K_{t,t}$ by adding any s $(1 \leq s \leq t(t-1))$ edges, then $\psi^*(G) = \psi^*(K_{t,t}) = t$.

Denote by $K_s(t)$ the complete s-partite graph with exactly t vertices in each part. By Theorem 2.6, it follows immediately that

Corollary 2.4 *For any two integers s, $t \geq 2$,*

$$\psi^*(K_s(t)) = \psi^*(K_t(s)) = \begin{cases} \frac{ts}{2} & if \quad st \quad is \quad even, \\ \frac{ts-1}{2} & if \quad st \quad is \quad odd. \end{cases}$$

Corollary 2.5 *For any four integers t, s, p, $q \geq 2$,*

$$\psi^*(K_s(t) \vee K_p(q)) = \begin{cases} \psi^*(K_s(t)) + \psi^*(K_p(q)) & if \text{ either } st \text{ or } pq \text{ is even}, \\ \psi^*(K_s(t)) + \psi^*(K_p(q)) + 1 & if \text{ both } st \text{ and } pq \text{ are odd}. \end{cases}$$

3 The strong pseudoachromatic number of join of graphs

Let G^c be the complement graph of G. It is well-known that $\chi(G \vee H) = \chi(G) + \chi(H)$ and $\alpha(G \vee H) = \alpha(G) + \alpha(H)$ for any graphs G and H (for instance, see [4]). But for any $k \geq 0$, there exist graphs G and H such that $\psi^*(G \vee H) = \psi^*(G) + \psi^*(H) + k$. For $k = 0$ or 1, see Corollary 2.5. If $k \geq 2$, let $G = H = K_k^c$. Then by Corollary 2.3, $\psi^*(G \vee H) = \psi^*(K_{k,k}) = k = \psi^*(G) + \psi^*(H) + k$.

A graph G is called a *strongly critical graph* if $\psi^*(G - v) < \psi^*(G)$ for any $v \in V(G)$. Similarly, G is called a *critical graph* if $\Psi(G - v) < \Psi(G)$ for any $v \in V(G)$. We shall characterize the class of all graphs $\mathcal{G}$ that $\psi^*(G \vee H) = \psi^*(G) + \psi^*(H)$ for any $G, H \in \mathcal{G}$.

First we establish the following crucial lemma.

Lemma 3.1 *Let G and H be two graphs. Then* $\psi^*(G \vee H) =$
$\max_{X \subseteq V(G), Y \subseteq V(H), |X| = |Y| \geq 0} \{\psi^*(G \setminus X) + \psi^*(H \setminus Y) + |X|$*: Either $G \setminus X$ or $H \setminus Y$ is strongly critical*$\}$.

Proof. For appropriate vertex subsets X, Y as in the hypothesis respectively of the graphs G and H, color their i-th vertex with the color i for $1 \leq i \leq |X|$. Then one can obtain a strong $(\psi^*(G \setminus X) + \psi^*(H \setminus Y) + |X|)$-coloring of $G \vee H$ from a strong $\psi^*(G \setminus X)$-coloring and a strong $\psi^*(H \setminus Y)$-coloring

of $G \setminus X$ and $H \setminus Y$ respectively with the help of $\psi^*(G \setminus X) + \psi^*(H \setminus Y)$ new colors.

Next consider a strong-$\psi^*(G \vee H)$-coloring of $G \vee H$. In this coloring, let A be the set of colors that appear only in $V(G)$, B the set of colors that appear only in $V(H)$ and C the set of colors that appear in both G and H. Then, $\psi^*(G \vee H) = |A| + |B| + |C|$.

Claim. Either $G \setminus X$ or $H \setminus Y$ is strongly critical where $X \subseteq V(G)$, $Y \subseteq V(H)$ with $|X| = |Y| = |C|$, $|A| = \psi^*(G \setminus X)$ and $|B| = \psi^*(H \setminus Y)$.

Let $X \subseteq V(G)$ and $Y \subseteq V(H)$ be the set of vertices colored by the colors from C. If two vertices of X (respectively, Y) are assigned the same color, then one of the two vertices can be colored by a color not in C, so that we have $X_1 \subseteq V(G)$ and $Y_1 \subseteq V(H)$ such that $|X_1| = |Y_1| = |C|$. Now suppose that $|X| = |Y| = |C|$ (Else, one can deal with X_1 and Y_1 using similar argument). Note that the $|A|$ coloring of $G \setminus X$ is a strong-$|A|$-coloring for $G \setminus X$. Then, $|A| \leq \psi^*(G \setminus X)$. Similarly, $|B| \leq \psi^*(H \setminus Y)$. But then, we have a strong-$(\psi^*(G \setminus X) + \psi^*(H \setminus Y) + |X|)$-coloring for $G \vee H$. So, $|A| = \psi^*(G \setminus X)$ and $|B| = \psi^*(H \setminus Y)$.

If $G \setminus X$ and $H \setminus Y$ are not strongly critical, then $\psi^*(G \setminus (X \cup \{u\})) = \psi^*(G \setminus X) = |A|$ and $\psi^*(H \setminus (Y \cup \{v\})) = \psi^*(H \setminus Y) = |B|$ holds good for some vertices $u \in G \setminus X$ and $v \in H \setminus Y$. Now one can color u and v with a new color, which is not appear in A, B, C. But then it results in a strong-$(|A| + |B| + |C| + 1)$-coloring for $G \vee H$, a contradiction. ∎

Theorem 3.1 *For any two graphs G and H, $\psi^*(G \vee H) = \psi^*(G) + \psi^*(H)$ if and only if $\psi^*(G) + \psi^*(H) = \max_{X \subseteq V(G), Y \subseteq V(H), |X| = |Y| \geq 0} \{\psi^*(G \setminus X) + \psi^*(H \setminus Y) + |X|$: Either $G \setminus X$ or $H \setminus Y$ is strongly critical$\}$.*

Proof. Follows from Lemma 3.1. ∎

Corollary 3.1 *For any two graphs G and H, $\psi^*(G \vee H) \geq \psi^*(G) + \psi^*(H) + 1$ if and only if either $G \setminus X$ or $H \setminus Y$ is strongly critical with $\psi^*(G \setminus X) + \psi^*(H \setminus Y) + |X| \geq \psi^*(G) + \psi^*(H) + 1$, where $X \subseteq V(G), Y \subseteq V(H)$ and $|X| = |Y| \geq 1$.*

In [9], it has been shown that $\Psi(G \vee K_n) = \Psi(G) + \Psi(K_n)$. But this does not hold good for ψ^*. Actually, for any integer t, there exists some positive integer k with $k(k-1) \geq t$, such that $\psi^*(C_{2k(k+1)} \vee K_{2k(k+1)}) - \psi^*(C_{2k(k+1)}) - \psi^*(K_{2k(k+1)}) = k(k-1) \geq t$ by Corollary 2.1 and Theorem 2.3. For the cases of $G \vee K_1$ and $G \vee K_2$, we have the following results.

Theorem 3.2 (1) *If G is strongly critical, then $\psi^*(K_1 \vee G) = \psi^*(G)$.* (2) *If G is not strongly critical, then $\psi^*(K_1 \vee G) = \psi^*(G) + 1$.*

Proof. By Proposition 2.2, for any graph G,

$$\psi^*(G) \leq \psi^*(K_1 \vee G) \leq \psi^*(G) + 1. \tag{3}$$

Case 1. G is strongly critical.

Note that $\psi^*(G \setminus X) + \psi^*(K_1 \backslash Y) + |X| \leq \psi^*(G) + \psi^*(K_1)$ for any $|X| = |Y| = 1$. Then, $\psi^*(K_1 \vee G) = \psi^*(G) + \psi^*(K_1) = \psi^*(G)$ by Theorem 3.1.

Case 2. G is not strongly critical.

Let $\psi^*(G) = s$ and $V(K_1) = \{u_0\}$. By the choice of G, suppose that $\psi^*(G - v) = \psi^*(G) = s$, where $v \in V(G)$. Then, $G - v$ has a strong-s-coloring. Now we color u_0 and v with the color $s + 1$. It is easy to see that $K_1 \vee G$ has a strong-$(s+1)$-coloring. Thus, $\psi^*(K_1 \vee G) = \psi^*(G) + 1$ follows from inequality (3). ∎

Corollary 3.2 *For any $n \geq 4$,*

$$\psi^*(W_n) = \begin{cases} 2k-1 & if \quad k(2k-1)+1 \leq n \leq k(2k-1)+2, \\ 2k & if \quad k(2k-1)+3 \leq n \leq 2k(k+1)+1, \\ 2k+1 & if \quad 2k(k+1)+2 \leq n \leq (2k+1)(k+1). \end{cases}$$

Proof. When $k(2k-1)+1 \leq n \leq (2k+1)(k+1)$, by Remark 2.1, Theorem 2.4, and the proof of Theorem 2.3, C_{n-1} is strongly critical if and only if either $n = k(2k-1)+1$ or $n = k(2k-1)+2$ or $n = 2k(k+1)+1$. Thus, the result follows from Theorems 2.3 and 3.2. ∎

By Remark 2.1 and Theorem 2.4, the following result can be proved on similar lines as in Corollary 3.2.

Corollary 3.3 *For any* $n \geq 3$,

$$\psi^*(F_n) = \begin{cases} 2k-1 & if \quad n = k(2k-1)+2 \\ 2k & if \quad k(2k-1)+3 \leq n \leq 2k(k+1)+1, \\ 2k+1 & if \quad 2k(k+1)+2 \leq n \leq (2k+1)(k+1)+1. \end{cases}$$

A graph G is called a *strongly 2-critical graph* if $\psi^*(G-u-v) < \psi^*(G)$ for any $u, v \in V(G)$. If G is strongly critical, by Proposition 2.2, $\psi^*(G-u-v) \leq \psi^*(G-u) < \psi^*(G)$ holds for any u, $v \in V(G)$. Thus, a strongly critical graph is a strongly 2-critical graph, but not the Vice-Versa. For instance, K_7 is strongly 2-critical, but it is not strongly critical.

Theorem 3.3 (1) *If* G *is strongly* 2*-critical, then* $\psi^*(K_2 \vee G) = \psi^*(G)+1$. (2) *If* G *is not strongly* 2*-critical, then* $\psi^*(K_2 \vee G) = \psi^*(G)+2$.

Proof. By inequality (3), it follows that

$$\psi^*(G)+1 \leq \psi^*(K_2 \vee G) \leq \psi^*(K_1 \vee G)+1 \leq \psi^*(G)+2. \qquad (4)$$

Case 1. G is strongly 2-critical.

Note that $\psi^*(K_2) = 1$. By Theorem 3.1, $\psi^*(K_2 \vee G) = \psi^*(G)+1$.

Case 2. G is not strongly 2-critical

Let $\psi^*(G) = s$ and $V(K_2) = \{u_0, v_0\}$. By the choice of G, suppose that $\psi^*(G-u-v) = \psi^*(G) = s$, where u, $v \in V(G)$. Then, $G-u-v$ has a strong-s-coloring. Now color u_0 and u with the color $s+1$, v_0 and v with the color $s+2$. This results in a strong-$(s+2)$-coloring for $G \vee K_2$. That is, $\psi^*(G \vee K_2) = \psi^*(G)+2$ by the inequality (4). ∎

4 The pseudoachromatic number of join of graphs

A graph G is called k *non-critical* (for some positive integer k) if $\Psi(G) \leq$

$\Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil - 1$ holds for some $X \subseteq V(G)$ with $|X| = k$. For any two graphs G and H, it is obvious that $\Psi(G \vee H) \geq \Psi(G) + \Psi(H)$. Balasubramanian et al. [1] characterized the class of all graphs that satisfies the graph equation $\Psi(G \vee H) = \Psi(G) + \Psi(H)$ via the characterization of all graphs that satisfies the graph inequality $\Psi(G \vee H) \geq \Psi(G) + \Psi(H) + 1$.

Theorem 4.1 [1] *For any two graphs G and H, $\Psi(G \vee H) \geq \Psi(G) + \Psi(H) + 1$ if and only if (i) both G and H are k non-critical for some positive integer k or (ii) there exists a non-negative integer k_0, and sets $X \subseteq V(G)$, $Y \subseteq V(H)$ with $|X| = |Y|$ such that $\Psi(G \setminus X) = \Psi(G) - \left\lceil \frac{|X|}{2} \right\rceil - k_0$ and $\Psi(H \setminus Y) \geq \Psi(H) - \left\lfloor \frac{|Y|}{2} \right\rfloor + k_0 + 1$ or vice versa.*

By employing a similar method as in Lemma 3.1, one can show that

Lemma 4.1 *For any two graphs G and H, $\Psi(G \vee H) =$ $\max_{X \subseteq V(G), Y \subseteq V(H), |X| = |Y| \geq 0} \{\Psi(G \setminus X) + \Psi(H \setminus Y) + |X|$: Either $G \setminus X$ or $H \setminus Y$ is critical$\}$.*

From Lemma 4.1 it follows that

Theorem 4.2 *For any two graphs G and H, $\Psi(G \vee H) \geq \Psi(G) + \Psi(H) + 1$ if and only if (iii) either $G \setminus X$ or $H \setminus Y$ is critical with $\Psi(G \setminus X) + \Psi(H \setminus Y) + |X| \geq \Psi(G) + \Psi(H) + 1$, where $X \subseteq V(G)$, $Y \subseteq V(H)$ and $|X| = |Y| \geq 1$ happens.*

Corollary 4.1 *For any two graphs G and H, $\Psi(G \vee H) = \Psi(G) + \Psi(H)$ if and only if $\Psi(G) + \Psi(H) = \max_{X \subseteq V(G), Y \subseteq V(H), |X| = |Y| \geq 0} \{\Psi(G \setminus X) + \Psi(H \setminus Y) + |X|$: Either $G \setminus X$ or $H \setminus Y$ is critical$\}$.*

Proposition 4.1 *The condition (iii) in Theorem 4.2 holds if and only if either the condition (i) or the condition (ii) in Theorem 4.1 holds.*

Proof. First we prove the sufficiency part under the supposition that the necessity part holds. If $|X| = |Y| = k$ such that $\Psi(G) \leq \Psi(G \setminus X) +$

$\left\lceil \frac{|X|}{2} \right\rceil - 1$ and $\Psi(H) \leq \Psi(H \setminus Y) + \left\lceil \frac{|Y|}{2} \right\rceil - 1$, then (i) holds. Otherwise, either $\Psi(G) \geq \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil$ or $\Psi(H) \geq \Psi(H \setminus Y) + \left\lceil \frac{|Y|}{2} \right\rceil$ for some $|X| = |Y| = k \geq 1$. Without loss of generality, suppose that $\Psi(G) \geq \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil$, where there exists some nonnegative integer k_0 such that $\Psi(G \setminus X) = \Psi(G) - \left\lceil \frac{|X|}{2} \right\rceil - k_0$. Now the condition (ii) of Theorem 4.1 follows as $\Psi(G \setminus X) + \Psi(H \setminus Y) + |X| \geq \Psi(G) + \Psi(H) + 1$ and $\Psi(H \setminus Y) \geq \Psi(H) - \left\lfloor \frac{|Y|}{2} \right\rfloor + k_0 + 1$. So, either (i) or (ii) holds.

Next we prove the necessity part under the supposition of the sufficiency part. Now two cases arise.

Case 1. The condition (i) of Theorem 4.1 holds.

Subcase 1.1. $\Psi(G \setminus X) > 0$ and $\Psi(H \setminus Y) > 0$.

Let $t = \min_{X \subseteq V(G), Y \subseteq V(H), |X| = |Y| \geq 0} \{s : \text{Either } G \setminus (X \cup (s-1)K_1) \text{ or } H \setminus (Y \cup (s-1)K_1) \text{ is critical}\}$. We may suppose that $G \setminus (X \cup (s-1)K_1)$ is critical. By the definition of t, $\Psi(G \setminus (X \cup tK_1)) < \Psi(G \setminus (X \cup (s-1)K_1)) = \Psi(G \setminus X)$ and $\Psi(H \setminus (Y \cup tK_1)) \leq \Psi(H \setminus (Y \cup (t-1)K_1)) = \Psi(H \setminus Y)$. Let $X_1 = X \cup (t-1)K_1$, and $Y_1 = Y \cup (t-1)K_1$. Then, $|X_1| = |Y_1| \geq 1$, and $G \setminus X_1$ is critical. Moreover,

$$\Psi(G) \leq \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil - 1 \leq \Psi(G \setminus X_1) + \left\lceil \frac{|X_1|}{2} \right\rceil - 1, \qquad (5)$$

$$\Psi(H) \leq \Psi(H \setminus Y) + \left\lceil \frac{|Y|}{2} \right\rceil - 1 \leq \Psi(H \setminus Y_1) + \left\lceil \frac{|Y_1|}{2} \right\rceil - 1. \qquad (6)$$

By inequalities (5)–(6), $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) + \Psi(H) + 1$. So, the condition (iii) of Theorem 4.2 holds.

Subcase 1.2. $\Psi(G \setminus X) = 0$ or $\Psi(H \setminus Y) = 0$.

Suppose that $\Psi(H \setminus Y) = 0$. Then, $|X| = |Y| = |V(H)|$ and $\Psi(H) \leq \left\lceil \frac{|Y|}{2} \right\rceil - 1$. If $y \in V(H)$, then we have $\Psi(H) \leq \Psi(y) + \left\lceil \frac{(|Y|-1)}{2} \right\rceil - 1$ as $\Psi(y) = 1$. Let $Y_1 = H \setminus Y$. Then, $H \setminus Y_1$ is critical.

Let $X_1 = X \setminus v$, provided v is such an element in X for which $\Psi(G) \leq \Psi(G \setminus X + v) + \left\lceil \frac{(|X|-1)}{2} \right\rceil - 1$ holds. Then, $|X_1| = |Y_1| \geq 1$, $\Psi(G \setminus X_1) +$

$\Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) + \Psi(H) + 1$. So the condition (iii) of Theorem 4.2 holds.

Otherwise, for any $v \in X$, we have

$$\Psi(G \setminus X + v) + \left\lceil \frac{(|X| - 1)}{2} \right\rceil \leq \Psi(G) \leq \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil - 1. \quad (7)$$

Note that $\Psi(G \setminus X + v) \geq \Psi(G \setminus X)$ (see [3]). By inequality (7), $|X|$ is odd and $\Psi(G) = \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil - 1 = \Psi(G \setminus X + v) + \left\lceil \frac{(|X|-1)}{2} \right\rceil$. Let $X_1 = X - v$. Then, $|X_1| = |Y_1| \geq 1$, $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) - \frac{|X_1|}{2} + \Psi(H) - \frac{|X_1|}{2} + 1 + |X_1| = \Psi(G) + \Psi(H) + 1$. So the condition (iii) of Theorem 4.2 holds.

Case 2. The condition (ii) of Theorem 4.1 holds.

We may suppose that there exists a non-negative integer k_0, and sets $X \subseteq V(G)$, $Y \subseteq V(H)$ with $|X| = |Y|$ such that $\Psi(G \setminus X) = \Psi(G) - \left\lceil \frac{|X|}{2} \right\rceil - k_0$ and $\Psi(H \setminus Y) \geq \Psi(H) - \left\lfloor \frac{|Y|}{2} \right\rfloor + k_0 + 1$. If $\Psi(G \setminus X) > 0$ and $\Psi(H \setminus Y) > 0$, then the condition (iii) of Theorem 4.2 can be proved on similar lines as in Subcase 1.1. Thus, we only need to consider the next two Subcases.

Subcase 2.1. $\Psi(G \setminus X) = 0$.

Then, $|X| = |V(G)| = |Y|$, and $\Psi(G) = \left\lceil \frac{|X|}{2} \right\rceil + k_0 \leq \Psi(x) + \left\lceil \frac{(|X|-1)}{2} \right\rceil + k_0$ holds for some $x \in X$. Let $X_1 = G \setminus X$. Then, $G \setminus X_1$ is critical.

Let $Y_1 = Y \setminus v$, provided v is such an element in Y for which $\Psi(H) \leq \Psi(H \setminus Y + v) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor - k_0 - 1$. Then, $|X_1| = |Y_1| \geq 1$, and $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) + \Psi(H) + 1$. So the condition (iii) of Theorem 4.2 holds. Otherwise, for any $v \in Y$,

$$\Psi(H \setminus Y + v) + \left\lfloor \frac{(|X| - 1)}{2} \right\rfloor - k_0 \leq \Psi(H \setminus Y) + \left\lfloor \frac{|X|}{2} \right\rfloor - k_0 - 1. \quad (8)$$

Since $\Psi(H \setminus Y + v) \geq \Psi(H \setminus Y)$, by inequality (8) we can deduce that $|X|$ is even. Then, $\Psi(G) + 1 = \Psi(x) + \left\lceil \frac{(|X|-1)}{2} \right\rceil + k_0$, and $\Psi(H \setminus Y_1) = \Psi(H) - \frac{(|X_1|-1)}{2} + k_0$. So, $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| = \Psi(G) + 1 -$

$\frac{(|X_1|+1)}{2} - k_0 + \Psi(H) - \frac{(|X_1|-1)}{2} + k_0 + |X_1| = \Psi(G) + \Psi(H) + 1$, and hence the condition (iii) of Theorem 4.2 holds.

Subcase 2.2. $\Psi(H \setminus Y) = 0$.

Then, $|Y| = |V(H)| = |X|$, and $\Psi(H) \leq \left\lfloor \frac{|X|}{2} \right\rfloor - k_0 - 1 \leq \Psi(y) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor - k_0 - 1$ holds for some $y \in Y$. Let $Y_1 = H \setminus Y$. Then, $H \setminus Y_1$ is critical. Let $X_1 = X - v$, provided v is such an element in X for which $\Psi(G) \leq \Psi(G \setminus X + v) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor + k_0$. Obviously, the condition (iii) of Theorem 4.2 holds. Otherwise, for any $v \in X$, we have

$$\Psi(G \setminus X + v) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor + k_0 + 1 \leq \Psi(G \setminus X) + \left\lceil \frac{|X|}{2} \right\rceil + k_0. \quad (9)$$

Since $\Psi(G \setminus X + v) \geq \Psi(G \setminus X)$, by inequality (9) we can deduce that $\Psi(G) = \Psi(G \setminus X + v) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor + k_0 + 1$. If $|X|$ is odd, then $\Psi(H \setminus Y_1) + \left\lfloor \frac{(|X|-1)}{2} \right\rfloor - k_0 - 1 = \left\lfloor \frac{|X|}{2} \right\rfloor - k_0 \geq \Psi(H) + 1$, and hence $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) - \frac{|X_1|}{2} - k_0 - 1 + \Psi(H) - \frac{|X_1|}{2} + k_0 + 2 + |X_1| = \Psi(G) + \Psi(H) + 1$. If $|X|$ is even, it can be proved on similar lines that $\Psi(G \setminus X_1) + \Psi(H \setminus Y_1) + |X_1| \geq \Psi(G) + \Psi(H) + 1$. Thus, the condition (iii) of Theorem 4.2 follows. ∎

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The nine smallest hyper-Wiener indices of trees and the eight smallest hyper-Wiener (Wiener) indices of unicyclic graphs*

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Abstract

The seven smallest hyper-Wiener indices of trees on $n \geq 17$ vertices have been determined. In this paper, the eighth to ninth smallest hyper-Wiener indices of trees on $n \geq 18$ vertices are identified. Moreover, the eight smallest Wiener indices, and the eight smallest hyper-Wiener indices of unicyclic graphs on $n \geq 13$ vertices are also determined, and we find that the unicyclic graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices of unicyclic graphs on $n \geq 13$ vertices for $1 \leq i \leq 8$.

1 Introduction

Let $G = (V, E)$ be a connected simple graph with $|V| = n$ and $|E| = m$. Sometimes we refer to G as an (n, m) graph. If $m = n - 1$, then G is called a *tree*. While if $m = n$, then G is called a *unicyclic graph*. Let $\mathcal{T}_n$ and $\mathcal{U}_n$ denote the class of trees and unicyclic graphs on n vertices, respectively. Let $N(u)$ be the first neighbor vertex set of u, then $d(u) = |N(u)|$ is called the degree of u. In particular, $\Delta = \Delta(G)$ denotes the *maximum degree* of vertices of G. As usual, let $K_{1,n-1}$ and C_n be the star and cycle of order n, respectively.

The *distance* $d(u, v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and

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v. Let $\gamma(G,k)$ denote the number of vertex pairs of G, the distance of which is equal to k. There are two important graph-based structure-descriptors, called Wiener index and hyper-Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ is denoted by [1]

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \sum_{k\geq 1} k\gamma(G,k), \tag{1}$$

and the *hyper-Wiener index* $WW(G)$ is defined as [2]

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2 = \frac{1}{2}\sum_{k\geq 1} k(k+1)\gamma(G,k). \tag{2}$$

The Wiener index is introduced long time ago [1], numerous of its chemical applications and mathematical properties were reported [3–5]. Whereas the hyper-Wiener index is conceived somewhat later [2]. It rapidly gained popularity and numerous results on it were raised [6–10]. The mathematical properties of hyper-Wiener index and its applications in chemistry can be referred to [8–13] and the references cited therein.

Gutman et al. firstly gave a partial order to Wiener index among the starlike trees in [14]. After then, the first up to fifteenth smallest and the first up to seventeenth greatest Wiener indices of trees on n vertices were identified in [15] and [16], respectively. Also, the similar order was considered for the hyper-Wiener index by Gutman et al.. Recently, the first up to seventh smallest [17–18] and the first up to fifteenth greatest [18] hyper-Wiener indices of trees on n vertices had been determined, respectively. In this paper, we identify the eighth to ninth smallest hyper-Wiener indices of trees on $n \geq 18$ vertices. Moreover, we determine the eight smallest Wiener indices, and the eight smallest hyper-Wiener indices of unicyclic graphs on $n \geq 13$ vertices. It's surprising that the unicyclic graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices of unicyclic graphs on $n \geq 13$ vertices for $1 \leq i \leq 8$.

2 Some preliminary lemmas

The *first Zagreb index* $M_1(G)$ is defined as [19]:

$$M_1(G) = \sum_{v\in V} d(v)^2, \tag{3}$$

it is also an important topological index and has been closely correlated with many chemical and mathematical properties [19–20]. The *diameter* of G, denoted by $diam(G)$, is $diam(G) = max\{d(u,v) : u,v \in V(G)\}$. For the relation between Wiener, hyper-Wiener and the first Zagreb index, Zhou et al. has proved that

Lemma 2.1 [12] *Let G be a connected (n, m) graph, which does not contain triangles and/or quadrangles. Then*

$$(1)\quad W(G) \geq \frac{3n(n-1)}{2} - \frac{1}{2}M_1(G) - m,$$

$$(2)\quad WW(G) \geq 3n(n-1) - \frac{3}{2}M_1(G) - 2m,$$

where both equalities hold if and only if $diam(G) \leq 3$.

The *girth* $g(G)$ of a connected graph G, is the length of a shortest cycle in G. A *pendant vertex* is a vertex of degree 1. The next lemma is useful in the sequel.

Lemma 2.2 *Suppose $U = (V, E) \in \mathcal{U}_n$. (1) If $g(U) = 3$, then $\gamma(U, 2) = \frac{1}{2}M_1(U) - n - 3$; (2) If $g(U) = 4$, then $\gamma(U, 2) = \frac{1}{2}M_1(U) - n - 2$.*

Proof. We only prove the first assertion because the second assertion can be proved analogously. Next we prove the first assertion by induction on n. If $n = 3$, then $U = C_3$. It is easy to see that $\gamma(U, 2) = 0 = \frac{1}{2}M_1(U) - n - 3$, thus the result follows. Now assume the assertion holds for all unicyclic graphs with less than $n \geq 4$ vertices and a cycle C_3. Suppose U is a unicyclic graph on n vertices and U has a cycle C_3.

Since $n \geq 4$ and $g(U) = 3$, then U contains at least one pendant vertex. Suppose u_0 is a pendant vertex of U, and denote by v_0 the unique neighbor of u_0 in U. Since u_0 is a pendant vertex, by the induction hypothesis and Eq. (3) it follows that

$$\begin{aligned}
\gamma(U, 2) &= \gamma(U - u_0, 2) + d(v_0) - 1 \\
&= \frac{1}{2}\sum_{x \in V \setminus \{u_0, v_0\}} d(x)^2 + \frac{1}{2}(d(v_0) - 1)^2 - (n-1) - 3 + d(v_0) - 1 \\
&= \frac{1}{2}\sum_{x \in V \setminus \{u_0, v_0\}} d(x)^2 + \frac{1}{2}d(v_0)^2 + \frac{1}{2} - n - 3 \\
&= \frac{1}{2}\sum_{x \in V} d(x)^2 - n - 3 \\
&= \frac{1}{2}M_1(U) - n - 3.
\end{aligned}$$

This completes the proof of this result. ∎

Proposition 2.3 *Suppose $U \in \mathcal{U}_n$. If $g(U) = 3$, then*

$$(1)\quad W(U) \geq \frac{n(3n-5)}{2} - \frac{1}{2}M_1(U) + 3,$$

$$(2)\quad WW(U) \geq 3n^2 - 5n - \frac{3}{2}M_1(U) + 9,$$

where both equalities hold if and only if $diam(U) \leq 3$.

Proof. (1) Clearly, $\gamma(U,1) = n$ and $\sum\limits_{k\geq 1}\gamma(U,k) = \binom{n}{2}$ (see [12]). Lemma 2.2 (1) implies that $\gamma(U,2) = \frac{1}{2}M_1(U) - n - 3$, thus by Eq. (1) it follows that

$$\begin{aligned} W(U) &= n + 2\left(\frac{1}{2}M_1(U) - n - 3\right) + \sum_{k\geq 3} k\gamma(U,k) \\ &\geq M_1(U) - n - 6 + 3\left(\binom{n}{2} - \frac{1}{2}M_1(U) + 3\right) \\ &= \frac{n(3n-5)}{2} - \frac{1}{2}M_1(U) + 3. \end{aligned}$$

(2) By the proof of (1) and Eq. (2), we have

$$\begin{aligned} WW(U) &= n + 3\left(\frac{1}{2}M_1(U) - n - 3\right) + \sum_{k\geq 3}\frac{1}{2}k(k+1)\gamma(U,k) \\ &\geq \frac{3}{2}M_1(U) - 2n - 9 + 6\left(\binom{n}{2} - \frac{1}{2}M_1(U) + 3\right) \\ &= 3n^2 - 5n - \frac{3}{2}M_1(U) + 9. \end{aligned}$$

It is easy to see that both equalities hold if and only if $diam(U) \leq 3$. By combining the above arguments, the results follow. ∎

In the proof of Proposition 2.3, if we replace Lemma 2.2 (1) by Lemma 2.2 (2), we can deduce the next results easily

Proposition 2.4 *Suppose* $U \in \mathcal{U}_n$. *If* $g(U) = 4$, *then*

$$(1)\quad W(U) \geq \frac{n(3n-5)}{2} - \frac{1}{2}M_1(U) + 2,$$

$$(2)\quad WW(U) \geq 3n^2 - 5n - \frac{3}{2}M_1(U) + 6,$$

where both equalities hold if and only if $diam(U) \leq 3$.

3 Main results

We recall the notation of *majorization* (see [21,22]). Suppose $(x) = (x_1, x_2, ..., x_n)$ and $(y) = (y_1, y_2, ..., y_n)$ are two non-increasing sequences of real

numbers, we say (x) is majorized by (y), denoted by $(x) \trianglelefteq (y)$, if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, ..., n$. It has been shown that

Lemma 3.1 [23] *Let G be a connected graph with degree sequence $(a) = (d_1, d_2, ..., d_n)$ and G' be a connected graph with degree sequence $(b) = (d'_1, d'_2, ..., d'_n)$. If $(a) \trianglelefteq (b)$, then $M_1(G) \leq M_1(G')$, where equality holds if and only if $(a) = (b)$.*

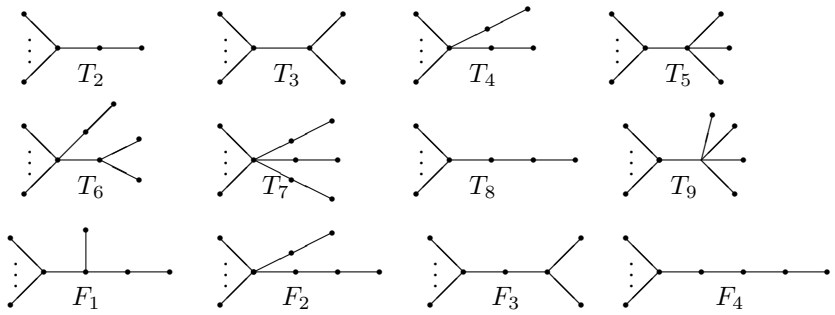


Fig. 1. The trees $T_2, ..., T_9$ and $F_1, ..., F_4$ of order $n \geq 17$.

In the following, let $T_1 = K_{1,n-1}$, $T_2, ..., T_9$ and $F_1, ..., F_4$ be the trees of order $n \geq 17$ as shown in Fig. 1. By Lemma 3.1, it follows that

Lemma 3.2 *Suppose $T \in \mathcal{T}_n$ with $\Delta(T) \leq n-5$, then $M_1(T) \leq n^2 - 9n + 48$, where equality holds if and only if $T \cong T_9$.*

Proof. Suppose $T \ncong T_9$. Let $(a) = (d_1, d_2, ..., d_n)$ be the degree sequence of T. Note that the degree sequence of T_9 is $(b) = (n-5, 5, 1, ..., 1)$, it is easy to see that $(a) \trianglelefteq (b)$ and $(a) \neq (b)$ because T_9 is the unique tree with (b) as its degree sequence. Thus, $M_1(T) < M_1(T_9) = n^2 - 9n + 48$ follows from Lemma 3.1. ∎

In [18], it has been proved that

Theorem A [18] Suppose $n \geq 17$ and $T \in \mathcal{T}_n \setminus \{T_1, T_2, T_3, T_4, T_5, T_6, T_7\}$, then $WW(T) > WW(T_7) > WW(T_6) > WW(T_5) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.

With the help of Lemma 3.2, we can improve Theorem A to be

Theorem 3.3 *Suppose $n \geq 18$ and $T \in \mathcal{T}_n \setminus \{T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9\}$, then $WW(T) > WW(T_9) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_5) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.*

Proof. We divide the proof into the next two cases.

Case 1. $n-4 \leq \Delta(T) \leq n-1$.

Clearly, T_1 is the unique tree with $\Delta = n-1$, T_2 is the unique tree with $\Delta = n-2$, T_3, T_4, T_8 are the all trees with $\Delta = n-3$, T_5, T_6, T_7 and F_1, F_2, F_3, F_4 are the all trees with $\Delta = n-4$. Since $T \in \mathcal{T}_n \setminus \{T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9\}$, then $T \cong F_1$ or $T \cong F_2$ or $T \cong F_3$ or $T \cong F_4$. By a directly calculation, we have $WW(T_8) = \frac{1}{2}(3n^2+13n-70)$, $WW(T_9) = \frac{1}{2}(3n^2+17n-140)$ and $WW(F_1) = \frac{1}{2}(3n^2+19n-114)$, $WW(F_2) = \frac{1}{2}(3n^2+19n-82)$, $WW(F_3) = \frac{1}{2}(3n^2+27n-154)$, $WW(F_4) = \frac{1}{2}(3n^2+37n-190)$. Since $n \geq 18$, by Theorem A it follows that $WW(F_4) > WW(F_3) > WW(F_2) > WW(F_1) > WW(T_9) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_5) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.

Case 2. $\Delta(T) \leq n-5$.

Since $T \ncong T_9$, by Lemmas 2.1 (2) and 3.2 we have

$$\begin{aligned} WW(T) &\geq 3n(n-1) - \frac{3}{2}M_1(T) - 2(n-1) \\ &> 3n(n-1) - \frac{3}{2}(n^2-9n+48) - 2(n-1) \\ &= WW(T_9). \end{aligned}$$

By combining the above arguments, the result follows. ∎

Lemma 3.4 *Suppose $U \in \mathcal{U}_n$ with $\Delta(U) \leq n-4$. (1) If $g(U) = 3$, then $M_1(U) \leq n^2-7n+42$; (2) If $g(U) = 4$, then $M_1(U) \leq n^2-7n+36$; (3) If $g(U) \geq 5$, then $M_1(U) \leq n^2-7n+32$.*

Proof. We only prove the first assertion, because the other assertions can be approved analogously. Suppose the degree sequence of U is $(a) = (d_1, d_2, d_3, ..., d_n)$, since $U \in \mathcal{U}_n$ and U has exactly one cycle C_3, then $n-4 \geq d_1 \geq d_2 \geq d_3 \geq 2$. Let $(b) = (n-4, 5, 2, 1, ..., 1)$, then $(a) \trianglelefteq (b)$. By Lemma 3.1, we can conclude that $M_1(U) \leq (n-4)^2+5^2+2^2+n-3 = n^2-7n+42$. This completes the proof of this result. ∎

In the following, let U_1, ..., U_{13} and H_1, H_2, H_3 be the unicyclic graphs of order $n \geq 13$ as depicted in Fig. 2.

Theorem 3.5 *Suppose $n \geq 13$ and $U \in \mathcal{U}_n \setminus \{U_1, U_2, ..., U_{13}\}$, then $W(U) > W(U_{13}) > W(U_{12}) = W(U_{11}) > W(U_{10}) = W(U_9) > W(U_8) = W(U_7) > W(U_6) = W(U_5) > W(U_4) > W(U_3) = W(U_2) > W(U_1)$.*

Proof. (1) We divide the proof into the next two cases.

Case 1. $n-3 \leq \Delta(U) \leq n-1$.

It is easy to see that U_1 is the unique unicyclic graph with $\Delta(U) = n-1$, U_2, U_3, U_4 are the all unicyclic graphs with $\Delta(U) = n-2$, $U_5, U_6, ..., U_{13}$

and H_1, H_2, H_3 are the all unicyclic graphs with $\Delta(U) = n-3$. Since $U \in \mathcal{U}_n \backslash \{U_1, U_2, ..., U_{13}\}$, then $U \cong H_1$ or $U \cong H_2$ or $U \cong H_3$. By a directly calculation, we have $W(U_1) = n^2 - 2n$, $W(U_2) = W(U_3) = n^2 - n - 4$, $W(U_4) = n^2 - n - 3$, $W(U_5) = W(U_6) = n^2 - 10$, $W(U_7) = W(U_8) = n^2 - 9$, $W(U_9) = W(U_{10}) = n^2 - 8$, $W(U_{11}) = W(U_{12}) = n^2 - 7$, $W(U_{13}) = n^2 - 6$, and $W(H_1) = n^2 + n - 14$, $W(H_2) = n^2 + n - 13$, $W(H_3) = n^2 + n - 11$. Since $n \geq 13$, then $W(H_3) > W(H_2) > W(H_1) > W(U_{13}) > W(U_{12}) = W(U_{11}) > W(U_{10}) = W(U_9) > W(U_8) = W(U_7) > W(U_6) = W(U_5) > W(U_4) > W(U_3) = W(U_2) > W(U_1)$. The result follows.

Case 2. $\Delta(U) \leq n-4$.

Three cases should be considered.

Subcase 1. $g(U) \geq 5$.

By Lemmas 2.1 (1) and 3.4 (3), we have

$$\begin{aligned} W(U) &\geq \frac{3n(n-1)}{2} - \frac{1}{2}M_1(U) - n \\ &\geq \frac{3n(n-1)}{2} - \frac{1}{2}(n^2 - 7n + 32) - n \\ &= n^2 + n - 16 \\ &> W(U_{13}). \end{aligned}$$

Subcase 2. $g(U) = 4$.

By Proposition 2.4 (1) and Lemma 3.4 (2), we have

$$\begin{aligned} W(U) &\geq \frac{3n^2 - 5n}{2} - \frac{1}{2}M_1(U) + 2 \\ &\geq \frac{3n^2 - 5n}{2} - \frac{1}{2}(n^2 - 7n + 36) + 2 \\ &= n^2 + n - 16 \\ &> W(U_{13}). \end{aligned}$$

Subcase 3. $g(U) = 3$.

By Proposition 2.3 (1) and Lemma 3.4 (1), we have

$$\begin{aligned} W(U) &\geq \frac{3n^2 - 5n}{2} - \frac{1}{2}M_1(U) + 3 \\ &\geq \frac{3n^2 - 5n}{2} - \frac{1}{2}(n^2 - 7n + 42) + 3 \\ &= n^2 + n - 18 \\ &> W(U_{13}). \end{aligned}$$

By combining the above arguments, the result follows. ∎

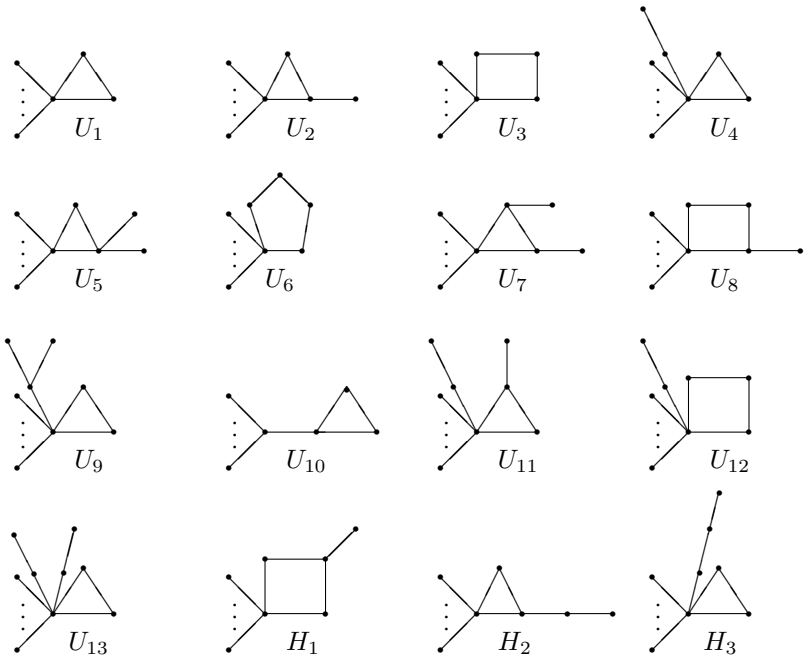


Fig. 2. The unicyclic graphs with $n-3 \leq \Delta \leq n-1$.

Theorem 3.6 *Suppose* $n \geq 13$ *and* $U \in \mathcal{U}_n \backslash \{U_1, U_2, ..., U_{13}\}$, *then* $WW(U) > WW(U_{13}) > WW(U_{12}) = WW(U_{11}) > WW(U_{10}) = WW(U_9) > WW(U_8) = WW(U_7) > WW(U_6) = WW(U_5) > WW(U_4) > WW(U_3) = WW(U_2) > WW(U_1)$.

Proof. (1) We divide the proof into the next two cases.

Case 1. $n-3 \leq \Delta(U) \leq n-1$.

By the proof of Theorem 3.5, $U_1, U_2, ..., U_{13}$ and H_1, H_2, H_3 are the all unicyclic graphs with $n-3 \leq \Delta(U) \leq n-1$. Since $U \in \mathcal{U}_n \setminus \{U_1, U_2, ..., U_{13}\}$, then $U \cong H_1$ or $U \cong H_2$ or $U \cong H_3$. By a directly calculation, we have $WW(U_1) = \frac{1}{2}(3n^2 - 7n)$, $WW(U_2) = WW(U_3) = \frac{1}{2}(3n^2 - n - 24)$, $WW(U_4) = \frac{1}{2}(3n^2 - n - 18)$, $WW(U_5) = WW(U_6) = \frac{1}{2}(3n^2 + 5n - 60)$, $WW(U_7) = WW(U_8) = \frac{1}{2}(3n^2 + 5n - 54)$, $WW(U_9) = WW(U_{10}) = \frac{1}{2}(3n^2 + 5n - 48)$, $WW(U_{11}) = WW(U_{12}) = \frac{1}{2}(3n^2 + 5n - 40)$, $WW(U_{13}) = \frac{1}{2}(3n^2 + 5n - 34)$, and $WW(H_1) = \frac{1}{2}(3n^2 + 13n - 94)$, $WW(H_2) = \frac{1}{2}(3n^2 + 13n - 88)$, $WW(H_3) = \frac{1}{2}(3n^2 + 13n - 74)$. Since $n \geq 13$, then $WW(H_3) > WW(H_2) > WW(H_1) > WW(U_{13}) > WW(U_{12}) = WW(U_{11}) > WW(U_{10})$

$= WW(U_9) > WW(U_8) = WW(U_7) > WW(U_6) = WW(U_5) > WW(U_4) > WW(U_3) = WW(U_2) > WW(U_1)$. The result follows.

Case 2. $\Delta(U) \leq n-4$.

We consider the next cases.

Subcase 1. $g(U) \geq 5$.

By Lemmas 2.1 (2) and 3.4 (3), we have

$$\begin{aligned} WW(U) &\geq 3n(n-1) - \frac{3}{2}M_1(U) - 2n \\ &\geq 3n(n-1) - \frac{3}{2}(n^2 - 7n + 32) - 2n \\ &= \frac{1}{2}(3n^2 + 11n - 96) \\ &> WW(U_{13}). \end{aligned}$$

Subcase 2. $g(U) = 4$.

By Proposition 2.4 (2) and Lemma 3.4 (2), we have

$$\begin{aligned} WW(U) &\geq 3n^2 - 5n - \frac{3}{2}M_1(U) + 6 \\ &\geq 3n^2 - 5n - \frac{3}{2}(n^2 - 7n + 36) + 6 \\ &= \frac{1}{2}(3n^2 + 11n - 96) \\ &> WW(U_{13}). \end{aligned}$$

Subcase 3. $g(U) = 3$.

By Proposition 2.3 (2) and Lemma 3.4 (1), we have

$$\begin{aligned} WW(U) &\geq 3n^2 - 5n - \frac{3}{2}M_1(U) + 9 \\ &\geq 3n^2 - 5n - \frac{3}{2}(n^2 - 7n + 42) + 9 \\ &= \frac{1}{2}(3n^2 + 11n - 108) \\ &> WW(U_{13}). \end{aligned}$$

By combining the above arguments, the result follows. ∎

Remark. By Theorems 3.2–3.3, we can conclude that the unicyclic graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices of unicyclic graphs on $n \geq 13$ vertices for $1 \leq i \leq 8$.

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The majorization theorem of extremal pseudographs ☆

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ABSTRACT

A pseudograph is a graph in which both loops and multiple edges are permitted. Suppose $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d'_1, d'_2, ..., d'_n)$ are two positive non-increasing degree sequences, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, ..., n$. Let $\Gamma(\pi)$ be the class of connected undirected pseudographs with degree sequence π. Let $\rho(G)$ and $\mu(G)$ be the spectral radius and signless Laplacian spectral radius of G, respectively. In this paper, the extremal pseudographs with the largest (respectively, signless Laplacian) spectral radii in $\Gamma(\pi)$ are characterized. Furthermore, we show that if $\pi \lhd \pi'$, G and G' are the pseudographs with the largest (respectively, signless Laplacian) spectral radii in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.

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1. Introduction

A *pseudograph* is a graph in which both loops and multiple edges are permitted. Thus, a simple graph is also a pseudograph, but not vice versa. Throughout this paper, $G = (V(G), E(G))$ is a connected undirected pseudograph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E(G)$. The degree of a vertex v of G, denoted $d(v)$, is the number of edges of G incident with v, each loop counting as two edges. Denote $N_G(v)$ the neighbor set of vertex v in G. Let $\Upsilon_{uv}(G)$ be the number of edges joining vertices u and v in G. In particular, $\Upsilon_{uu}(G)$ indicates the number of loops incident with vertex u in G. If there is no confusion, we simplify $N_G(v)$ and $\Upsilon_{uv}(G)$ as $N(v)$ and Υ_{uv}, respectively.

The adjacency matrix of G is an $n \times n$ matrix $A(G) = (a_{ij})$, where a_{ij} is the number of edges joining vertices v_i and v_j, each loop counting as two edges.

In the following, let G be a graph with n vertices and let $f \neq 0$ be a column vector defined on $V(G)$, i.e., $f = (f(v_1), f(v_2), ..., f(v_n))^T$. If there exists a real number q such that for each $u \in V(G)$,

$$qf(u) = \big(A(G)f\big)(u) = \sum_{v \in N(u)\setminus\{u\}} \Upsilon_{uv} f(v) + 2\Upsilon_{uu} f(u), \tag{1.1}$$

then q is called an eigenvalue of $A(G)$. The *spectral radius* of G, denoted $\rho(G)$, is the largest eigenvalue of $A(G)$.

The *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees of G. If there exists a real number p such that for each $u \in V(G)$,

$$pf(u) = \big(Q(G)f\big)(u) = \sum_{v \in N(u)\setminus\{u\}} \Upsilon_{uv}\big(f(u) + f(v)\big) + 4\Upsilon_{uu} f(u), \tag{1.2}$$

then p is called an eigenvalue of $Q(G)$. It is easy to see that $Q(G)$ is positive semidefinite [4] and hence we use $\mu(G)$ to denote the largest eigenvalue of $Q(G)$. Hereafter, $\mu(G)$ is called the *signless Laplacian spectral radius* of G.

When G is a connected simple graph, the *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$. When G is a connected simple graph, it is well known that [13] $L(G)$ is also positive semidefinite so that we can use $\lambda(G)$ to denote the largest eigenvalue of $L(G)$. Hereafter, $\lambda(G)$ is called the *Laplacian spectral radius* of G.

By Eqs. (1.1) and (1.2), we have $\mathcal{R}_{A(G)}(f) = f^T A(G) f = 2\sum_{uv \in E(G)} \Upsilon_{uv} f(u) f(v)$ and $\mathcal{R}_{Q(G)}(f) = f^T Q(G) f = \sum_{uv \in E(G)} \Upsilon_{uv}(f(u) + f(v))^2$. By the famous Rayleigh–Ritz Theorem (see e.g. [5, pp. 172–178]) it follows that

Proposition 1.1. *(See [5].) Let G be a connected undirected pseudograph, and let f be an n-tuple unit vector on $V(G)$. Then,*

$$\rho(G) \geq \mathcal{R}_{A(G)}(f) \quad \textit{and} \quad \mu(G) \geq \mathcal{R}_{Q(G)}(f),$$

where the first (respectively, second) inequality implies that f is an eigenvector corresponding to $\rho(G)$ (respectively, $\mu(G)$). Furthermore, there is a unique positive unit eigenvector corresponding to $\rho(G)$ (respectively, $\mu(G)$).

By Proposition 1.1, in the coming discussion, $f = (f(v_1), ..., f(v_n))^T$ always indicates the unique positive unit eigenvector corresponding to $\rho(G)$ or $\mu(G)$, and f is called the *Perron vector* of G.

If $d_i = d(v_i) \geq 1$ for $i = 1, 2, ..., n$, then we call the sequence $\pi = (d_1, d_2, ..., d_n)$ the *degree sequence* of G. Throughout this paper, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n \geq 1$. We use $\Gamma(\pi)$ to denote the class of connected undirected pseudographs with degree sequence π, and we use $S(\pi)$ to denote the class of connected simple graphs with degree sequence π.

Suppose $G \in \Gamma(\pi)$. If $\rho(G) \geq \rho(G')$ (respectively, $\mu(G) \geq \mu(G')$) for any other $G' \in \Gamma(\pi)$, then we call G has *largest* (respectively, *signless Laplacian*) *spectral radius* in $\Gamma(\pi)$. Furthermore, we call G an *extremal pseudograph* of $\Gamma(\pi)$ if G has the largest spectral radius or largest signless Laplacian spectral radius in $\Gamma(\pi)$.

Suppose $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d'_1, d'_2, ..., d'_n)$ are two non-increasing integer sequences, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, ..., n$. Such an ordering is sometimes called *majorization* [12].

Note that a tree, a unicyclic graph, a bicyclic graph and a tricyclic graph on n vertices is a connected simple graph with $n-1$, n, $n+1$ and $n+2$ edges, respectively. The work on determining the graph which has largest spectral radius among some class of graphs, can be traced back to 1985 when Brualdi and Hoffman [2] investigated the (not necessarily connected) graph with the largest spectral radius in the set of all graphs with a given number of vertices and edges. Their work was followed by other people, in the connected graph case as well as in the general case. In this line, Bıyıkoğlu et al. [1] firstly considered the relation between the spectral radii of the extremal graphs in two classes of trees with given degree sequences, and Zhang [14] later considered the similar problem for the Laplacian spectral radii (i.e., the signless Laplacian spectral radii since $L(G)$ and $Q(G)$ share the same spectra [13] when G is a simple bipartite graph), and they showed that

Theorem 1.2. *Let π and π' be two different non-increasing degree sequences of trees and $\pi \lhd \pi'$. Suppose T and T' are the extremal trees in $S(\pi)$ and $S(\pi')$, respectively. Then* [1] *$\rho(T) < \rho(T')$ and* [14] *$\lambda(T) < \lambda(T')$.*

Such relation is called the *majorization theorem* [6,7]. In the sequel, the majorization theorems for unicyclic and bicyclic graphs were also proved [6,7,10,15].

Theorem 1.3. *Let π and π' be two different non-increasing degree sequences of unicyclic (respectively, bicyclic) graphs and $\pi \lhd \pi'$.*

(1) *Suppose U and U' are the extremal unicyclic graphs in $S(\pi)$ and $S(\pi')$, respectively. Then,* [10] $\rho(U) < \rho(U')$, [15] $\mu(U) < \mu(U')$;
(2) *Suppose B and B' are the extremal bicyclic graphs in $S(\pi)$ and $S(\pi')$, respectively. Then* [7] $\rho(B) < \rho(B')$, [6] $\mu(B) < \mu(B')$,

In 1981, Cvetković [3] indicated 12 directions in further investigations of graph spectra, one of which is "classifying and ordering graphs". Not long before, we found that the majorization theorem is a good tool to deal with Cvetković's above problem [9], i.e., the order of graphs according to their largest (signless Laplacian) spectral radii. Unfortunately, the majorization theorem cannot hold for all the connected simple graphs, since there are already counterexamples for tricyclic graphs [7,8,11].

In this note, we will show that the majorization theorem does hold for all the connected undirected pseudographs, and our main result can be stated as follows:

Theorem 1.4. *Let π and π' be two different positive non-increasing degree sequences and $\pi \lhd \pi'$. Suppose G and G' are the extremal pseudographs in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then, $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.*

Recall that a connected graph on n vertices is a tree if and only if it contains $n-1$ edges. Thus, if π is a degree sequence of trees, then $S(\pi) = \Gamma(\pi)$. So, Theorem 1.2 immediately follows from Theorem 1.4, and hence Theorem 1.4 is an extension to Theorem 1.2.

The main idea to prove our main result mainly follows that used in [1,14,15]. Firstly, we will use the "shifting" and "switching" graph perturbations to characterize the extremal pseudographs of $\Gamma(\pi)$ in Section 2. Secondly, we will use the "Muirhead Lemma" to prove Theorem 1.4 in Section 3.

2. The characterizations of the extremal pseudographs in $\Gamma(\pi)$

Lemma 2.1. *Let G and G' be two connected undirected pseudographs with $V(G) = V(G')$ and let f be the Perron vector of G. Suppose $R_{A(G')}(f) \geq R_{A(G)}(f)$ and $R_{Q(G')}(f) \geq R_{Q(G)}(f)$. If there exists a vertex $v \in V(G)$ such that either $\Upsilon_{uv}(G) < \Upsilon_{uv}(G')$ and $\Upsilon_{vx}(G) \leq \Upsilon_{vx}(G')$ for $x \in V(G) \setminus \{u\}$ or $\Upsilon_{uv}(G') < \Upsilon_{uv}(G)$ and $\Upsilon_{vx}(G') \leq \Upsilon_{vx}(G)$ for $x \in V(G) \setminus \{u\}$, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.*

Proof. Here, we only prove that $\mu(G') > \mu(G)$, as $\rho(G') > \rho(G)$ can be proved similarly. By Proposition 1.1, we have $\mu(G') \geq R_{Q(G')}(f) \geq R_{Q(G)}(f) = \mu(G)$.

If $\mu(G) = \mu(G')$, then $\mu(G') = R_{Q(G')}(f)$, and hence f is also the Perron vector of G' by Proposition 1.1. From Eq. (1.2) corresponding to the vertex v, we have

$$\mu(G)f(v) = \big(Q(G)f\big)(v) = \sum_{z\in N_G(v)\setminus\{v\}} \Upsilon_{vz}(G)\big(f(v)+f(z)\big) + 4\Upsilon_{vv}(G)f(v)$$

$$= \mu\big(G'\big)f(v) = \big(Q\big(G'\big)f\big)(v) = \sum_{z\in N_{G'}(v)\setminus\{v\}} \Upsilon_{vz}\big(G'\big)\big(f(v)+f(z)\big) + 4\Upsilon_{vv}\big(G'\big)f(v).$$

It is a contradiction to either $\Upsilon_{uv}(G) < \Upsilon_{uv}(G')$ and $\Upsilon_{vx}(G) \leq \Upsilon_{vx}(G')$ for $x \in V(G)\backslash\{u\}$ or $\Upsilon_{uv}(G') < \Upsilon_{uv}(G)$ and $\Upsilon_{vx}(G') \leq \Upsilon_{vx}(G)$ for $x \in V(G) \setminus \{u\}$. So, $\mu(G) < \mu(G')$. □

Let $G-uv$ denote the pseudograph obtained from G by deleting the edge $uv \in E(G)$. Similarly, denote by $G+uv$ the pseudograph obtained from G by adding an edge $uv \notin E(G)$. Suppose u, v are two different vertices of G and suppose that $uw \in E(G)$. Let $G' = G - uw + vw$ ($w = u$ or $w = v$ is permitted) or let G' be a new pseudograph obtained from G by deleting a loop incident with u and then add a new loop incident with v. In both cases, we say that G' is obtained from G by shifting an edge from u to v.

Lemma 2.2 *(Shifting). Let u, v be two different vertices of a connected undirected pseudograph G, and $E_1 = \{e_1, e_2, ..., e_k\}$ be $k \geq 1$ different edges of G. Let f be the Perron vector of G. Suppose E_1 are incident with u, and we obtain G' from G by shifting E_1 from u to v. If $f(v) \geq f(u)$ and G' is connected, then $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$.*

Proof. Here, we only prove that $\mu(G') > \mu(G)$, as $\rho(G') > \rho(G)$ can be proved similarly. Without loss of generality, suppose G' is obtained from G by deleting the loops e_1, ..., e_s incident with u, and then add s loops incident with v, and then replace the edges e_{s+1}, ..., e_k incident with u and $w_1, w_2, ..., w_{k-s}$, respectively, by $k-s$ edges incident with v and $w_1, w_2, ..., w_{k-s}$, respectively. Then,

$$\begin{aligned} R_{Q(G')}(f) - R_{Q(G)}(f) &= \sum_{yz\in E(G')} \Upsilon_{yz}(G')\big(f(y)+f(z)\big)^2 \\ &\quad - \sum_{yz\in E(G)} \Upsilon_{yz}(G)\big(f(y)+f(z)\big)^2 \\ &= 4s\big(f^2(v)-f^2(u)\big) + \sum_{i=1}^{k-s}\Big(\big(f(v)+f(w_i)\big)^2 - \big(f(u)+f(w_i)\big)^2\Big) \\ &\geq 0. \end{aligned}$$

Suppose there are exactly t copies of u in $w_1, w_2, ..., w_{k-s}$.

We firstly consider the cases of $s > 0$. If $t > 0$, then $\Upsilon_{vv}(G) < \Upsilon_{vv}(G')$ and $\Upsilon_{vx}(G) \leq \Upsilon_{vx}(G')$ for $x \in V(G) \setminus \{v\}$. If $t = 0$, then $\Upsilon_{uu}(G') < \Upsilon_{uu}(G)$ and $\Upsilon_{ux}(G') \leq \Upsilon_{ux}(G)$ for $x \in V(G) \setminus \{u\}$. In both cases, the result follows from Lemma 2.1.

We secondly consider the case of $s = 0$. If $t > 0$, then $\Upsilon_{uv}(G) < \Upsilon_{uv}(G')$ and $\Upsilon_{vx}(G) \leq \Upsilon_{vx}(G')$ for $x \in V(G) \setminus \{u\}$. If $t = 0$, since $s = 0$ and $k \geq 1$, there must exist some $w \in V(G) \setminus \{u\}$ such that $\Upsilon_{uw}(G') < \Upsilon_{uw}(G)$ and $\Upsilon_{ux}(G') \leq \Upsilon_{ux}(G)$ for $x \in V(G) \setminus \{w\}$. In both cases, the result follows from Lemma 2.1. □

Lemma 2.3. *Suppose G is an extremal pseudograph in $\Gamma(\pi)$ and f is the Perron vector of G. If $d(u) > d(v)$, then $f(u) > f(v)$. Moreover, if $f(u) = f(v)$, then $d(u) = d(v)$.*

Proof. Assume to the contrary, that there exist vertices u and v such that $d(u) > d(v)$, but $f(u) \leq f(v)$. Since G is connected (because $G \in \Gamma(\pi)$), there exists a shortest path, say P_{uv}, from u to v. Note that $d(u) - d(v) = k > 0$. Then, there must exist edges $e_i = uu$ (a loop) and $e'_j = uw_j$, where $0 \leq i \leq s$ and $0 \leq j \leq t$, such that $2s + t = k$ and uw_1, uw_2, ..., $uw_t \notin E(P_{uv})$. We can obtain a new pseudograph G' from G by shifting $\{e_1, ..., e_s, e'_1, ..., e'_t\}$ from u to v such that $G' \in \Gamma(\pi)$. Since $f(u) \leq f(v)$, we have $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$ by Lemma 2.2, contradicting the choice of G. □

Lemma 2.4 *(Switching). Let $G = (V, E)$ be a connected undirected pseudograph. Let u_1, v_1 and v_2 be three different vertices of G such that $u_1v_1 \in E(G)$, $u_2v_2 \in E(G)$ and $u_2 \neq v_1$. Let $G' = G + v_1v_2 + u_1u_2 - u_1v_1 - u_2v_2$. Suppose f is the Perron vector of G and G' is also connected. If $f(v_1) \geq f(u_2)$ and $f(v_2) \geq f(u_1)$, then $\rho(G') \geq \rho(G)$ and $\mu(G') \geq \mu(G)$. Both equalities are strict if either $f(v_1) > f(u_2)$ or $f(v_2) > f(u_1)$.*

Proof. Here, we only prove the case of signless Laplacian spectral radius, as the case of spectral radius can be proved similarly.

$$\begin{aligned} R_{Q(G')}(f) - R_{Q(G)}(f) &= \big(f(v_1) + f(v_2)\big)^2 + \big(f(u_1) + f(u_2)\big)^2 \\ &\quad - \big(f(u_1) + f(v_1)\big)^2 - \big(f(u_2) + f(v_2)\big)^2 \\ &= 2\big(f(v_2) - f(u_1)\big)\big(f(v_1) - f(u_2)\big) \\ &\geq 0. \end{aligned}$$

By Proposition 1.1, we have $\mu(G') \geq \mu(G)$.

Now, suppose that $f(v_2) > f(u_1)$ and $\mu(G') = \mu(G)$. If $f(v_1) > f(u_2)$, then $R_{Q(G')}(f) > R_{Q(G)}(f)$. By Proposition 1.1, $\mu(G') > \mu(G)$, a contradiction. Thus, $f(v_1) = f(u_2)$, and hence f is also the Perron vector of $\mu(G')$ by Proposition 1.1.

Since $\mu(G') = \mu(G)$, by Eq. (1.2), we have

$$\mu(G)f(u_2) = \sum_{x \in N_G(u_2)\setminus\{u_2\}} \Upsilon_{u_2x}(G)\big(f(u_2) + f(x)\big) + 4\Upsilon_{u_2u_2}(G)f(u_2) \tag{2.1}$$

$$= \mu\big(G'\big)f(u_2) = \sum_{x \in N_{G'}(u_2)\setminus\{u_2\}} \Upsilon_{u_2x}\big(G'\big)\big(f(u_2) + f(x)\big) + 4\Upsilon_{u_2u_2}\big(G'\big)f(u_2) \tag{2.2}$$

If $u_2 \in \{u_1, v_2\}$, by Eqs. (2.1) and (2.2), we have $4f(u_2) = f(u_1)+f(v_2)+f(v_1)+f(u_2)$, contradicting $f(v_2) > f(u_1)$ and $f(v_1) = f(u_2)$. If $u_2 \notin \{u_1, v_2\}$, by Eqs. (2.1) and (2.2), we have $f(v_2) = f(u_1)$, contradicting $f(v_2) > f(u_1)$.

Thus, $f(v_2) > f(u_1)$ implies that $\mu(G') > \mu(G)$. It can be proved similarly that $f(v_1) > f(u_2)$ also implies $\mu(G') > \mu(G)$. □

Lemma 2.5. *Suppose G is a pseudograph in $\Gamma(\pi)$ and f is the Perron vector of G. If there exist three different vertices u, v and w such that $uv \in E(G)$, $uw \notin E(G)$,*

$f(v) < f(w) \leq f(u)$ and $f(u) \geq f(x)$ for all $x \in N(w)$. Then, G is not an extremal pseudograph in $\Gamma(\pi)$.

Proof. Assume to the contrary, that G is an extremal pseudograph in $\Gamma(\pi)$. Since G is connected and $uw \notin E(G)$, there exists a shortest path, say $P_{uw} = u \cdots yw$, from u to w, where $u \neq y \neq w$. Since $f(w) > f(v)$, by Lemma 2.3 we have $d(w) \geq d(v)$. We consider the following two cases.

Case 1. $uv \notin E(P_{uw})$.

If $vy \notin E(G)$, let $G' = G+uw+vy-uv-wy$. Note that $f(u) \geq f(y)$ and $f(w) > f(v)$. Then, $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$ by Lemma 2.4. Clearly, $G' \in \Gamma(\pi)$, contrary to the choice of G.

Thus, $vy \in E(G)$. If there exists some vertex, say x, such that $\Upsilon_{wx}(G) > \Upsilon_{vx}(G)$, let $G' = G + uw + vx - uv - wx$. Then, $G' \in \Gamma(\pi)$. Since $f(u) \geq f(x)$ and $f(w) > f(v)$, by Lemma 2.4, $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$, contradicting the choice of G.

Thus, $\Upsilon_{wx}(G) \leq \Upsilon_{vx}(G)$ holds for each $x \in V(G)$, and hence $\Upsilon_{ww}(G) \leq \Upsilon_{vw}(G) = \Upsilon_{wv}(G) \leq \Upsilon_{vv}(G)$. Furthermore, since $u \in N(v)\backslash N(w)$, we have $\Upsilon_{wu}(G) < \Upsilon_{vu}(G)$. Now,

$$\begin{aligned} d(w) &= \sum_{x \in V(G)\backslash\{u,v,w\}} \Upsilon_{wx}(G) + \Upsilon_{wv}(G) + \Upsilon_{wu}(G) + 2\Upsilon_{ww}(G) \\ &< \sum_{x \in V(G)\backslash\{u,v,w\}} \Upsilon_{vx}(G) + \Upsilon_{vw}(G) + \Upsilon_{vu}(G) + 2\Upsilon_{vv}(G) = d(v), \end{aligned}$$

a contradiction.

Case 2. $uv \in E(P_{uw})$.

Assume that there exists a vertex x in $N(w)$ such that $x \notin P_{uw}$ (or $w \in N(w)$). Let $G' = G + uw + vx - uv - wx$. Then, $G' \in \Gamma(\pi)$. Note that $f(u) \geq f(x)$ and $f(w) > f(v)$. By Lemma 2.4, we have $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$, a contradiction. Thus, $x \in P_{uw}$ holds for each $x \in N(w)$ and $w \notin N(w)$, which implies that $d(w) = 1$. Now, since $uv \in E(P_{uw})$ and $v \neq w$, we have $d(v) \geq 2 > 1 = d(w)$, a contradiction. □

Theorem 2.6. *Let G be an extremal pseudograph in $\Gamma(\pi)$ and f the Perron vector of G. Then, there exists an ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ such that*

(1) *$d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$, $f(v_1) \geq f(v_2) \geq \cdots \geq f(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1;*
(2) *let $v \in N(u)\backslash N(x)$, $y \in N(x)\backslash N(u)$ such that $h(u) = h(x) = h(v) - 1 = h(y) - 1$, if $u \prec x$, then $v \prec y$.*

Proof. Clearly, there exists an ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G) = \{v_1, v_2, ..., v_n\}$ such that $v_i \prec v_j$ whenever $f(v_i) > f(v_j)$, or $f(v_i) = f(v_j)$ and $d(v_i) \geq d(v_j)$. Thus, $f(v_1) \geq f(v_2) \geq \cdots \geq f(v_n)$. Moreover, Lemma 2.3 implies that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. To complete the proof of (1), it suffices to show that $h(v_i) \leq h(v_{i+1})$ holds for $i = 1, 2, ..., n-1$ by induction. The result clearly holds for $i = 1$. Now, we assume that the result already holds for $1 \leq i \leq k-1$, namely, we already have $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_{k-1}) \leq h(v_k)$, and we will prove that $h(v_k) \leq h(v_{k+1})$.

Case 1. $f(v_k) > f(v_{k+1})$.

Since G is connected, there exists the smallest integer $s \in \{1, 2, ..., k\}$ such that v_s is adjacent to some vertex v_r in $\{k+1, ..., n\}$. We claim that $h(v_s) \geq h(v_k) - 1$. Otherwise, assume to the contrary that $h(v_s) < h(v_k) - 1$. Then, $s \neq k$, and hence $1 \leq s \leq k-1$. Let $t = \min\{j : v_j \in N(v_k)\}$. If $v_t \prec v_s$ or $v_t = v_s$, since $t \in \{1, 2, ..., k-1\}$, by the induction hypothesis we have $h(v_k) \leq h(v_t) + 1 \leq h(v_s) + 1 < h(v_k)$, a contradiction. Thus, $v_s \prec v_t$, and hence $f(v_s) \geq f(v_t) \geq f(v_j)$ holds for each $v_j \in N(v_k)$ by the choice of t. Since $s \leq k-1$ and $r \geq k+1$, we have $f(v_s) \geq f(v_k) > f(v_{k+1}) \geq f(v_r)$, contradicting Lemma 2.5. Thus, $h(v_s) \geq h(v_k) - 1$.

Let $P_{v_1 v_{k+1}}$ be a shortest path from v_1 to v_{k+1}, and v_q be the last vertex belonging to $\{1, 2, ..., k\}$ on the path $P_{v_1 v_{k+1}}$. If $s \leq k-1$, then $h(v_s) \leq h(v_q)$ by the induction hypothesis and the choice of v_s. If $s = k$, by the choice of v_s we have $q = s = k$, and hence $h(v_s) = h(v_q)$. Thus,

$$h(v_{k+1}) \geq h(v_q) + 1 \geq h(v_s) + 1 \geq h(v_k).$$

So, (1) holds.

Case 2. $f(v_k) = f(v_{k+1})$.

Let $q = \min\{i : f(v_i) = f(v_{k+1})\}$. Then, $q \leq k$ and $f(v_q) = f(v_{q+1}) = \cdots = f(v_{k+1})$. By Lemma 2.3, we have $d(v_q) = d(v_{q+1}) = \cdots = d(v_{k+1})$. Now, we relabel $V(G)$ by the following method: If $j \notin \{q, q+1, ..., k+1\}$, let $v'_j = v_j$; if $j \in \{q, q+1, ..., k+1\}$, let $v'_{q+t-1} = v_j$ if and only if $h(v_j)$ is the t-th smallest value among $\{h(v_q), h(v_{q+1}), ..., h(v_{k+1})\}$.

By the choice of q and the induction hypothesis, we have $h(v'_1) \leq h(v'_2) \leq \cdots \leq h(v'_{q-1})$, $h(v'_q) \leq h(v'_{q+1}) \leq \cdots \leq h(v'_k) \leq h(v'_{k+1})$, $f(v'_1) \geq f(v'_2) \geq \cdots \geq f(v'_n)$, $d(v'_1) \geq d(v'_2) \geq \cdots \geq d(v'_n)$ and $f(v'_{q-1}) > f(v'_q)$. If $q = 1$, the result already holds. If $q \geq 2$, by the proof of Case 1, we have $h(v'_{q-1}) \leq h(v'_q)$. Thus, (1) also holds.

Now we turn to prove (2).

Assume to the contrary, that there exist $v \in N(u) \backslash N(x)$, $y \in N(x) \backslash N(u)$ such that $h(u) = h(x) = h(v) - 1 = h(y) - 1$ and $u \prec x$, but $y \prec v$. If $f(y) = f(v)$, then $d(y) = d(v)$ by Lemma 2.3. We interchange the positions of y and v in the ordering $\prec$. Then, (1) and (2) hold. So, we may suppose that $f(y) > f(v)$ and $f(u) \geq f(x)$, as $u \prec x$ and $y \prec v$.

Since $h(u) = h(x) = h(v) - 1 = h(y) - 1$, there exists a path P_{ux} from u to x such that $v_1 \in V(P_{ux})$, $v \notin V(P_{ux})$ and $y \notin V(P_{ux})$. Let $G' = G + uy + xv - uv - xy$. Then, $G' \in \Gamma(\pi)$. By Lemma 2.4, $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$, contradicting the choice of G.

Therefore, (2) holds. □

If G is a connected simple graph and there exists an ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ such that both (1) and (2) of Theorem 2.6 hold, then G is called a *BFS-graph* [1,15]. By Theorem 2.6, it immediately follows that

Corollary 2.7. *(See [1,14].) A tree with degree sequence π is an extremal tree in $S(\pi)$ if and only if it is a BFS-tree. Furthermore, the extremal tree of $S(\pi)$ is uniquely determined up to isomorphism.*

3. The proof of Theorem 1.4

Suppose $\pi = (d_1, d_2, \ldots, d_n)$, $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two different positive non-increasing degree sequences. In the following, we write $\pi \lhd^* \pi'$ if and only if $\pi \lhd \pi'$, and π and π' differ only in two positions, where the difference is 1, that is, $d_i = d'_i$, $i \notin \{s, q\}$, $1 \le s < q \le n$, and $d'_s = d_s + 1$, $d'_q = d_q - 1$. So, $\pi \lhd^* \pi'$ is also a special majorization, and is called a *star majorization* in [7].

If $\pi = (d_1, ..., d_n)$ is a non-increasing integer sequence and $d_i \ge d_j + 2$, then the following operation is called a *unit transformation* from i to j on π: subtract 1 from d_i and add 1 to d_j. The following famous lemma about majorization in integer sequences is due to Muirhead (for instance, see [12]).

Lemma 3.1 *(Muirhead Lemma). If π and π' are two non-increasing integer sequences and $\pi \lhd \pi'$, then π can be obtained from π' by a finite sequence of unit transformations.*

Lemma 3.2. *Suppose π and π' are two positive non-increasing degree sequences and G and G' are the extremal pseudographs in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd^* \pi'$, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.*

Proof. We assume here that the vertices of G are already ordered as described in Theorem 2.6. Let f be the Perron vector of G, and let $P_{v_s v_q}$ be a shortest path from v_s to v_q. By the choice of G and $s < q$, $f(v_s) \ge f(v_q)$ follows from Theorem 2.6. Since $d_q = d'_q + 1 \ge 2$, there must exist some edge, say $e = v_q w$, such that $e \notin E(P_{v_s v_q})$. Let $G^* = G + v_s w - v_q w$. Then, G^* is connected and $G^* \in \Gamma(\pi')$. Since $f(v_s) \ge f(v_q)$, Lemma 2.2 implies that $\rho(G) < \rho(G^*) \le \rho(G')$ and $\mu(G) < \mu(G^*) \le \mu(G')$. □

Proof of Theorem 1.4. By the proof of Lemma 3.2, if $\pi \lhd^* \pi'$ and there exists a pseudograph G with π as its degree sequence, then there also exists a connected graph G'

with π' as its degree sequence. Now, Theorem 1.4 immediately follows from Lemmas 3.1 and 3.2. □

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On the Laplacian spectral radii of tricyclic graphs *

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Abstract

A graph G of order n is called a tricyclic graph if G is connected and the number of edges of G is $n+2$. Let $\mathcal{T}_n$ denote the set of all tricyclic graphs on n vertices. In this paper, we determine the first to nineteenth largest Laplacian spectral radii among the all graphs in the class $\mathcal{T}_n$ $(n \geq 11)$ together with the corresponding graphs.

1 Introduction

Throughout the paper, $G = (V, E)$ is a connected undirected simple graph with $V = \{v_1, v_2, ..., v_n\}$ and $E = \{e_1, e_2, ..., e_m\}$, i.e., $|V| = n$ and $|E| = m$. If $m = n + c - 1$, then G is called a $c-$cyclic graph. Especially, if $c = 1, 2, 3$, then G is called a unicyclic, bicyclic, or tricyclic graph, respectively. The notation $\mathcal{T}_n$ is used to denote the class of tricyclic graphs of order n. The neighbors of a vertex v is denoted by $N(v)$. Write $d(v)$ for the degree of vertex v. Specially, Δ denotes the maximum degree of G.

The adjacency matrix $A(G) = [a_{ij}]$ of G is an $n \times n$ symmetric matrix of 0's and 1's with $a_{ij} = 1$ if and only if v_i and v_j is joined by an edge. Suppose the degree of vertex v_i equals $d(v_i)$ for $i = 1, 2, ..., n$, and let $D(G)$ be the diagonal matrix whose (i, i)-entry is $d(v_i)$. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$, and the *Lapalacian characteristic polynomial* of G is denoted by $\Phi(G, \lambda)$, i.e., $\Phi(G, \lambda)$=det$(\lambda I - L(G))$. The maximum eigenvalue of $L(G)$, denoted by $\mu(G)$, is called the *Laplacian spectral radius*

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of $L(G)$. Our terminology and notation are standard except as indicated. For terminology and notation not defined here, we refer the readers to [1-10] and the references therein.

The investigation on the spectral radii of $L(G)$ is an important topic in the theory of graph spectral. Up to now, the first to fourteenth largest spectral radii of $L(G)$ were determined in the class of trees in [1-3]. The first to thirteenth largest spectral radii of $L(G)$ were given in the class of unicyclic graphs in [4-6]. Recently, Jia-Yu Shao et al. [7] obtained the first four largest spectral radii of $L(G)$ in the class of bicyclic graphs. Actually, we have determined the first eight largest spectral radii of $L(G)$ by using the different method from [1-7] in [8]. In this paper, we obtain the first to nineteenth largest Laplacian spectral radii among the all graphs in the class $\mathcal{T}_n$ $(n \geq 11)$ together with the corresponding graphs.

2 Main results

A vertex of degree 1 is called a *pendant vertex* of G. Suppose B is a square matrix, let $a_{ii}(B)$ denote the entry appearing in the i-th row and the i-th column of B. In [9], we have obtained a new method to calculate the Lapalacian characteristic polynomial of an n-vertex graph as follows

Lemma 2.1 [9] *Let G be a graph on $n-k$ $(1 \leq k \leq n-2)$ vertices with $V(G) = \{v_n, v_{n-1}, ..., v_{k+1}\}$. If G' is obtained from G by attaching k new pendant vertices, say v_1, ..., v_k, to v_{k+1}, then*

$$\Phi(L(G'), \lambda) = (\lambda - 1)^k \cdot det(\lambda I_{n-k} - L(G) - B_{n-k}),$$

where $a_{11}(L(G))$ is corresponding to the vertex v_{k+1}, and $B_{n-k} = diag\{k + \frac{k}{\lambda-1}, 0, ..., 0\}$.

Example 2.2 *Let G', G be the graphs as shown in Fig 1. It is easy to see that G' is obtained from G by attaching $n-4$ new pendant vertices to the vertex v_{n-3} of G. By Lemma 2.1, we have*

$\Phi(L(G'), \lambda) = (\lambda - 1)^{n-4} det(M)$,

where $M = \begin{pmatrix} \lambda - (n-2) - \frac{n-4}{\lambda-1} & 1 & 1 & 0 \\ 1 & \lambda - 3 & 1 & 1 \\ 1 & 1 & \lambda - 2 & 0 \\ 0 & 1 & 0 & \lambda - 1 \end{pmatrix}$.

By using "Matlab", it is easy to obtain that

$\Phi(L(G'), \lambda) = \lambda(\lambda-1)^{n-5}(\lambda^4 - (n+5)\lambda^3 + (6n+3)\lambda^2 - (9n-5)\lambda + 3n)$.

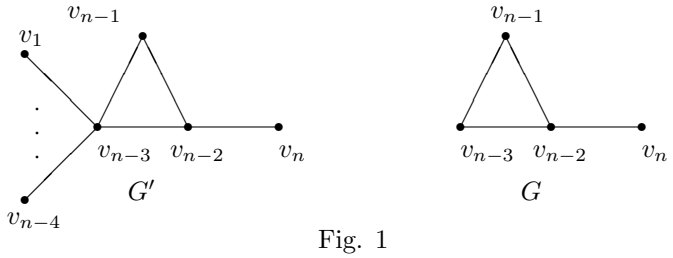


Fig. 1

Lemma 2.3 [10] $\mu(G) \leq max\{d(v) + m(v) : v \in V\}$, *where* $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.

Lemma 2.4 [11] $\Delta + 1 \leq \mu(G) \leq n$, *the left equality holds if and only if* $\Delta = n - 1$.

Proposition 2.5 *Suppose* $c \geq 0$ *and* G *is a* $c-$*cyclic graph with* $\Delta \leq n-3$. *If* $n \geq max\{c + 7, 2c + 5\}$, *then* $\mu(G) \leq n - 1$.

Proof. By Lemma 2.3, we only need to prove that $max\{d(v) + m(v) : v \in V\} \leq n - 1$.

Suppose $max\{d(v) + m(v) : v \in V\}$ occurs at the vertex u. Three cases arise $d(u) = 1$, $d(u) = 2$, or $3 \leq d(u) \leq n - 3$.

Case 1. $d(u) = 1$. Suppose $v \in N(u)$. Since $d(v) \leq \Delta \leq n - 3$, thus $d(u) + m(u) = d(u) + d(v) \leq n - 2 < n - 1$.

Case 2. $d(u) = 2$. Suppose that v,$w \in N(u)$. Note that G is a $c-$cyclic graph, then $|N(v) \cap N(w)| \leq c + 1$ and $|N(v) \cup N(w)| \leq n$. Therefore, $d(u) + m(u) = 2 + \frac{d(v)+d(w)}{2} \leq 2 + \frac{n+c+1}{2} \leq n - 1$.

Case 3. $3 \leq d(u) \leq n - 3$. Note that $3 \leq d(u) \leq n - 3$, then $d(u) + m(u) \leq d(u) + \frac{2m-d(u)-2}{d(u)} = d(u) - 1 + \frac{2m-2}{d(u)}$. Next we shall prove that $d(u) - 1 + \frac{2m-2}{d(u)} \leq n - 1$, equivalently, $d(u)(n - d(u)) \geq 2m - 2$. Once this is proved, we are done. Let $f(x) = (n - x)x$.

When $x \in [3, \frac{n}{2}]$, since $f'(x) = n-2x \geq 0$, then $f(x) \geq f(3) = 3(n-3) \geq 2(n + c - 1) - 2 = 2m - 2$.

When $x \in [\frac{n}{2}, n - 3]$, since $f'(x) = n - 2x \leq 0$, then $f(x) \geq f(n - 3) = 3(n - 3) \geq 2(n + c - 1) - 2 = 2m - 2$.

By combining the above discussion, the conclusion follows.

Corollary 2.6 *Suppose* $G \in \mathcal{T}_n$. *If* $n \geq 11$ *and* $\Delta \leq n - 3$, *then* $\mu(G) \leq n - 1$.

Let $H_1 - H_{27}$ be the tricyclic graphs on $n \geq 11$ vertices as shown in Fig. 2. For convenience, $V \backslash \{v\}$ is written as $V - v$.

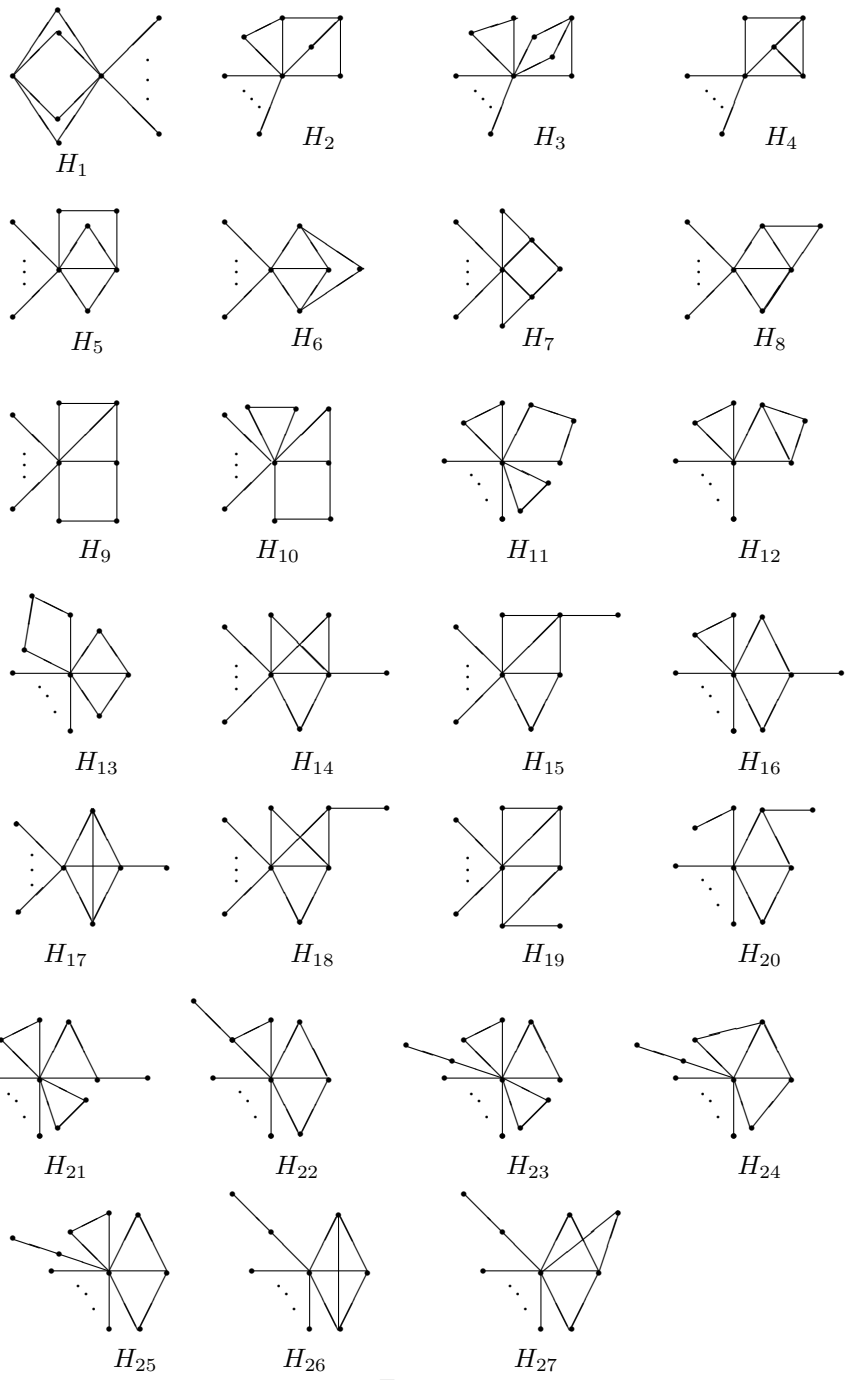

H_1
H_2
H_3
H_4
H_5
H_6
H_7
H_8
H_9
H_{10}
H_{11}
H_{12}
H_{13}
H_{14}
H_{15}
H_{16}
H_{17}
H_{18}
H_{19}
H_{20}
H_{21}
H_{22}
H_{23}
H_{24}
H_{25}
H_{26}
H_{27}

Fig. 2.

Lemma 2.7 *Suppose $G \in \mathcal{T}_n$ and $n \geq 11$. If G has the property $n-1 < \mu(G) < n$, then G should be the graphs $H_1 - H_{27}$.*

Proof. Suppose $\Delta = n-1$, Lemma 2.4 implies that $\mu(G) = n$. Combining with Corollary 2.6, if G has the property $n-1 < \mu(G) < n$, then $\Delta = n-2$. Next we shall show that $G \cong H_i$, where $1 \leq i \leq 27$.

Assume that $u_0 \in V(G)$ such that $d(u_0) = n-2$ and $v_0 \notin N(u_0)$. Note that $N(v_0) \subseteq N(u_0)$. It is easy to see that $1 \leq d(v_0) \leq 4$ because $G \in \mathcal{T}_n$. We consider the next four cases.

Case 1. $d(v_0) = 1$. Three subcases should be considered.

Subcase 1. $max\{|N(u_0) \cap N(v)| : v \in V - u_0\} = 1$. It is easy to see that $G \cong H_{21}$ or H_{23}.

Subcase 2. $max\{|N(u) \cap N(v)| : v \in V - u_0\} = 2$. It is easy to see that $G \cong H_{15}$ or H_{16} or H_{17} or H_{19} or H_{20} or H_{22} or H_{24} or H_{25} or H_{26}.

Subcase 3. $max\{|N(u) \cap N(v)| : v \in V - u_0\} = 3$. It is easy to see that $G \cong H_{14}$ or H_{18} or H_{27}.

Case 2. $d(v_0) = 2$. Two subcase should be considered.

Subcase 1. $max\{|N(u_0) \cap N(v)| : v \in V - u_0\} = 1$. It is easy to see that $G \cong H_7$ or H_{10} or H_{11} or H_{12}.

Subcase 2. $max\{|N(u) \cap N(v)| : v \in V - u_0\} = 2$. It is easy to see that $G \cong H_5$ or H_6 or H_8 or H_9 or H_{13}.

Case 3. $d(v_0) = 3$. It is easy to see that $G \cong H_2$ or H_3 or H_4.

Case 4. $d(v_0) = 4$. It is easy to see that $G \cong H_1$.

Lemma 2.8 *Suppose $n \geq 11$, then $n-1 < \mu(H_i) < n$ holds for $1 \leq i \leq 27$.*

Proof. By Lemma 2.1, we have

(1a) $\Phi(H_1, \lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)^3(\lambda^3 - (n+5)\lambda^2 + (6n-2)\lambda - 4n)$.

(2a) $\Phi(H_2, \lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda^5 - (n+9)\lambda^4 + (10n+23)\lambda^3 - (33n+11)\lambda^2 + (41n-10)\lambda - 16n)$.

(3a) $\Phi(H_3, \lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)^2(\lambda-3)(\lambda^3 - (n+4)\lambda^2 + (5n-2)\lambda - 3n)$.

(4a) $\Phi(H_4, \lambda) = \lambda(\lambda-1)^{n-6}(\lambda-2)(\lambda-4)(\lambda^3-(n+4)\lambda^2+(5n-2)\lambda-3n)$.

(5a) $\Phi(H_5, \lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda^5 - (n+9)\lambda^4 + (10n+22)\lambda^3 - (32n+8)\lambda^2 + (38n-12)\lambda - 14n)$.

(6a) $\Phi(H_6, \lambda) = \lambda(\lambda-1)^{n-6}(\lambda-3)(\lambda^4-(n+7)\lambda^3+(8n+9)\lambda^2-(17n-7)\lambda + 8n)$.

(7a) $\Phi(H_7, \lambda) = \lambda(\lambda-1)^{n-7}(\lambda^2-5\lambda+5)(\lambda^4-(n+6)\lambda^3+(7n+6)\lambda^2-(13n-5)\lambda + 6n)$.

(8a) $\Phi(H_8,\lambda) = \lambda(\lambda-1)^{n-6}(\lambda^5-(n+10)\lambda^4+(11n+29)\lambda^3-(40n+16)\lambda^2+(54n-19)\lambda-21n)$.

(9a) $\Phi(H_9,\lambda) = \lambda(\lambda-1)^{n-7}(\lambda^6-(n+11)\lambda^5+(12n+41)\lambda^4-(53n+55)\lambda^3+(106n+4)\lambda^2-(94n-26)\lambda+29n)$.

(10a) $\Phi(H_{10},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-3)(\lambda^5-(n+8)\lambda^4+(9n+18)\lambda^3-(27n+6)\lambda^2+(31n-10)\lambda-11n)$.

(11a) $\Phi(H_{11},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda-3)^2(\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-2n)$.

(12a) $\Phi(H_{12},\lambda) = \lambda(\lambda-1)^{n-6}(\lambda-3)(\lambda-4)(\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-2n)$.

(13a) $\Phi(H_{13},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)^2(\lambda-4)(\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-2n)$.

(14a) $\Phi(H_{14},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)^2(\lambda^4-(n+7)\lambda^3+(8n+5)\lambda^2-(13n-7)\lambda+5n)$.

(15a) $\Phi(H_{15},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda^6-(n+11)\lambda^5+(12n+39)\lambda^4-(51n+45)\lambda^3+(95n-9)\lambda^2-(77n-31)\lambda+21n)$.

(16a) $\Phi(H_{16},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda-3)(\lambda^4-(n+6)\lambda^3+(7n+4)\lambda^2-(11n-6)\lambda+4n)$.

(17a) $\Phi(H_{17},\lambda) = \lambda(\lambda-1)^{n-6}(\lambda-4)(\lambda^4-(n+6)\lambda^3+(7n+4)\lambda^2-(11n-6)\lambda+4n)$.

(18a) $\Phi(H_{18},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda^5-(n+9)\lambda^4+(10n+21)\lambda^3-(31n+3)\lambda^2+(33n-16)\lambda-10n)$.

(19a) $\Phi(H_{19},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda^6-(n+11)\lambda^5+(12n+40)\lambda^4-(52n+48)\lambda^3+(99n-10)\lambda^2-(80n-34)\lambda+21n)$.

(20a) $\Phi(H_{20},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-3)(\lambda^5-(n+8)\lambda^4+(9n+17)\lambda^3-(26n+2)\lambda^2+(27n-13)\lambda-8n)$.

(21a) $\Phi(H_{21},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-3)^2(\lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n)$.

(22a) $\Phi(H_{22},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda-4)(\lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n)$.

(23a) $\Phi(H_{23},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-3)^3(\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n)$.

(24a) $\Phi(H_{24},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-3)(\lambda^2-6\lambda+7)(\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n)$.

(25a) $\Phi(H_{25},\lambda) = \lambda(\lambda-1)^{n-7}(\lambda-2)(\lambda-3)(\lambda-4)(\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n)$.

(26a) $\Phi(H_{26},\lambda)=\lambda(\lambda-1)^{n-6}(\lambda-4)^2(\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n)$.

(27a) $\Phi(H_{27},\lambda)=\lambda(\lambda-1)^{n-7}(\lambda-2)^2(\lambda-5)(\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n)$.

By Lemma 2.4, $n-1<\mu(H_i)\leq n$ holds for $1\leq i\leq 27$. Moreover, when $1\leq i\leq 27$, since $\Phi(H_i,n)\neq 0$, thus $n-1<\mu(H_i)<n$ follows.

Let $S(n,3)$ denote the class of graphs obtained by adding 3 edges to pendants of $K_{1,n-1}$. By combining Lemmas 2.3-2.8 and Corollary 2.6, we have

Corollary 2.9 *If $G\in\mathcal{T}_n$ and $n\geq 11$, then $\mu(G)=n$ if and only if $G\in S(n,3)$.*

Lemma 2.10 *Suppose $G\in\mathcal{T}_n$ and $n\geq 11$, then $\mu(H_1)>\mu(H_2)>\mu(H_3)=\mu(H_4)>\mu(H_5)>\mu(H_6)>\mu(H_7)>\mu(H_8)>\mu(H_9)>\mu(H_{10})>\mu(H_{11})=\mu(H_{12})=\mu(H_{13})>\mu(H_{14})>\mu(H_{15})>\mu(H_{16})=\mu(H_{17})>\mu(H_{18})>\mu(H_{19})>\mu(H_{20})>\mu(H_{21})=\mu(H_{22})>\mu(H_{23})=\mu(H_{24})=\mu(H_{25})=\mu(H_{26})=\mu(H_{27})$.*

Proof. By Lemma 2.8, $n-1<\mu(H_i)<n$ holds for $1\leq i\leq 27$. Next we shall divide the proof into the next 17 process.

(1) $\mu(H_1)>\mu(H_2)$. Rewrite equality (1a) as $\Phi(H_1,\lambda)=\lambda(\lambda-1)^{n-7}(\lambda-2)f_1(\lambda)$, where $f_1(\lambda)=\lambda^5-(n+9)\lambda^4+(10n+22)\lambda^3-(32n+12)\lambda^2+(40n-8)\lambda-16n$. Let $f_2(\lambda)=\lambda^5-(n+9)\lambda^4+(10n+23)\lambda^3-(33n+11)\lambda^2+(41n-10)\lambda-16n$. Thus, $\mu(H_1)$ and $\mu(H_2)$ equals the maximum root of the equation $f_1(\lambda)=0$ and $f_2(\lambda)=0$, respectively. When $\lambda\geq n-1$, since $f_2(\lambda)-f_1(\lambda)=\lambda(\lambda(\lambda+1-n)+n-2)>0$, thus $\mu(H_1)>\mu(H_2)$.

(2) $\mu(H_2)>\mu(H_3)=\mu(H_4)$. By equalities (3a) and (4a), it follows that $\mu(H_3)=\mu(H_4)$. Rewrite equality (3a) as $\Phi(H_3,\lambda)=\lambda(\lambda-1)^{n-7}(\lambda-2)f_3(\lambda)$, where $f_3(\lambda)=\lambda^5-(n+9)\lambda^4+(10n+24)\lambda^3-(34n+14)\lambda^2+(45n-12)\lambda-18n$. Thus, $\mu(H_3)$ equals the maximum root of the equation $f_3(\lambda)=0$. Let $\psi_1(\lambda)=f_3(\lambda)-f_2(\lambda)=\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-2n$, and α_1 denote the maximum root of $\psi_1(\lambda)=0$. Since $\psi_1(0)=-2n<0$, $\psi_1(1)=n-4>0$, $\psi_1(n-1)=-2<0$ and $\psi_1(n)=n(n-4)>0$, then $n-1<\alpha_1<n$.

It is easy to see that $f_2(\lambda)=(\lambda^2-6\lambda+7)\psi_1(\lambda)+\gamma_1(\lambda)$ and $f_3(\lambda)=(\lambda^2-6\lambda+8)\psi_1(\lambda)+\gamma_1(\lambda)$, where $\gamma_1(\lambda)=-2\lambda^2+(n+4)\lambda-2n$. Since $f_2(\alpha_1)=f_3(\alpha_1)=\gamma_1(\alpha_1)<\alpha_1(6-n)-2n<0$, thus $\mu(H_2),\mu(H_3)\in(\alpha_1,n)$. Moreover, since $\lim\limits_{\lambda\longrightarrow+\infty}\psi_1(\lambda)=+\infty$, thus $\psi_1(\lambda)>\psi_1(\alpha_1)=0$ when $\lambda>\alpha_1$. This implies that $f_3(\lambda)>f_2(\lambda)$ when $\lambda>\alpha_1$. Therefore, $\mu(H_2)>\mu(H_3)$.

(3) $\mu(H_4)>\mu(H_5)$. Rewrite equality (4a) as $\Phi(H_4,\lambda)=\lambda(\lambda-1)^{n-6}f_4(\lambda)$, where $f_4(\lambda)=\lambda^5-(n+10)\lambda^4+(11n+30)\lambda^3-(41n+20)\lambda^2+(58n-16)\lambda-24n$.

Thus, $\mu(H_4)$ equals the maximum root of the equation $f_4(\lambda) = 0$. Let $f_5(\lambda) = \lambda^5 - (n+9)\lambda^4 + (10n+22)\lambda^3 - (32n+8)\lambda^2 + (38n-12)\lambda - 14n$. By equality (5a), $\mu(H_5)$ equals the maximum root of the equation $f_5(\lambda) = 0$. Let $\psi_2(\lambda) = f_5(\lambda) - f_4(\lambda) = \lambda^4 - (n+8)\lambda^3 + (9n+12)\lambda^2 - (20n-4)\lambda + 10n$. When $\lambda \geq n-1$, since $\psi_2''(\lambda) = 12\lambda^2 - (6n+48)\lambda + (18n+24) > 0$, thus $\psi_2'(\lambda) = 4\lambda^3 - (3n+24)\lambda^2 + (18n+24)\lambda - (20n-4) \geq \psi_2'(n-1) = n^3 - 12n^2 + 43n - 48 > 0$. Therefore, when $\lambda \geq n-1$, $\psi_2(\lambda) \geq \psi_2(n-1) = n^2 - 8n + 17 > 0$. Thus, $f_5(\lambda) > f_4(\lambda)$ when $\lambda \geq n-1$, this implies that $\mu(H_4) > \mu(H_5)$.

(4) $\mu(H_5) > \mu(H_6)$. Let $f_6(\lambda) = \lambda^4 - (n+7)\lambda^3 + (8n+9)\lambda^2 - (17n-7)\lambda + 8n$. By equality (6a), $\mu(H_6)$ equals the maximum root of the equation $f_6(\lambda) = 0$. It is easy to see that $f_5(\lambda) = f_6(\lambda)(\lambda - 2) + \gamma_2(\lambda)$, where $\gamma_2(\lambda) = -\lambda^3 + (n+3)\lambda^2 - (4n-2)\lambda + 2n$. Let α_2 denote the maximum root of $\gamma_2(\lambda) = 0$. Since $\gamma_2(0) = 2n > 0$, $\gamma_2(1) = 4 - n < 0$, $\gamma_2(n-1) = 2 > 0$, $\gamma_2(n) = n(4-n) < 0$, thus $n - 1 < \alpha_2 < n$.

Note that $f_6(\lambda) = \gamma_2(\lambda)(4 - \lambda) + \lambda(n - 1 - \lambda)$, then $f_6(\alpha_2) = \alpha_2(n - 1 - \alpha_2) < 0$. Moreover since $\lim_{\lambda \longrightarrow +\infty} f_6(\lambda) = +\infty$, thus $\mu(H_6) > \alpha_2$. Note that $\lim_{\lambda \longrightarrow +\infty} \gamma_2(\lambda) = -\infty$, thus $f_5(\mu(H_6)) = \gamma_2(\mu(H_6)) < 0$. This implies that $\mu(H_5) > \mu(H_6)$ because $\lim_{\lambda \longrightarrow +\infty} f_5(\lambda) = +\infty$.

(5) $\mu(H_6) > \mu(H_7)$. Let $f_7(\lambda) = \lambda^4 - (n+6)\lambda^3 + (7n+6)\lambda^2 - (13n-5)\lambda + 6n$, by equality (7a), $\mu(H_7)$ equals the maximum root of the equation $f_7(\lambda) = 0$.

Note that $f_7(\lambda) - f_6(\lambda) = \lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n = \psi_1(\lambda)$, by the proof of $\mu(H_2) > \mu(H_3)$, $n - 1 < \alpha_1 < n$, where α_1 is the maximum root of $\psi_1(\lambda) = 0$.

It is easy to see that $f_6(\lambda) = (\lambda - 4)\psi_1(\lambda) + \gamma_3(\lambda)$ and $f_7(\lambda) = (\lambda - 3)\psi_2(\lambda) + \gamma_3(\lambda)$, where $\gamma_3(\lambda) = -\lambda^2 + (n-1)\lambda$. Note that $n - 1 < \alpha_1 < n$, thus $f_7(\alpha_1) = f_6(\alpha_1) = \gamma_3(\alpha_1) = \alpha_1(n - 1 - \alpha_1) < 0$, which implies that $\mu(H_6), \mu(H_7) \in (\alpha_1, n)$. Moreover, since $\lim_{\lambda \longrightarrow +\infty} \psi_1(\lambda) = +\infty$, thus $\psi_1(\lambda) > \psi_1(\alpha_1) = 0$ when $\lambda > \alpha_1$. This implies that $f_7(\lambda) > f_6(\lambda)$ when $\lambda > \alpha_1$. Therefore, $\mu(H_6) > \mu(H_7)$.

(6) $\mu(H_7) > \mu(H_8)$. Rewrite equality (7a) as $\Phi(H_7, \lambda) = \lambda(\lambda-1)^{n-7} f_8(\lambda)$, where $f_8(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+41)\lambda^4 - (53n+55)\lambda^3 + (106n+5)\lambda^2 - (95n-25)\lambda + 30n$. Thus, $\mu(H_7)$ equals the maximum root of the equation $f_8(\lambda) = 0$. Rewrite equality (8a) as $\Phi(H_8, \lambda) = \lambda(\lambda-1)^{n-7} f_9(\lambda)$, where $f_9(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+39)\lambda^4 - (51n+45)\lambda^3 + (94n-3)\lambda^2 - (75n-19)\lambda + 21n$. Thus, $\mu(H_8)$ equals the maximum root of the equation $f_9(\lambda) = 0$. Let $\psi_3(\lambda) = f_8(\lambda) - f_9(\lambda) = 2\lambda^4 - (2n+10)\lambda^3 + (12n+8)\lambda^2 - (20n-6)\lambda + 9n$, α_3 and α_4 denote the maximum and the second largest root of $\psi_3(\lambda) = 0$, respectively. Since $\psi_3(0) = 9n > 0$, $\psi_3(1) = 6 - n < 0$, $\psi_3(2) = n - 4 > 0$, $\psi_3(n-1) = 14 - 5n < 0$, and

$\psi_3(n) = 2n^2(n-6) + 15n > 0$, thus $n-1 < \alpha_3 < n$, $2 < \alpha_4 < n-1$.

It is easy to see that $f_8(\lambda) = \frac{\lambda^2-6\lambda+7}{2}\psi_3(\lambda) + \gamma_4(\lambda)$ and $f_9(\lambda) = \frac{\lambda^2-6\lambda+5}{2}\psi_3(\lambda) + \gamma_4(\lambda)$, where $\gamma_4(\lambda) = \frac{2\lambda^3-(n+10)\lambda^2+(4n+8)\lambda-3n}{2}$. By straightly computation, $\frac{n+10+\sqrt{n^2-4n+52}}{6}$ is the maximum root of $\gamma_4'(\lambda) = 3\lambda^2 - (n+10)\lambda + 2n + 4 = 0$. Note that $\frac{n+10+\sqrt{n^2-4n+52}}{6} < n-1$ and $\lim_{\lambda \longrightarrow +\infty} \gamma_4'(\lambda) = +\infty$, thus when $\lambda \geq \alpha_3$, $f_8(\lambda) \geq \gamma_4(\alpha_3) > \gamma_4(n-1) = \frac{1}{2}((n-1)(n-9)n + 17n - 20) > 0$. Thus, $\mu(H_7) \in (n-1, \alpha_3)$. With the same reason, we have $\mu(H_8) \in (n-1, \alpha_3)$.

Moreover, since $\alpha_4 \in (2, n-1)$, $\psi_3(n-1) < 0$, and $\lim_{\lambda \longrightarrow +\infty} \psi_3(\lambda) = +\infty$, thus $\psi_3(\lambda) < \psi_3(\alpha_3) = 0$ when $\lambda \in (n-1, \alpha_3)$. Note that $\mu(H_8) \in (n-1, \alpha_3)$, thus $f_8(\mu(H_8)) = \psi_3(\mu(H_8)) < 0$. Moreover, since $\lim_{\lambda \longrightarrow +\infty} f_8(\lambda) = +\infty$, then $\mu(H_7) > \mu(H_8)$.

(7) $\mu(H_8) > \mu(H_9)$. Let $f_{10}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+41)\lambda^4 - (53n+55)\lambda^3 + (106n+4)\lambda^2 - (94n-26)\lambda + 29n$, by equality (9a), $\mu(H_9)$ equals the maximum root of the equation $f_{10}(\lambda) = 0$. Let $\psi_4(\lambda) = f_{10}(\lambda) - f_9(\lambda) = 2\lambda^4 - (2n+10)\lambda^3 + (12n+7)\lambda^2 - (19n-7)\lambda + 8n$, α_5 denote the maximum root of $\psi_4(\lambda) = 0$. Since $\psi_4(0) = 8n > 0$, $\psi_4(1) = 6 - n < 0$, $\psi_4(2) = 2n - 6 > 0$, $\psi_4(n-1) = 12 - 4n < 0$, and $\psi_4(n) = n(2n^2 - 12n + 15) > 0$, thus $n-1 < \alpha_5 < n$.

It is easy to see that $f_9(\lambda) = \frac{\lambda^2-6\lambda+5.5}{2}\psi_4(\lambda) + \gamma_5(\lambda)$ and $f_{10}(\lambda) = \frac{\lambda^2-6\lambda+7.5}{2}\psi_4(\lambda) + \gamma_5(\lambda)$, where $\gamma_5(\lambda) = \frac{-5\lambda^2+(5n-1)\lambda-4n}{4}$. When $\lambda \geq n-1$, since $\gamma_5'(\lambda) = \frac{-10\lambda+(5n-1)}{4} < 0$, thus $\gamma_5(\lambda) \leq \gamma_5(n-1) = -1 < 0$. Therefore, $f_9(\alpha_5) = f_{10}(\alpha_5) = \gamma_5(\alpha_5) < 0$. Thus, $\mu(H_8), \mu(H_9) \in (\alpha_5, n)$.

Moreover, since $\lim_{\lambda \longrightarrow +\infty} \psi_4(\lambda) = +\infty$, thus $\psi_4(\lambda) > \psi_4(\alpha_5) = 0$ when $\lambda > \alpha_5$. This implies that $f_{10}(\lambda) > f_9(\lambda)$ when $\lambda > \alpha_5$. Therefore, $\mu(H_8) > \mu(H_9)$.

(8) $\mu(H_9) > \mu(H_{10})$. Rewrite equality (10a) as $\Phi(H_{10}, \lambda) = \lambda(\lambda-1)^{n-7} f_{11}(\lambda)$, where $f_{11}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+42)\lambda^4 - (54n+60)\lambda^3 + (112n+8)\lambda^2 - (104n-30)\lambda + 33n$. Thus, $\mu(H_{10})$ equals the maximum root of the equation $f_{11}(\lambda) = 0$. Let $\psi_5(\lambda) = f_{11}(\lambda) - f_{10}(\lambda) = \lambda^4 - (n+5)\lambda^3 + (6n+4)\lambda^2 - (10n-4)\lambda + 4n$, and α_6 denote the maximum root of $\psi_5(\lambda) = 0$. Since $\psi_5(0) = 4n > 0$, $\psi_5(1) = 4 - n < 0$, $\psi_5(3) = n - 6 > 0$, $\psi_5(n-1) = 6 - 2n < 0$ and $\psi_5(n) = n(n^2 - 6n + 8) > 0$, then $n-1 < \alpha_6 < n$.

It is easy to see that $f_{10}(\lambda) = (\lambda^2 - 6\lambda + 7)\psi_5(\lambda) + \gamma_6(\lambda)$ and $f_{11}(\lambda) = (\lambda^2 - 6\lambda + 8)\psi_5(\lambda) + \gamma_6(\lambda)$, where $\gamma_6(\lambda) = n - 2\lambda$. Thus, $f_{11}(\alpha_6) = f_{10}(\alpha_6) = \gamma_6(\alpha_6) = n - 2\alpha_6 < 0$, which implies that $\mu(H_9), \mu(H_{10}) \in (\alpha_6, n)$. Moreover, since $\lim_{\lambda \longrightarrow +\infty} \psi_5(\lambda) = +\infty$, thus $\psi_5(\lambda) > \psi_5(\alpha_6) = 0$ when $\lambda > \alpha_6$. This implies that $f_{11}(\lambda) > f_{10}(\lambda)$ when $\lambda > \alpha_6$. Therefore, $\mu(H_9) > \mu(H_{10})$.

(9) $\mu(H_{10}) > \mu(H_{11}) = \mu(H_{12}) = \mu(H_{13})$. By equalities (11a), (12a) and (13a), it follows that $\mu(H_{11}) = \mu(H_{12}) = \mu(H_{13})$. Rewrite equality (11a) as $\Phi(H_{11}, \lambda) = \lambda(\lambda-1)^{n-7} f_{12}(\lambda)$, where $f_{12}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+43)\lambda^4 - (55n+65)\lambda^3 + (118n+12)\lambda^2 - (114n-36)\lambda + 36n$. Thus, $\mu(H_{11})$ equals the maximum root of the equation $f_{12}(\lambda) = 0$. Let $\psi_6(\lambda) = f_{12}(\lambda) - f_{11}(\lambda) = \lambda^4 - (n+5)\lambda^3 + (6n+4)\lambda^2 - (10n-6)\lambda + 3n$, and α_7 denote the maximum root of $\psi_6(\lambda) = 0$. Since $\psi_6(0) = 3n > 0$, $\psi_6(1) = 6 - 2n < 0$, $\psi_6(2.8) = 0.088n - 0.1344 > 0$, $\psi_6(n-1) = 4 - n < 0$ and $\psi_6(n) = n(n^2 - 6n + 9) > 0$, then $n - 1 < \alpha_7 < n$.

It is easy to see that $f_{11}(\lambda) = (\lambda^2 - 6\lambda + 8)\psi_6(\lambda) + \gamma_7(\lambda)$ and $f_{12}(\lambda) = (\lambda^2 - 6\lambda + 9)\psi_6(\lambda) + \gamma_7(\lambda)$, where $\gamma_7(\lambda) = -2\lambda^3 + (n+12)\lambda^2 - (6n+18)\lambda + 9n$. Note that the maximum root of $\gamma_7'(\lambda) = -6\lambda^2 + (2n+24)\lambda - (6n+18)$ is $\frac{n}{3} + 1$. Moreover, since $\frac{n}{3} + 1 < n - 1$ and $\lim\limits_{\lambda \longrightarrow +\infty} \gamma_7'(\lambda) = -\infty$, thus $\gamma_7(\lambda) \leq \gamma_7(n-1) = (n-1)n(9-n) - 23n + 32 < 0$ when $\lambda \geq n-1$. Therefore, $f_{11}(\alpha_7) = f_{12}(\alpha_7) = \gamma_7(\alpha_7) < 0$. Thus, $\mu(H_{10}), \mu(H_{11}) \in (\alpha_7, n)$.

Moreover, since $\lim\limits_{\lambda \longrightarrow +\infty} \psi_6(\lambda) = +\infty$, thus $\psi_6(\lambda) > \psi_6(\alpha_7) = 0$ when $\lambda > \alpha_7$. This implies that $f_{12}(\lambda) > f_{11}(\lambda)$ when $\lambda > \alpha_7$. Therefore, $\mu(H_{10}) > \mu(H_{11})$.

(10) $\mu(H_{13}) > \mu(H_{14})$. Let $f_{13}(\lambda) = \lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n$, by equality (13a), $\mu(H_{13})$ equals the maximum root of the equation $f_{13}(\lambda) = 0$. Let $f_{14}(\lambda) = \lambda^4 - (n+7)\lambda^3 + (8n+5)\lambda^2 - (13n-7)\lambda + 5n$, by equality (14a), $\mu(H_{14})$ equals the maximum root of the equation $f_{14}(\lambda) = 0$. It is easy to see that $f_{14}(\lambda) = (\lambda - 5) f_{13}(\lambda) + \gamma_8(\lambda)$, where $\gamma_8(\lambda) = \lambda^3 - (n+8)\lambda^2 + (9n-3)\lambda - 5n$. Note that $\gamma_8'(\lambda) = 3\lambda^2 - (2n+16)\lambda + 9n - 3$, and the maximum root of $\gamma_8'(\lambda) = 0$ is $\frac{n+8+\sqrt{n^2-11n+73}}{3}$. When $\lambda > n-1$, since $\frac{n+8+\sqrt{n^2-11n+73}}{3} < n-1$ and $\lim\limits_{\lambda \longrightarrow +\infty} \gamma_8'(\lambda) = +\infty$, then $\gamma_8'(\lambda) > 0$. Thus, when $\lambda \geq \mu(H_{13})$, $f_{14}(\lambda) \geq \gamma_8(\mu(H_{13})) > \gamma_8(n-1) = n - 6 > 0$. This implies that $\mu(H_{13}) > \mu(H_{14})$.

(11) $\mu(H_{14}) > \mu(H_{15})$. Let $f_{15}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+39)\lambda^4 - (51n+45)\lambda^3 + (95n-9)\lambda^2 - (77n-31)\lambda + 21n)$, by equality (15a), $\mu(H_{15})$ equals the maximum root of the equation $f_{15}(\lambda) = 0$. It is easy to see that $f_{15}(\lambda) = (\lambda^2 - 4\lambda + 6) f_{14}(\lambda) + \gamma_9(\lambda)$, where $\gamma_9(\lambda) = 10\lambda^3 - (10n+11)\lambda^2 + (21n-11)\lambda - 9n$. By straightly computation, $\frac{10n+11+\sqrt{100n^2-410n+451}}{30}$ is the maximum root of $\gamma_9'(\lambda) = 30\lambda^2 - (20n+22)\lambda + 21n - 11 = 0$. When $\lambda > n-1$, since $\frac{10n+11+\sqrt{100n^2-410n+451}}{30} < n-1$ and $\lim\limits_{\lambda \longrightarrow +\infty} \gamma_9'(\lambda) = +\infty$, then $\gamma_9'(\lambda) > 0$. Thus, when $\lambda \geq \mu(H_{14})$, $f_{15}(\lambda) \geq \gamma_9(\mu(H_{14})) > \gamma_9(n-1) = n - 10 > 0$. This implies that $\mu(H_{14}) > \mu(H_{15})$.

(12) $\mu(H_{15}) > \mu(H_{16}) = \mu(H_{17})$. By equalities (16a) and (17a), it follows that $\mu(H_{16}) = \mu(H_{17})$. Rewrite equality (16a) as $\Phi(H_{16}, \lambda) = \lambda(\lambda-1)^{n-7} f_{16}(\lambda)$, where $f_{16}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+40)\lambda^4 - (52n+$

$50)\lambda^3+(101n-6)\lambda^2-(86n-36)\lambda+24n$. Thus, $\mu(H_{16})$ equals the maximum root of the equation $f_{16}(\lambda)=0$. Let $\psi_7(\lambda)=f_{16}(\lambda)-f_{15}(\lambda)=\lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n$, and α_8 denote the maximum root of $\psi_7(\lambda)=0$. Since $\psi_7(0)=3n>0$, $\psi_7(1)=4-n<0$, $\psi_7(2)=n-2>0$, $\psi_7(n-1)=4-n<0$ and $\psi_7(n)=n(n^2-6n+8)>0$, then $n-1<\alpha_8<n$.

It is easy to see that $f_{15}(\lambda)=(\lambda^2-6\lambda+6)\psi_7(\lambda)+\gamma_{10}(\lambda)$ and $f_{16}(\lambda)=(\lambda^2-6\lambda+7)\psi_7(\lambda)+\gamma_{10}(\lambda)$, where $\gamma_{10}(\lambda)=-2\lambda^3+(2n+3)\lambda^2-(5n-1)\lambda+3n$. By straightly computation, $\frac{2n+3+\sqrt{4n^2-18n+15}}{6}$ is the maximum root of $\gamma'_{10}(\lambda)=-6\lambda^2+(4n+6)\lambda-(5n-1)=0$. When $\lambda\geq n-1$, since $\frac{2n+3+\sqrt{4n^2-18n+15}}{6}<n-1$ and $\lim\limits_{\lambda\longrightarrow+\infty}\gamma'_{10}(\lambda)=-\infty$, then $\gamma_{10}(\lambda)\leq\gamma_{10}(n-1)=4-n<0$. Thus, $f_{15}(\alpha_8)=f_{16}(\alpha_8)=\gamma_{10}(\alpha_8)<0$, which yields that $\mu(H_{15}),\mu(H_{16})\in(\alpha_8,n)$. Moreover, since $\lim\limits_{\lambda\longrightarrow+\infty}\psi_7(\lambda)=+\infty$, thus $\psi_7(\lambda)>\psi_7(\alpha_8)=0$ when $\lambda>\alpha_8$. This implies that $f_{16}(\lambda)>f_{15}(\lambda)$ when $\lambda>\alpha_8$. Therefore, $\mu(H_{15})>\mu(H_{16})$.

(13) $\mu(H_{17})>\mu(H_{18})$. Rewrite equality (17a) as $\Phi(H_{17},\lambda)=\lambda(\lambda-1)^{n-7}f_{17}(\lambda)$, where $f_{17}(\lambda)=\lambda^6-(n+11)\lambda^5+(12n+38)\lambda^4-(50n+38)\lambda^3+(87n-14)\lambda^2-(64n-24)\lambda+16n$. Thus, $\mu(H_{17})$ equals the maximum root of the equation $f_{17}(\lambda)=0$. Rewrite equality (18a) as $\Phi(H_{18},\lambda)=\lambda(\lambda-1)^{n-7}f_{18}(\lambda)$, where $f_{18}(\lambda)=\lambda^6-(n+11)\lambda^5+(12n+39)\lambda^4-(51n+45)\lambda^3+(95n-10)\lambda^2-(76n-32)\lambda+20n$. Thus, $\mu(H_{18})$ equals the maximum root of the equation $f_{18}(\lambda)=0$. Let $\psi_8(\lambda)=f_{18}(\lambda)-f_{17}(\lambda)=\lambda^4-(n+7)\lambda^3+(8n+4)\lambda^2-(12n-8)\lambda+4n$, then $\psi'_8(\lambda)=4\lambda^3-(3n+21)\lambda^2+(16n+8)\lambda-(12n-8)$. When $\lambda\geq n-1$, since $\psi''_8(\lambda)=12\lambda^2-(6n+42)\lambda+(16n+8)\geq(n-1)(6n-54)+(16n+8)>0$, thus $\psi'_8(\lambda)\geq\psi'_8(n-1)=(n-1)(n^2-10n)+21n-25>0$. So when $\lambda\geq n-1$, $f_{18}(\lambda)-f_{17}(\lambda)=\psi_8(\lambda)\geq\psi_8(n-1)=4>0$. Thus, $\mu(H_{17})>\mu(H_{18})$.

(14) $\mu(H_{18})>\mu(H_{19})$. Let $f_{19}(\lambda)=\lambda^6-(n+11)\lambda^5+(12n+40)\lambda^4-(52n+48)\lambda^3+(99n-10)\lambda^2-(80n-34)\lambda+21n$. By equality (19a), $\mu(H_{19})$ equals the maximum root of the equation $f_{19}(\lambda)=0$. Let $\psi_9(\lambda)=f_{19}(\lambda)-f_{18}(\lambda)=\lambda^4-(n+3)\lambda^3+4n\lambda^2-(4n-2)\lambda+n$, and α_9 denote the maximum root of $\psi_9(\lambda)=0$. Since $\psi_9(0)=n>0$, $\psi_9(\frac{1}{2})=\frac{11-2n}{16}<0$, $\psi_9(2)=n-4>0$, $\psi_9(n-1)=2-n<0$ and $\psi_9(n)=n(n^2-4n+3)>0$, then $n-1<\alpha_9<n$.

It is easy to see that $f_{18}(\lambda)=(\lambda^2-8\lambda+15)\psi_9(\lambda)+\gamma_{11}(\lambda)$ and $f_{19}(\lambda)=(\lambda^2-8\lambda+16)\psi_9(\lambda)+\gamma_{11}(\lambda)$, where $\gamma_{11}(\lambda)=-2\lambda^3+(2n+6)\lambda^2-(8n-2)\lambda+5n$. By straightly computation, $\frac{n+3+\sqrt{n^2-6n+12}}{3}$ is the maximum root of $\gamma'_{11}(\lambda)=-6\lambda^2+(4n+12)\lambda-(8n-2)=0$. When $\lambda\geq n-1$, since $\frac{n+3+\sqrt{n^2-6n+12}}{3}<n-1$ and $\lim\limits_{\lambda\longrightarrow+\infty}\gamma'_{11}(\lambda)=-\infty$, then $\gamma_{11}(\lambda)\leq\gamma_{11}(n-1)=6-n<0$. Thus, $f_{18}(\alpha_9)=f_{19}(\alpha_9)=\gamma_{11}(\alpha_9)<0$, which implies that $\mu(H_{18}),\mu(H_{19})\in(\alpha_9,n)$. Moreover, since $\lim\limits_{\lambda\longrightarrow+\infty}\psi_9(\lambda)=+\infty$, thus

$\psi_9(\lambda) > \psi_9(\alpha_9) = 0$ when $\lambda > \alpha_9$. This implies that $f_{19}(\lambda) > f_{18}(\lambda)$ when $\lambda > \alpha_9$. Therefore, $\mu(H_{18}) > \mu(H_{19})$.

(15) $\mu(H_{19}) > \mu(H_{20})$. Rewrite equality (20a) as $\Phi(H_{20}, \lambda) = \lambda(\lambda - 1)^{n-7} f_{20}(\lambda)$, where $f_{20}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+41)\lambda^4 - (53n+53)\lambda^3 + (105n-7)\lambda^2 - (89n-39)\lambda + 24n$. Thus, $\mu(H_{20})$ equals the maximum root of the equation $f_{20}(\lambda) = 0$. Note that $f_{20}(\lambda) - f_{19}(\lambda) = \lambda^4 - (n+5)\lambda^3 + (6n+3)\lambda^2 - (9n-5)\lambda + 3n = \psi_7(\lambda)$. By the proof of $\mu(H_{15}) > \mu(H_{16})$, we have $n - 1 < \alpha_8 < n$, where α_8 is the maximum root of $\psi_7(\lambda) = 0$.

It is easy to see that $f_{19}(\lambda) = (\lambda^2 - 6\lambda + 7)\psi_7(\lambda) + \gamma_3(\lambda)$ and $f_{20}(\lambda) = (\lambda^2 - 6\lambda + 8)\psi_7(\lambda) + \gamma_3(\lambda)$, where $\gamma_3(\lambda) = -\lambda^2 + (n-1)\lambda$. Since $f_{19}(\alpha_8) = f_{20}(\alpha_8) = \gamma_3(\alpha_8) < 0$, thus $\mu(H_{19}), \mu(H_{20}) \in (\alpha_8, n)$. Moreover, since $\lim_{\lambda \longrightarrow +\infty} \psi_7(\lambda) = +\infty$, thus $\psi_7(\lambda) > \psi_7(\alpha_8) = 0$ when $\lambda > \alpha_8$. This implies that $f_{20}(\lambda) > f_{19}(\lambda)$ when $\lambda > \alpha_8$. Therefore, $\mu(H_{19}) > \mu(H_{20})$.

(16) $\mu(H_{20}) > \mu(H_{21}) = \mu(H_{22})$. By equalities (21a) and (22a), it follows that $\mu(H_{21}) = \mu(H_{22})$. Rewrite equality (22a) as $\Phi(H_{22}, \lambda) = \lambda(\lambda-1)^{n-7} f_{21}(\lambda)$, where $f_{21}(\lambda) = \lambda^6 - (n+11)\lambda^5 + (12n+41)\lambda^4 - (53n+53)\lambda^3 + (105n-6)\lambda^2 - (90n-40)\lambda + 24n$. Thus, $\mu(H_{22})$ equals the maximum root of the equation $f_{21}(\lambda) = 0$. When $\lambda > n - 1$, since $f_{21}(\lambda) - f_{20}(\lambda) = \lambda(\lambda + 1 - n) > 0$, thus $f_{21}(\lambda) > f_{20}(\lambda)$. Recall that $\mu(H_{20})$, $\mu(H_{22}) \in (n-1, n)$, then $\mu(H_{20}) > \mu(H_{22})$.

(17) $\mu(H_{22}) > \mu(H_{23}) = \mu(H_{24}) = \mu(H_{25}) = \mu(H_{26}) = \mu(H_{27})$. By equalities (23a)-(27a), it follows that $\mu(H_{23}) = \mu(H_{24}) = \mu(H_{25}) = \mu(H_{26}) = \mu(H_{27})$. Let $f_{22}(\lambda) = \lambda^4 - (n+5)\lambda^3 + (6n+3)\lambda^2 - (9n-5)\lambda + 3n$, $f_{23}(\lambda) = \lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n$. By equalities (22a) and (23a), $\mu(H_{22})$ and $\mu(H_{23})$ equals the maximum root of the equation $f_{22}(\lambda) = 0$ and $f_{23}(\lambda) = 0$, respectively. Clearly, $f_{22}(\lambda) = (\lambda - 3)f_{23}(\lambda) + \gamma_3(\lambda)$, where $\gamma_3(\lambda) = -\lambda^2 + (n-1)\lambda$. Since $\mu(H_{23}) > n - 1$, thus $f_{22}(\mu(H_{23})) = \gamma_3(\mu(H_{23})) = -\mu(H_{23})(\mu(H_{23}) + 1 - n) < 0$. Moreover, since $\lim_{\lambda \longrightarrow +\infty} f_{22}(\lambda) = +\infty$, thus $\mu(H_{22}) > \mu(H_{23})$.

By combining equalities (1a)-(27a), Lemmas 2.7-2.10 and Corollaries 2.6-2.9, we have

Theorem 2.11 *Suppose $G \in \mathcal{T}_n$ and $n \geq 11$.*

(1) *Then $\mu(G) \leq n$, the equality holds if and only if $G \in S(n, 3)$.*

(2) *If $G \notin S(n, 3)$, then $\mu(G) \leq \mu(H_1)$, the equality holds if and only if $G \cong H_1$, where $\mu(H_1)$ is the maximum root of the equation $\lambda^3 - (n+5)\lambda^2 + (6n-2)\lambda - 4n = 0$.*

(3) *If $G \notin S(n, 3)$ and $G \ncong H_1$, then $\mu(G) \leq \mu(H_2)$, the equality holds if and only if $G \cong H_2$, where $\mu(H_2)$ is the maximum root of the equation $\lambda^5 - (n+9)\lambda^4 + (10n+23)\lambda^3 - (33n+11)\lambda^2 + (41n-10)\lambda - 16n = 0$.*

(4) *If $G \notin S(n, 3)$ and $G \ncong H_i$ $(1 \leq i \leq 2)$, then $\mu(G) \leq \mu(H_3)$,*

the equality holds if and only if $G \cong H_3$ *or* $G \cong H_4$, *where* $\mu(H_3)$ *is the maximum root of the equation* $\lambda^3 - (n+4)\lambda^2 + (5n-2)\lambda - 3n = 0$.

(5) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 4)$, *then* $\mu(G) \le \mu(H_5)$, *the equality holds if and only if* $G \cong H_5$, *where* $\mu(H_5)$ *is the maximum root of the equation* $\lambda^5-(n+9)\lambda^4+(10n+22)\lambda^3-(32n+8)\lambda^2+(38n-12)\lambda-14n = 0$.

(6) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 5)$, *then* $\mu(G) \le \mu(H_6)$, *the equality holds if and only if* $G \cong H_6$, *where* $\mu(H_6)$ *is the maximum root of the equation* $\lambda^4 - (n+7)\lambda^3 + (8n+9)\lambda^2 - (17n-7)\lambda + 8n = 0$.

(7) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 6)$, *then* $\mu(G) \le \mu(H_7)$, *the equality holds if and only if* $G \cong H_7$, *where* $\mu(H_7)$ *is the maximum root of the equation* $\lambda^4 - (n+6)\lambda^3 + (7n+6)\lambda^2 - (13n-5)\lambda + 6n = 0$.

(8) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 7)$, *then* $\mu(G) \le \mu(H_8)$, *the equality holds if and only if* $G \cong H_8$, *where* $\mu(H_8)$ *is the maximum root of the equation* $\lambda^5-(n+10)\lambda^4+(11n+29)\lambda^3-(40n+16)\lambda^2+(54n-19)\lambda-21n = 0$.

(9) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 8)$, *then* $\mu(G) \le \mu(H_9)$, *the equality holds if and only if* $G \cong H_9$, *where* $\mu(H_9)$ *is the maximum root of the equation* $\lambda^6-(n+11)\lambda^5+(12n+41)\lambda^4-(53n+55)\lambda^3+(106n+4)\lambda^2-(94n-26)\lambda+29n = 0$.

(10) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 9)$, *then* $\mu(G) \le \mu(H_{10})$, *the equality holds if and only if* $G \cong H_{10}$, *where* $\mu(H_{10})$ *is the maximum root of the equation* $\lambda^5-(n+8)\lambda^4+(9n+18)\lambda^3-(27n+6)\lambda^2+(31n-10)\lambda-11n = 0$.

(11) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 10)$, *then* $\mu(G) \le \mu(H_{11})$, *the equality holds if and only if* $G \cong H_{11}$ *or* $G \cong H_{12}$ *or* $G \cong H_{13}$, *where* $\mu(H_{11})$ *is the maximum root of the equation* $\lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n = 0$.

(12) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 13)$, *then* $\mu(G) \le \mu(H_{14})$, *the equality holds if and only if* $G \cong H_{14}$, *where* $\mu(H_{14})$ *is the maximum root of the equation* $\lambda^4 - (n+7)\lambda^3 + (8n+5)\lambda^2 - (13n-7)\lambda + 5n = 0$.

(13) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 14)$, *then* $\mu(G) \le \mu(H_{15})$, *the equality holds if and only if* $G \cong H_{15}$, *where* $\mu(H_{15})$ *is the maximum root of the equation* $\lambda^6 - (n+11)\lambda^5 + (12n+39)\lambda^4 - (51n+45)\lambda^3 + (95n-9)\lambda^2 - (77n-31)\lambda + 21n = 0$.

(14) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 15)$, *then* $\mu(G) \le \mu(H_{16})$, *the equality holds if and only if* $G \cong H_{16}$ *or* $G \cong H_{17}$, *where* $\mu(H_{16})$ *is the maximum root of the equation* $\lambda^4-(n+6)\lambda^3+(7n+4)\lambda^2-(11n-6)\lambda+4n = 0$.

(15) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 17)$, *then* $\mu(G) \le \mu(H_{18})$, *the equality holds if and only if* $G \cong H_{18}$, *where* $\mu(H_{18})$ *is the maximum root of the equation* $\lambda^5-(n+9)\lambda^4+(10n+21)\lambda^3-(31n+3)\lambda^2+(33n-16)\lambda-10n = 0$.

(16) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ $(1 \le i \le 18)$, *then* $\mu(G) \le \mu(H_{19})$, *the equality holds if and only if* $G \cong H_{19}$, *where* $\mu(H_{19})$ *is the maximum root of the equation* $\lambda^6 - (n+11)\lambda^5 + (12n+40)\lambda^4 - (52n+48)\lambda^3 + (99n-10)\lambda^2 - (80n-34)\lambda + 21n = 0$.

(17) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ *(*$1 \leq i \leq 19$*), then* $\mu(G) \leq \mu(H_{20})$*, the equality holds if and only if* $G \cong H_{20}$*, where* $\mu(H_{20})$ *is the maximum root of the equation* $\lambda^5-(n+8)\lambda^4+(9n+17)\lambda^3-(26n+2)\lambda^2+(27n-13)\lambda-8n=0$.

(18) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ *(*$1 \leq i \leq 20$*), then* $\mu(G) \leq \mu(H_{21})$*, the equality holds if and only if* $G \cong H_{21}$ *or* $G \cong H_{22}$*, where* $\mu(H_{21})$ *is the maximum root of the equation* $\lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n=0$.

(19) *If* $G \notin S(n,3)$ *and* $G \ncong H_i$ *(*$1 \leq i \leq 22$*), then* $\mu(G) \leq \mu(H_{23})$*, the equality holds if and only if* $G \cong H_{23}$ *or* $G \cong H_{24}$ *or* $G \cong H_{25}$ *or* $G \cong H_{26}$ *or* $G \cong H_{27}$*, where* $\mu(H_{23})$ *is the maximum root of the equation* $\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n=0$.

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The First to Ninth Greatest LEL-invariants of Connected Graphs *

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Abstract

Let G be a connected graph with n vertices, and $\mu_1, \mu_2, ..., \mu_n$ be the Laplacian eigenvalues of G. The Laplacian-energy-like invariant (short for LEL-invariant) of a graph, denoted as $LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}$, has been defined and investigated in [J. Liu, B. Liu, A Laplacian-energy-like invariant of a graph, *MATCH Commun. Math. Comput. Chem.*, **59** (2008), 355–372]. In this paper, the first to ninth greatest LEL-invariants, together with the corresponding graphs among the class of connected n-vertex graphs are determined.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with n vertices and m edges. The adjacency matrix, degree matrix of G is defined as $A(G) = [a_{ij}]$, $D(G) = diag\{d(v_1), d(v_2), \cdots, d(v_n)\}$, respectively. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$. Let $\lambda_1, \lambda_2, ..., \lambda_n$ be the adjacency spectrum of G, and $\mu_1, \mu_2, ..., \mu_n$ be the Laplacian spectrum of G. The *energy* $E(G)$ of a graph G is defined as [2] $E(G) = \sum_{i=1}^{n} |\lambda_i|$. This quantity has a long known application in molecular-orbital theory of organic molecules (see [3–4]) and has been much investigated. In this line, the maximal, second-maximal, minimal and second-minimal energy among the all n-vertex trees are determined in [5]. The maximal energy graphs and the maximal energy

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bipartite graphs are identified in [6–7]. For other similar results on the maximal or minimal energy of graphs see [8–10] and the references therein.

Motivated by the definition of $E(G)$, Gutman and Zhou [11] proposed the definition of *Laplacian energy* of a graph $G = (V, E)$, and it is defined as $LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|$, where $|V| = n$ and $|E| = m$. It is proved that [11] there is a great deal of analogy between the properties of $E(G)$ and $LE(G)$, but also some significant differences. Various properties of Laplacian energy and the relation between $E(G)$ and $LE(G)$ may be found in [11–14].

The *Laplacian-energy-like invariant* (short for *LEL-invariant*) of a graph, denoted as $LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}$, has been defined and investigated in [1]. It is found that the quantities $E(G)$ and $LEL(G)$ have a number of analogous properties [1, 16, 18]. And Gutman et al. [16] also proved that $E(G)$ can be expressed in terms of eigenvalues of the line graph, whereas $LEL(G)$ in terms of singular values of the incidence matrix of a directed graph. Moreover, it is also found that the Laplacian coeffcients have relation with Laplacian-energy-like invariant. For the related results, one can refer to [21–25]. As reported above, a good deal of attention has been paid to the ordinary energy, i.e., the energy of adjacency matrix, but the graph which shares the greatest energy among the class of connected n-vertex graphs has not been determined. In this paper, we identify the first to ninth greatest LEL-invariants, together with the corresponding graphs among the class of connected n-vertex graphs.

Comparing with the ordinary energy and Laplacian energy, the LEL-invariant seems to be relatively less well known. Up to now, there are only few references [1,15,17,19,23] concerning with this quantity. Very recently, Stevanović et al. [19] showed that LEL-invariant is a good designed molecular descriptor, which has great application in chemistry. Thus, we hope this work would inspire others to investigate this invariant.

2 Main results

Let $G_1 \cup G_2$ denote the graph consisting of two (disconnected) components G_1 and G_2, and kG denote the graph consisting of k ($k > 0$ be an integer) copies of the graph G. The join $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph having vertex set $V(G_1 \vee G_2) = V(G_1 \cup G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{(u, v) : u \in V(G_1), v \in V(G_2)\}$. As usual, K_n, P_n and C_n denote the complete graph, the path and the cycle of order n, respectively. Specially, K_1 denotes an isolated vertex.

Let G^c be the complement of G. It is well known that

Lemma 2.1 [20] *Let G be a graph with n vertices. If $\lambda_i(G)$, $i = 1, ..., n$ are the eigenvalues of $L(G)$, then the eigenvalues of $L(G^c)$ are $n - \lambda_{n-i}(G)$,*

$i = 1, 2, ..., n-1$ *and* 0.

Let $W_1(n) = K_n$, $W_2(n) = K_{n-2} \vee (2K_1)$, $W_3(n) = K_{n-4} \vee C_4$, $W_4(n) = K_{n-3} \vee (K_1 \cup K_2)$, $W_5(n) = K_{n-6} \vee (C_4 \vee 2K_1)$, $W_6(n) = K_{n-5} \vee ((K_2 \cup K_1) \vee 2K_1)$, $W_7(n) = K_{n-4} \vee P_4$, $W_8(n) = K_{n-3} \vee (3K_1)$, $W_9(n) = K_{n-4} \vee (K_1 \cup K_3)$. For example, the graphs $W_2(8)$, $W_3(8)$, $W_4(8)$, $W_5(8)$, $W_6(8)$, $W_7(8)$, $W_8(8)$, $W_9(8)$ are shown in Fig. 1.

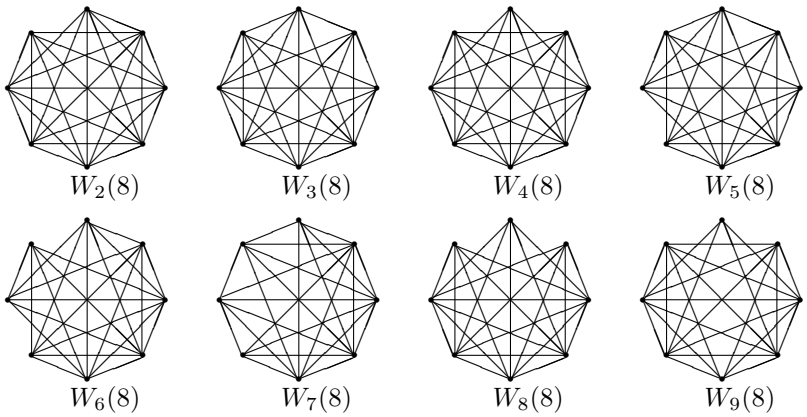


Fig. 1. The graphs $W_2(8)$, $W_3(8)$, ..., $W_9(8)$.

For convenience, we write $S(G) = (\mu_1, \mu_2, ..., \mu_n)$ to denote the fact that the Laplacian spectrum of G is $\mu_1, \mu_2, ..., \mu_n$. By an elementary calculation, we have

(1a) $S((W_1(n))^c) = (\underbrace{0, 0, \cdots, 0}_{n})$.

(2a) $S((W_2(n))^c) = (2, \underbrace{0, 0, \cdots, 0}_{n-1})$.

(3a) $S((W_3(n))^c) = (2, 2, \underbrace{0, 0, \cdots, 0}_{n-2})$.

(4a) $S((W_4(n))^c) = (3, 1, \underbrace{0, 0, \cdots, 0}_{n-2})$.

(5a) $S((W_5(n))^c) = (2, 2, 2, \underbrace{0, 0, \cdots, 0}_{n-3})$.

(6a) $S((W_6(n))^c) = (3, 2, 1, \underbrace{0, 0, \cdots, 0}_{n-3})$.

(7a) $S((W_7(n))^c) = (2+\sqrt{2}, 2, 2-\sqrt{2}, \underbrace{0, 0, \cdots, 0}_{n-3})$.

(8a) $S((W_8(n))^c) = (3, 3, \underbrace{0, 0, \cdots, 0}_{n-2})$.

(9a) $S((W_9(n))^c) = (4, 1, 1, \underbrace{0, 0, \cdots, 0}_{n-3})$.

By equalities (1a)–(9a) and Lemma 2.1, it follows that

(1b) $S(W_1(n)) = (\underbrace{n, n, \cdots, n}_{n-1}, 0)$.

(2b) $S(W_2(n)) = (\underbrace{n, n, \cdots, n}_{n-2}, n-2, 0)$.

(3b) $S(W_3(n)) = (\underbrace{n, n, \cdots, n}_{n-3}, n-2, n-2, 0)$.

(4b) $S(W_4(n)) = (\underbrace{n, n, \cdots, n}_{n-3}, n-1, n-3, 0)$.

(5b) $S(W_5(n)) = (\underbrace{n, n, \cdots, n}_{n-4}, n-2, n-2, n-2, 0)$.

(6b) $S(W_6(n)) = (\underbrace{n, n, \cdots, n}_{n-4}, n-1, n-2, n-3, 0)$.

(7b) $S(W_7(n)) = (\underbrace{n, n, \cdots, n}_{n-4}, n-2+\sqrt{2}, n-2, n-2-\sqrt{2}, 0)$.

(8b) $S(W_8(n)) = (\underbrace{n, n, \cdots, n}_{n-3}, n-3, n-3, 0)$.

(9b) $S(W_9(n)) = (\underbrace{n, n, \cdots, n}_{n-4}, n-1, n-1, n-4, 0)$.

Lemma 2.2 [1] *For any connected graph G with n vertices and m edges, $LEL(G) \leq \sqrt{2m(n-1)}$. Equality holds if and only if $G \cong K_n$.*

Lemma 2.3 *For $n \geq 6$, $LEL(W_1(n)) > LEL(W_2(n)) > \cdots > LEL(W_9(n))$.*

Proof. By equalities (1b)–(9b), it is easily checked that $LEL(W_1(n)) > LEL(W_2(n)) > LEL(W_3(n)) > LEL(W_4(n))$ and $LEL(W_5(n)) > LEL(W_6(n)) > LEL(W_7(n))$. Thus, we only need to consider the next cases.

Case 1. $LEL(W_4(n)) > LEL(W_5(n))$.

We only need to prove that $\sqrt{n}+\sqrt{n-1}+\sqrt{n-3} > 3\sqrt{n-2}$. It is sufficient to prove that $\sqrt{n}+\sqrt{n-3} > 3\sqrt{n-2}-\sqrt{n-1}$, equivalently, we only need to prove that $(\sqrt{n}+\sqrt{n-3})^2 > (3\sqrt{n-2}-\sqrt{n-1})^2$.

Thus, we only need to prove that

(1c) $\sqrt{n(n-3)}+3\sqrt{(n-1)(n-2)} > 4n-8$.

Note that $\sqrt{n(n-3)}+3\sqrt{(n-1)(n-2)} > 4\sqrt{n(n-3)} > 4n-8$ because $n \geq 6$, then inequality (1c) holds. This implies that $LEL(W_4(n)) > LEL(W_5(n))$.

Case 2. $LEL(W_7(n)) > LEL(W_8(n))$.

We only need to prove that $\sqrt{n-2}+\sqrt{n-2+\sqrt{2}}+\sqrt{n-2-\sqrt{2}} > \sqrt{n}+2\sqrt{n-3}$. It is sufficient to prove that $(\sqrt{n-2}+\sqrt{n-2+\sqrt{2}}+\sqrt{n-2-\sqrt{2}})^2 > (\sqrt{n}+2\sqrt{n-3})^2$, so we only need to prove that $\sqrt{n-2}(\sqrt{n-2+\sqrt{2}}+\sqrt{n-2-\sqrt{2}}) > n-3+2\sqrt{n(n-3)}-\sqrt{n^2-4n+2}$.

Thus, it is sufficient to prove that $(n-2)(\sqrt{n-2+\sqrt{2}}+\sqrt{n-2-\sqrt{2}})^2 > (n-3+2\sqrt{n(n-3)}-\sqrt{n^2-4n+2})^2$, equivalently, we only need to prove that $\sqrt{n^2-4n+2}\cdot(4n-10+4\sqrt{n(n-3)}) > 4n^2-14n+3+4(n-3)\sqrt{n(n-3)}$.

Therefore, it is sufficient to prove that $(n^2-4n+2)\cdot(4n-10+4\sqrt{n(n-3)})^2 > (4n^2-14n+3+4(n-3)\sqrt{n(n-3)})^2$, equivalently, we only need to prove that

(2c) $24n^2-140n+191+8(3n-11)\sqrt{n(n-3)} > 0$.

Recall that $n \geq 6$, then inequality (2c) holds. Thus, $LEL(W_7(n)) > LEL(W_8(n))$.

Case 3. $LEL(W_8(n)) > LEL(W_9(n))$.

We only need to prove that $2\sqrt{n-3}+\sqrt{n} > \sqrt{n-4}+2\sqrt{n-1}$. It is sufficient to prove that $(2\sqrt{n-3}+\sqrt{n})^2 > (\sqrt{n-4}+2\sqrt{n-1})^2$, equivalently, we only need to prove that $\sqrt{n(n-3)}-\sqrt{(n-1)(n-4)} > 1$.

Thus, it is sufficient to prove that $(\sqrt{n(n-3)}-\sqrt{(n-1)(n-4)})^2 > 1$, equivalently, we only need to prove that

(3c) $(2n^2-8n+3)^2 > 4n(n-1)(n-3)(n-4)$.

Note that inequality (3c) is equivalent with $9 > 0$, then inequality (3c) holds. Thus, $LEL(W_8(n)) > LEL(W_9(n))$.

This completes the proof of this lemma. ∎

Lemma 2.4 *Let $n \geq 6$ and G be a connected graph with n vertices. If $G \notin \{W_1(n), W_2(n), ..., W_9(n)\}$, then $LEL(W_9(n)) > LEL(G)$.*

Proof. Suppose G has m edges. It is easy to see that $W_1(n)$ is the unique n-vertex graph with $\frac{n(n-1)}{2}$ edges, there exists exactly one n-vertex graph, $W_2(n)$, with $\frac{n(n-1)}{2} - 1$ edges, there exist exactly two n-vertex graphs, $W_3(n)$, $W_4(n)$, with $\frac{n(n-1)}{2} - 2$ edges, and there exist exactly five n-vertex graphs, $W_5(n)$, $W_6(n)$, $W_7(n)$, $W_8(n)$, $W_9(n)$, with $\frac{n(n-1)}{2} - 3$ edges. Now since $G \notin \{W_1(n), W_2(n), ..., W_9(n)\}$, then $m \leq \frac{n(n-1)}{2} - 4$. By Lemma 2.2, we have $LEL(G) \leq \sqrt{(n^2 - n - 8)(n-1)}$.

Next we shall prove that, for all $n \geq 6$, the next inequality (4c) follows.

(4c) $(n-4)\sqrt{n} + 2\sqrt{n-1} + \sqrt{n-4} > \sqrt{(n^2 - n - 8)(n-1)}$

To deduce inequality (4c), we only need to prove that $(n-4)\sqrt{n} + \sqrt{n-4} > \sqrt{n-1} \cdot (\sqrt{n^2 - n - 8} - 2\ )$. It is sufficient to prove that $((n-4)\sqrt{n} + \sqrt{n-4}\ )^2 > (n-1)(\sqrt{n^2 - n - 8} - 2\ )^2$, equivalently, we only need to prove that $(n-4)\sqrt{n(n-4)} + 2(n-1) \cdot \sqrt{n^2 - n - 8} > 3n^2 - 10n + 4$.

Therefore, we only need to prove that $((n-4)\sqrt{n(n-4)} + 2(n-1) \cdot \sqrt{n^2 - n - 8}\ )^2 > (3n^2 - 10n + 4\ )^2$, equivalently, we only need to prove that$(n-1)(n-4)\sqrt{n(n-4)(n^2 - n - 8)} > n^4 - 9n^3 + 24n^2 - 19n + 12$, equivalently, we only need to prove that $(n-1)\sqrt{n(n-4)(n^2 - n - 8)} > n^3 - 5n^2 + 4n - 3$.

Thus, we only need to prove that $((n-1)\sqrt{n(n-4)(n^2 - n - 8)}\ )^2 > (n^3 - 5n^2 + 4n - 3\ )^2$, equivalently, we only need to prove that

(5c) $3n^5 - 26n^4 + 81n^3 - 114n^2 + 56n - 9 > 0$.

Bearing in mind that $n \geq 6$, then inequality (5c) holds. Thus, inequality (4c) follows.

Combining with equality (9b) and inequality (4c), it follows that $LEL(G) < LEL(W_9(n))$ for all $n \geq 6$. This completes the proof. ∎

By combining Lemmas 2.3–2.4, we can conclude that

Theorem 2.5 *Let $n \geq 6$ and G be a connected graph with n vertices. If $G \notin \{W_1(n), W_2(n), ..., W_9(n)\}$, then $LEL(W_1(n)) > LEL(W_2(n)) > \cdots > LEL(W_9(n)) > LEL(G)$.*

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The proof of a conjecture on the lewin number of primitive non-powerful signed digraphs ☆

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ABSTRACT

Suppose S is a primitive non-powerful signed digraph. A pair of *SSSD* walks of S are two directed walks of S, which have the same initial vertex, same terminal vertex and same length, but different signs. The lewin number of S, denoted $l(S)$, is the least positive integer k such that there are both *SSSD* walks of lengths k and $k+1$ from some vertex u to some vertex v (possibly u again) of S. This paper presents a proof of a conjecture on $l(S)$, which was put forward by You et al. [L.H. You, M.H. Liu, B.L. Liu, Bounds on the lewin number for primitive non-powerful signed digraphs, Acta Math. Appl. Sinica 35 (2012) 396–407].

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1. Introduction

Let $D = (V, A)$ be a digraph on n vertices. We permit loops but no multiple arcs. A $u \longrightarrow v$ walk in D is a sequence of vertices $u, u_1, \ldots, u_k, v$ and a sequence of arcs $(u, u_1), (u_1, u_2), \ldots, (u_k, v)$. Furthermore, if $u \longrightarrow v$ is a walk with distinct vertices, then $u \longrightarrow v$ is called a path. A closed walk is a $u \longrightarrow v$ walk, where $u = v$. A cycle is a closed $u \longrightarrow v$ walk with distinct vertices except for $u = v$,

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and a cycle on k vertices is denoted by C_k. The length of a walk W is the number of arcs of W, and is denoted by $|W|$.

Suppose D is a digraph. If we assign a sign 1 or -1 to each arc of D, the resulting digraph S is called a signed digraph. If W is a walk of a signed digraph S, the sign $sgn(W)$ of W is defined as $sgn(W) = \prod_{e_i \in A(W)} sgn(e_i)$. Two walks W_1 and W_2 in a signed digraph are called a pair of *SSSD* walks, if they have the same initial vertex, same terminal vertex and same length, but they have different signs. If the signed digraph S contains no pairs of *SSSD* walks, then S is called powerful. Otherwise, S is non-powerful.

It is well known that matrices and digraphs are closely related. Let $A = (a_{ij})$ be a square sign pattern matrix of order n. The associated digraph $D(A)$ of A (possibly with loops) is defined to be the digraph with vertex set $V = \{1, 2, \ldots, n\}$ and arc set $E = \{(i, j)|a_{ij} \neq 0\}$. The associated signed digraph $S(A)$ of A is obtained from $D(A)$ by assigning the sign of a_{ij} to each arc (i, j) in $D(A)$. For any positive integer k, the entries $(A^k)_{ij} \neq 0$ of the power A^k if and only if there is a walk of length k from vertex i to vertex j in $D(A)$; the sign of the entries $(A^k)_{ij}$ is 1 (or -1) if and only if all walks of length k from vertex i to vertex j have the same sign 1 (or -1) in $S(A)$; and the sign of the entries $(A^k)_{ij}$ is the ambiguous sign, say # in [4], if and only if there is a pair of *SSSD* walks of length k from vertex i to vertex j in $S(A)$. We call A powerful if each power of A contains no # entry, that is, A is powerful if and only if $S(A)$ contains no pair of *SSSD* walks.

A nonnegative square matrix A is primitive if some power $A^k > 0$. A square sign pattern matrix A is called primitive if $|A|$ is primitive, where $|A|$ denotes the (0,1)-matrix obtained from A by replacing each nonzero entry by 1.

The notation $u \xrightarrow{k} v$ is used to indicate that there is a $u \to v$ walk of length k. By $u \xrightarrow{k_1,\ k_2} v$, we mean that $u \xrightarrow{k_1} v$ and $u \xrightarrow{k_2} v$. We use the notation $u \xrightarrow{k\ SSSD} v$ to indicate that there is a pair of *SSSD* walks of length k from u to v, and we use the notation $u \xrightarrow{k_1,\ k_2\ SSSD} v$ to indicate that $u \xrightarrow{k_1\ SSSD} v$ and $u \xrightarrow{k_2\ SSSD} v$. Now, from the above definitions, $u \not\xrightarrow{k} v$ and $u \not\xrightarrow{k\ SSSD} v$ imply that there is no walk, no pair of *SSSD* walks of length k from u to v, respectively.

Let S be a signed digraph, and D be the corresponding underlying digraph of S. Recall that D is primitive if and only if there exists some positive integer k such that there is a walk $u \xrightarrow{k} v$ whenever $u, v \in V(D)$. If D is primitive, then we call S primitive.

In 2007, You et al. [11] showed that a square sign pattern matrix A is primitive non-powerful if and only if there exists some positive integer k such that $A^k = \#J$. The least such k is called the base of A, and denoted by $b(A)$. Namely, S is a primitive non-powerful signed digraph if and only if there exists some positive integer k such that $u \xrightarrow{k\ SSSD} v$ whenever $u, v \in V(S)$. The least such k is called the base of S, and denoted by $b(S)$. Clearly, $b(A) = b(S(A))$.

Furthermore, the local base is defined in [1,3,6,9]. The research on the (local) bases of primitive non-powerful sign pattern matrices (signed digraphs) attracted much attention of the mathematics scholars [12].

In 1971, Lewin [2] presents a characterization of primitive matrices: A nonnegative irreducible square matrix is primitive if and only if for some positive integer k there is an ordered pair (u, v) such that $(A^k)_{uv}(A^{k+1})_{uv} > 0$. The result implies that a strongly connected digraph D is primitive if and only if there exists a positive integer k such that $u \xrightarrow{k,\ k+1} v$ for some $u, v \in V(D)$. Therefore, if D is primitive, then D must have a smallest k such that $u \xrightarrow{k,\ k+1} v$ for some $u, v \in V(D)$. Such smallest k is called the lewin number of D, and denoted by $l(D)$ in [8]. To be more precise, $l(D) = \min\{t : u \xrightarrow{t,\ t+1} v$ for some $u, v \in V(D)\}$.

Recently, based on the Lewin's result for primitive digraphs, You et al. [10] showed that a strongly connected signed digraph S is primitive non-powerful if and only if there exists a positive integer k such that $u \xrightarrow{k,\ k+1\ SSSD} v$ for some $u, v \in V(S)$. Moreover, motivated by the concept of lewin number

of a primitive digraph, You et al. [10] defined the lewin number $l(S)$ of a primitive non-powerful signed digraph S as $l(S) = \min\{t : u \xrightarrow{t,\ t+1\ SSSD} v \text{ for some } u, v \in V(S)\}$.

By the relationship between digraphs and matrices, it is easy to know that the lewin number $l(A)$ of a primitive non-powerful sign pattern matrix A is the smallest positive integer t such that the signs of $(A^t)_{uv}$ and $(A^{t+1})_{uv}$ are the ambiguous sign, #, for some u, v, where $1 \leqslant u, v \leqslant n$. Clearly, $l(A) = l(S(A))$.

In the coming discussion, we are only concerned with the primitive non-powerful signed digraphs, and to avoid repetition, S always indicates a primitive non-powerful signed digraph, and D denotes the corresponding underlying primitive digraph of S.

Now, from the definitions of $l(D)$, $b(S)$, and $l(S)$, it easily follows that $l(D) \leqslant l(S) \leqslant b(S)$.

In the sequel, let q and s be two positive integers such that $2 \leqslant s < q \leqslant n$, the greatest common divisor of q and s is equal to 1, i.e., $\gcd(q, s) = 1$, and $q + s \geqslant n + 1$, and let $D_{n,q,s} = (V, A)$ be the digraph, where $V = \{v_1, v_2, \ldots, v_n\}$ and $A = \{(v_i, v_{i+1}) : 1 \leqslant i \leqslant n-1\} \cup \{(v_s, v_1), (v_n, v_{n-q+1})\}$ (see [8]). It is well known that D is primitive if and only if D is strongly connected and the greatest common divisor of the lengths of all the cycles of D is 1 (for instance, see [5]). Note that $D_{n,q,s}$ has exactly two cycles, say C_q and C_s, and $\gcd(q, s) = 1$. Thus, $D_{n,q,s}$ is primitive. Throughout this paper, $S_{n,q,s}$ denotes a non-powerful primitive signed digraph such that the corresponding underlying digraph of $S_{n,q,s}$ is $D_{n,q,s}$.

In [10], some bounds on the lewin number for primitive non-powerful signed digraphs were given, and the next conjecture was put forward.

Conjecture 1.1 [10]. *For any primitive non-powerful signed digraph S of order n,*

$$l(S) \leqslant \begin{cases} \frac{3n^2-15n+20}{2}, & \text{if } n \geqslant 12 \text{ is even;} \\ \frac{3n^2-9n+6}{2}, & \text{if } n \geqslant 7 \text{ is odd.} \end{cases}$$

Moreover, equality in the above two cases holds if and only if S is isomorphic to $S_{n,n-1,n-3}$ or $S_{n,n,n-2}$, respectively.

Unfortunately, when $n = 14$, the following theorem shows that there are exceptional signed digraphs for the equality of Conjecture 1.1. However, for the other cases, Conjecture 1.1 holds, since we have the next result, which will be shown in Section 3.

Theorem 1.2. *For any primitive non-powerful signed digraph S of order n,*

$$l(S) \leqslant \begin{cases} \frac{3n^2-15n+20}{2}, & \text{if } n \text{ is even and } n \geqslant 12; \\ \frac{3n^2-9n+6}{2}, & \text{if } n \text{ is odd and } n \geqslant 7. \end{cases}$$

Moreover, equality in the former case holds if and only if $S \cong S_{n,n-1,n-3}$ or $S \cong S_{14,14,11}$, and equality in the later case holds if and only if $S \cong S_{n,n,n-2}$.

2. The lewin number of $S_{n,q,s}$

Based on the characterization for powerful irreducible sign pattern matrices [4], You et al. [11] obtained an important characterization for primitive non-powerful signed digraphs in term of graph parameter.

Proposition 2.1 [11]. *Suppose S is a primitive signed digraph. Then, S is non-powerful if and only if S contains a pair of cycles C_{p_1} and C_{p_2} satisfying one of the following two conditions:*

(A_1) *p_1 is odd and p_2 is even and $sgn(C_{p_2}) = -1$.*
(A_2) *Both p_1 and p_2 are odd and $sgn(C_{p_1}) = -sgn(C_{p_2})$.*

A pair of cycles C_{p_1} and C_{p_2} satisfying (A_1) or (A_2) is called a "distinguished cycle pair" in [11]. It is easy to check that if C_{p_1} and C_{p_2} are a distinguished cycle pair, then the (closed) walks $W_1 = p_2C_{p_1}$ (walk around C_{p_1} by p_2 times) and $W_2 = p_1C_{p_2}$ have the same length p_1p_2, but different signs:

$$(sgn(C_{p_1}))^{p_2} = -(sgn(C_{p_2}))^{p_1}. \tag{2.1}$$

The following lemma is well-known. For instance, see [7].

Lemma 2.2. *Let a, b, c, x_0, y_0 be five integers. Suppose that $\gcd(a, b) = 1$, and $(x, y) = (x_0, y_0)$ is one solution of $ax + by = c$. Then, all the other integer solutions of $ax + by = c$ are of the form: $(x, y) = (x_0 + bt, y_0 - at)$, where t is an arbitrary integer.*

Let W_1 and W_2 be two walks of D. In the sequel, we always write $W_1 \cup W_2$ as $W_1 + W_2$.

Lemma 2.3. *Let v_{t_1} and v_{t_2} be two vertices of $S_{n,q,s}$, and P_1 and P_2 be two different paths from v_{t_1} to v_{t_2}, where $|P_2| \geqslant |P_1|$. Suppose $v_{t_1} \xrightarrow{m\ SSSD} v_{t_2}$. Then,*

(1) *either $m = |P_1| + (q-1)s$ or $m \geqslant |P_1| + qs$;*
(2) *if $m \geqslant |P_1| + qs$, then $v_{t_1} \xrightarrow{m-qs} v_{t_2}$.*

Proof. By the definition of $D_{n,q,s}$, since there are two different paths from v_{t_1} to v_{t_2}, we can conclude that $n - q + 1 \leqslant t_2 < t_1 \leqslant s$ and $|P_2| = |P_1| + q - s$. Furthermore, there exists no other path, except for P_1 and P_2, from v_{t_1} to v_{t_2}. Suppose W_1 and W_2 are a pair of *SSSD* walks of length m from v_{t_1} to v_{t_2}. Then, there exist nonnegative integers a_i, b_i, where $i = 1, 2$, such that one of the following three conditions holds:

(B_1) $W_i = P_i + a_iC_q + b_iC_s$, where $i = 1, 2$;
(B_2) $W_i = P_1 + a_iC_q + b_iC_s$, where $i = 1, 2$;
(B_3) $W_i = P_2 + a_iC_q + b_iC_s$, where $i = 1, 2$.

We divide the proof into the following two cases.

Case 1. (B_1) holds.

Note that $|W_1| = |W_2|$. Thus, $m = |P_1| + a_1q + b_1s = |P_2| + a_2q + b_2s$, and hence $(a_1 - a_2)q + (b_1 - b_2)s = q - s$. Since $1 \times q + (-1) \times s = q - s$ and $\gcd(q, s) = 1$, by Lemma 2.2 there exists some integer x such that

$$\begin{cases} a_1 = a_2 + 1 + sx \\ b_1 = b_2 - 1 - qx \end{cases} \tag{2.2}$$

If $x \geqslant 1$, then $a_1 \geqslant s+1$ by Eq. (2.2). Thus, $m = |W_1| \geqslant |P_1| + a_1q \geqslant |P_1| + q(s+1) > |P_1| + qs$. So, (1) holds. Moreover, $P_1 + (a_1 - s)C_q + b_1C_s$ is a walk of length $m - qs$ from v_{t_1} to v_{t_2}, and hence (2) holds.

If $x = 0$, then $a_1 = a_2 + 1$ and $b_2 = b_1 + 1$ by Eq. (2.2). Let Q be the unique path from v_{t_2} to v_{t_1}. Then, $W_1 + Q = a_1C_q + (b_1 + 1)C_s = (a_2 + 1)C_q + b_2C_s = W_2 + Q$, and hence $sgn(W_1) = sgn(W_2)$. This contradicts the fact that W_1 and W_2 are a pair of *SSSD* walks.

If $x \leqslant -2$, then $b_1 \geqslant 2q - 1 > q$ by Eq. (2.2). Thus, $m = |W_1| \geqslant |P_1| + b_1s \geqslant |P_1| + s(2q-1) > |P_1| + qs$. So, (1) holds. Moreover, $P_1 + a_1C_q + (b_1 - q)C_s$ is a walk of length $m - qs$ from v_{t_1} to v_{t_2}, and hence (2) holds.

If $x = -1$, then $a_1 = a_2 + 1 - s$ and $b_1 = b_2 - 1 + q$ by Eq. (2.2). Thus, $a_2 = a_1 + s - 1 \geqslant s - 1$ and $b_1 \geqslant q - 1$.

If $a_2 = s - 1$ and $b_1 = q - 1$, then $a_1 = b_2 = 0$, and hence $m = |W_1| = |P_1| + (q-1)s$. So, (1) holds. If $a_2 \geqslant s$, then $m = |W_2| \geqslant |P_2| + a_2q > |P_1| + a_2q \geqslant |P_1| + qs$. So, (1) holds. Moreover,

$P_2 + (a_2 - s)C_q + b_2C_s$ is a walk of length $m - qs$ from v_{t_1} to v_{t_2}. So, (2) holds. (1) and (2) can be proved similarly when $a_2 \geqslant s$.

Case 2. Either (B_2) or (B_3) holds.

We may suppose that (B_2) holds, since the proof is similar when (B_3) holds.

Note that $|W_1| = |W_2|$. Thus, $m = |P_1| + a_1q + b_1s = |P_1| + a_2q + b_2s$, and hence

$$(a_1 - a_2)q = (b_2 - b_1)s. \tag{2.3}$$

Since W_1 and W_2 are two *SSSD* walks, $a_1 \neq a_2$. By symmetry, we may suppose that $a_1 > a_2$. Note that $\gcd(q, s) = 1$. From Eq. (2.3), it follows that $b_2 - b_1 = qx$, where x is a positive integer. Hence, $b_2 \geqslant q$. Now, $m = |W_2| = |P_1| + a_2q + b_2s \geqslant |P_1| + qs$. So, (1) holds. Furthermore, $P_1 + a_2C_q + (b_2 - q)C_s$ is a walk of length $m - qs$ from v_{t_1} to v_{t_2}. So, (2) holds. □

Lemma 2.4. $l(S_{n,q,s}) \leqslant l(D_{n,q,s}) + qs$.

Proof. Suppose u and v are two vertices of $S_{n,q,s}$ such that $u \xrightarrow{l(D_{n,q,s}),\ l(D_{n,q,s})+1} v$. Let Q_1 and Q_2 be two walks of lengths $l(D_{n,q,s})$ and $l(D_{n,q,s})+1$, respectively, from u to v. Set $V_1 = \{v_{n-q+1}, v_{n-q+2}, \ldots, v_s\}$. Since $n - q + 1 \leqslant s$, $V_1 \neq \emptyset$. It is easy to see that $V(Q_1) \cap V_1 \neq \emptyset$ and $V(Q_2) \cap V_1 \neq \emptyset$. Choose $u_1 \in V(Q_1) \cap V_1$ and $u_2 \in V(Q_2) \cap V_1$. Then, $u_1 \in V(C_q) \cap V(C_s)$ and $u_2 \in V(C_q) \cap V(C_s)$, where C_q and C_s are two cycles of $D_{n,q,s}$.

Note that C_q and C_s are all the cycles of $D_{n,q,s}$ and $S_{n,q,s}$ is non-powerful. Then, C_q and C_s must be a distinguished cycle pair by Proposition 2.1. By Eq. (2.1), qC_s and sC_q have different signs. Let $W_1 = qC_s$ and $W_2 = sC_q$. Then, W_1 and W_2 are a pair of *SSSD* walks from u_1 to u_1, and W_1 and W_2 are also a pair of *SSSD* walks from u_2 to u_2. Thus, $Q_1 + W_1$ and $Q_1 + W_2$ are a pair of *SSSD* walks (of length $l(D_{n,q,s}) + qs$) from u to v, and $Q_2 + W_1$ and $Q_2 + W_2$ are a pair of *SSSD* walks (of length $l(D_{n,q,s}) + qs + 1$) from u to v. So,

$$u \xrightarrow{l(D_{n,q,s})+qs,\ l(D_{n,q,s})+qs+1\ SSSD} v.$$

Therefore, $l(S_{n,q,s}) \leqslant l(D_{n,q,s}) + qs$. □

Theorem 2.5. $l(S_{n,q,s}) = l(D_{n,q,s}) + qs$.

Proof. Let u, v be two arbitrary vertices (possible $u = v$) of $S_{n,q,s}$. In view of Lemma 2.4, it suffices to show that either $u \not\xrightarrow{k\ SSSD} v$ or $u \not\xrightarrow{k+1\ SSSD} v$ for any $k \in \{1, 2, \ldots, l(D_{n,q,s}) + qs - 1\}$.

Suppose there exists some integer $k \in \{1, 2, \ldots, l(D_{n,q,s}) + qs - 1\}$ such that $u \xrightarrow{k,\ k+1\ SSSD} v$ holds for some $u, v \in V(S_{n,q,s})$. As there are at most two different paths from u to v, we divide the proof into the following two cases.

Case 1. There is a unique path from u to v.

Let P be the unique path from u to v, where $|P| = 0$ if and only if $u = v$. Suppose W_1 and W_2 are a pair of *SSSD* walks of length k, and W_3 and W_4 are a pair of *SSSD* walks of length $k + 1$ from u to v. Then, there exist nonnegative integers a_i, b_i such that

$$W_i = P + a_iC_q + b_iC_s, \quad i = 1, 2, 3, 4.$$

Since W_1 and W_2 are a pair of *SSSD* walks, we have $|W_1| = |W_2| = k$ and hence Eq. (2.3) holds. Without loss of generality, we may suppose that $b_2 > b_1$. By Eq. (2.3), it follows that $b_2 = b_1 + xq$, where $x \geqslant 1$. Similarly, we may suppose that $b_4 > b_3$, and hence $b_4 = b_3 + yq$, where $y \geqslant 1$. Thus, $P + a_2C_q + (b_2 - q)C_s$ and $P + a_4C_q + (b_4 - q)C_s$ are two walks of lengths $k - qs$ and $k + 1 - qs$, respectively, from u to v. Therefore, $l(D_{n,q,s}) \leqslant k - qs \leqslant (l(D_{n,q,s}) + qs - 1) - qs = l(D_{n,q,s}) - 1$, a contradiction.

Case 2. There are two different paths from u to v.

Let P_1 and P_2 be two different paths from u to v, where $|P_2| \geqslant |P_1| \geqslant 1$. Since there are at most two different paths from u to v, $k \geqslant |P_1| + qs$ and $k+1 \geqslant |P_1| + qs$ by (1) of Lemma 2.3 and $s \geqslant 2$. Now, (2) of Lemma 2.3 implies that

$$u \xrightarrow{k-qs,\ k+1-qs} v.$$

Thus, $l(D_{n,q,s}) \leqslant k - qs \leqslant (l(D_{n,q,s}) + qs - 1) - qs = l(D_{n,q,s}) - 1$, a contradiction. □

By Theorem 2.5 and $l(D_{n,n,n-1}) = 1$, we have

Corollary 2.6 [10]. $l(S_{n,n,n-1}) = n(n-1) + 1$.

Lemma 2.7 [8]. *For any primitive digraph D of order $n \geqslant 7$,*

$$l(D) \leqslant \begin{cases} \frac{n^2-7n+14}{2}, & \text{if } n \text{ is even;} \\ \frac{n^2-5n+6}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore, equality in the above two cases holds if and only if D is isomorphic to $D_{n,n-1,n-3}$ or $D_{n,n,n-2}$, respectively.

From Theorem 2.5 and Lemma 2.7, it immediately follows that

Corollary 2.8. *Suppose $n \geqslant 7$. Then,*

(1) $l(S_{n,n,n-2}) = \frac{3n^2-9n+6}{2}$ *if n is odd;*
(2) $l(S_{n,n-1,n-3}) = \frac{3n^2-15n+20}{2}$ *if n is even.*

Corollary 2.9. $l(S_{14,14,11}) = 199$.

Proof. In view of Theorem 1.2, it suffices to prove that $l(D_{14,14,11}) = 45$. Let v_{t_1}, v_{t_2} be two arbitrary vertices of $S_{14,14,11}$. We only need to show that either $v_{t_1} \overset{k}{\not\longrightarrow} v_{t_2}$ or $v_{t_1} \overset{k+1}{\not\longrightarrow} v_{t_2}$ for any $k \in \{1, 2, \ldots, 44\}$. Assume to the contrary that there exists some positive integer $k \in \{1, 2, \ldots, 44\}$ such that W_1 and W_2 are two walks of lengths k and $k+1$, respectively, from v_{t_1} to v_{t_2}. Because there are at most two different paths from v_{t_1} to v_{t_2}, we consider the following two cases.

Case 1. There is a unique path from v_{t_1} to v_{t_2}.

Let P be the unique path from v_{t_1} to v_{t_2}, where $|P| = 0$ if and only if $t_1 = t_2$. Then, there exist nonnegative integers a_i, b_i such that

$$W_i = P + a_i C_{14} + b_i C_{11}, \quad i = 1, 2.$$

Since $|W_2| = |W_1| + 1$, we get $14(a_2 - a_1) + 11(b_2 - b_1) = 1$. Since $14 \times 4 + 11 \times (-5) = 1$ and $\gcd(14, 11) = 1$, by Lemma 2.2 there exists some integer x such that

$$\begin{cases} a_2 = a_1 + 4 + 11x \\ b_2 = b_1 - 5 - 14x \end{cases}$$

This contradicts $|W_1| < |W_2| \leqslant 45$.

Case 2. There are two different paths from v_{t_1} to v_{t_2}.

Let P_1 and P_2 be two different paths from v_{t_1} to v_{t_2}, where $|P_2| \geqslant |P_1| \geqslant 1$. It is easy to see that $1 \leqslant t_2 < t_1 \leqslant 11$ and $|P_2| = |P_1| + 3$. By virtue of Case 1, we may assume that there are nonnegative integers a_i, b_i, where $i = 1, 2$, such that one of the following two cases holds:

(*i*) $W_1 = P_1 + a_1C_{14} + b_1C_{11}$, $W_2 = P_2 + a_2C_{14} + b_2C_{11}$;
(*ii*) $W_1 = P_2 + a_1C_{14} + b_1C_{11}$, $W_2 = P_1 + a_2C_{14} + b_2C_{11}$.

If (*i*) holds, since $|W_2| = |W_1|+1$, we get $14(a_1-a_2)+11(b_1-b_2) = 2$. Since $14\times(-3)+11\times4 = 2$ and $\gcd(14, 11) = 1$, by Lemma 2.2 there exists some integer x such that

$$\begin{cases} a_1 = a_2 - 3 + 11x \\ b_1 = b_2 + 4 - 14x \end{cases}$$

This contradicts $|W_1| < |W_2| \leqslant 45$, $|P_2| \geqslant 4$ and $|P_1| \geqslant 1$.

If (*ii*) holds, then $14(a_2-a_1)+11(b_2-b_1) = 4$ by $|W_2| = |W_1|+1$. Since $14\times5+11\times(-6) = 4$ and $\gcd(14, 11) = 1$, by Lemma 2.2 there exists some integer x such that

$$\begin{cases} a_2 = a_1 + 5 + 11x \\ b_2 = b_1 - 6 - 14x \end{cases}$$

This contradicts $|W_1| < |W_2| \leqslant 45$.

By combining the above arguments, we can conclude that $l(S_{14,14,11}) = 199$. □

3. The proof of Theorem 1.2.

Lemma 3.1. *Let C_{p_1} and C_{p_2} be two cycles of a primitive digraph D. If $p_1 + p_2 \geqslant n + 1$ and $p_2 = p_1 + 1$, then $l(D) \leqslant p_1$.*

Proof. Since $p_1 + p_2 \geqslant n + 1$, C_{p_1} and C_{p_2} have a common vertex, say v. Thus, C_{p_1} and C_{p_2} are two walks of lengths p_1 and p_2 from v to v, respectively. So, $l(D) \leqslant p_1$. □

Lemma 3.2. *Let S be a signed digraph on n vertices, C_{p_1} and C_{p_2} be a distinguished cycle pair of S. Then, $l(S) \leqslant l(D) + p_1p_2 + 2n - p_1 - p_2$.*

Proof. Suppose W_1 and W_2 are two walks of lengths $l(D)$ and $l(D) + 1$, respectively, from u to v. Let P_1 be a shortest path from $V(C_{p_1})$ to u and P_2 be a shortest path from v to $V(C_{p_2})$.

By Eq. (2.1), $P_1+W_1+P_2+p_2C_{p_1}$ and $P_1+W_1+P_2+p_1C_{p_2}$ are a pair of *SSSD* walks of length $l(D)+|P_1|+|P_2|+p_1p_2$ from some vertex $x \in V(C_{p_1})$ to some vertex $y \in V(C_{p_2})$. Similarly, $P_1+W_2+P_2+p_2C_{p_1}$ and $P_1+W_2+P_2+p_1C_{p_2}$ are a pair of *SSSD* walks of length $l(D)+1+|P_1|+|P_2|+p_1p_2$ from x to y. Since $|P_1| \leqslant n - p_1$ and $|P_2| \leqslant n - p_2$, $l(S) \leqslant l(D) + |P_1| + |P_2| + p_1p_2 \leqslant l(D) + 2n - p_1 - p_2 + p_1p_2$. □

Lemma 3.3. *Let S be a signed digraph on n vertices, C_{p_1} and C_{p_2} be a distinguished cycle pair of S. If $p_1 = p_2$, then $l(S) \leqslant l(D) + 2n - p_1$.*

Proof. Since C_{p_1} and C_{p_2} are a distinguished cycle pair of S and $p_1 = p_2$, by Proposition 2.1 we get $sgn(C_{p_1}) = -sgn(C_{p_2})$. It can be proved similarly with Lemma 3.2. □

Lemma 3.4. *Let C_{p_1} and C_{p_2} be a distinguished cycle pair of S, and let W_1 and W_2 be two walks of lengths k and $k+1$, respectively, from u to v in S. If $V(W_i) \cap V(C_{p_j}) \neq \emptyset$ for $1 \leqslant i \leqslant j \leqslant 2$, then $l(S) \leqslant k+p_1p_2$.*

Proof. It is easy to see that $W_1 + p_2C_{p_1}$ and $W_1 + p_1C_{p_2}$ are a pair of *SSSD* walks of length $k+p_1p_2$ from u to v by Eq. (2.1). Similarly, $W_2 + p_2C_{p_1}$ and $W_2 + p_1C_{p_2}$ are a pair of *SSSD* walks of length $k+1+p_1p_2$ from u to v. Thus, $l(S) \leqslant k + p_1p_2$. □

The *girth* of D, denoted $g(D)$, is the length of a shortest cycle in D.

Corollary 3.5. *Let S be a signed digraph on n vertices, and C_{p_1} and C_{p_2} be a distinguished cycle pair of S. If $l(D) \geqslant n$ and $g(D) \geqslant \left\lceil \frac{n+1}{2} \right\rceil$, then $l(S) \leqslant l(D) + p_1 p_2$.*

Proof. Suppose W_1 and W_2 are two walks of lengths $l(D)$ and $l(D)+1$, respectively, from u to v in D. Since $l(D) \geqslant n$, W_1 contains at least one cycle C_t. Note that $g(D) \geqslant \left\lceil \frac{n+1}{2} \right\rceil$. Then, $V(C_t) \cap V(C_{p_1}) \neq \emptyset$ and $V(C_t) \cap V(C_{p_2}) \neq \emptyset$. Similarly, W_2 contains at least one cycle C_s such that $V(C_s) \cap V(C_{p_1}) \neq \emptyset$ and $V(C_s) \cap V(C_{p_2}) \neq \emptyset$. Now, the result follows from Lemma 3.4. □

When $g(D) = 1$, we easily get $l(D) = 1$. For $g(D) \geqslant 2$, Shen and Neufeld [8] had shown that

Lemma 3.6 [8]. *Let D be a primitive digraph with $n \geqslant 7$ vertices and $2 \leqslant g(D) \leqslant 3$. Then, $l(D) \leqslant n-2$.*

Lemma 3.7 [8]. *Let D be a primitive digraph with $n \geqslant 7$ vertices and girth $g \geqslant 4$. Then,*

$$l(D) \leqslant \begin{cases} \frac{g(n-5)}{2} + 1, & \text{if } g \text{ is even;} \\ \frac{g(n-4)}{2} + 1, & \text{if } g \text{ is odd and } n \text{ is even;} \\ \frac{g(n-3)}{2}, & \text{if } g \text{ is odd and } n \text{ is odd.} \end{cases}$$

Lemma 3.8. *Let S be a signed digraph on 14 vertices, and $D_{14,14,11}$ be a subgraph of D. If C_{11} and C_{14} are a distinguished cycle pair of S, then $l(S) \leqslant 199$, with the equality if and only if $S \cong S_{14,14,11}$.*

Proof. Since C_{14} and C_{11} are a distinguished cycle pair of S and $D_{14,14,11}$ is a subgraph of D, we have $l(S) \leqslant l(S_{14,14,11}) = 199$ by Corollary 2.9.

If $S \cong S_{14,14,11}$, then $l(S) = 199$ by Corollary 2.9. Next we shall show that $l(S) = 199$ implies that $S \cong S_{14,14,11}$. Assume to the contrary that $l(S) = 199$, but $D \ncong D_{14,14,11}$. Then, D contains at least another cycle C_p, where $1 \leqslant p \leqslant 13$.

If $g(D) \leqslant 7$, by Lemmas 3.6–3.7 we get $l(D) \leqslant 36$. Now, Lemma 3.2 implies that $l(S) \leqslant 36 + 11 \times 14 + 3 = 193$, a contradiction. If $g(D) \geqslant 8$ and $l(D) \leqslant 13$, then $l(S) \leqslant 13 + 11 \times 14 + 3 = 170$ by Lemma 3.2, a contradiction. If $g(D) \geqslant 8$ and $14 \leqslant l(D) \leqslant 44$, then $l(S) \leqslant 44 + 11 \times 14 = 198$ by Corollary 3.5, a contradiction.

Thus, $g(D) \geqslant 8$ and $l(D) \geqslant 45$, and hence $8 \leqslant p \leqslant 13$.

If $p = 8$, since there exists some vertex $u \in V(C_8) \cap V(C_{11})$ such that $4C_8$ and $3C_{11}$ are two walks of lengths 32 and 33, respectively, from u to u, we get $l(D) \leqslant 32$, a contradiction.

If $p = 9$, since there exists some vertex $v \in V(C_9) \cap V(C_{14})$ such that $3C_9$ and $2C_{14}$ are two walks of lengths 27 and 28, respectively, from v to v, we get $l(D) \leqslant 27$, a contradiction.

If $p \in \{10, 12, 13\}$, by Lemma 3.1 we have $l(D) \leqslant 13$, a contradiction.

So, $p = 11$. Since $l(D) \geqslant 45$, $D_{14,14,11} \subset D \subseteq \mathscr{D}_{14,14,11}$, where $\mathscr{D}_{14,14,11}$ is the digraph obtained from $D_{14,14,11}$ by adding the arcs $\{(v_{12}, v_2), (v_{13}, v_3), (v_{14}, v_4), (v_8, v_{12}), (v_9, v_{13}), (v_{10}, v_{14})\}$.

If $(v_{12}, v_2) \in A(D)$, then there are two paths P_1 and P_2 of lengths 3 and 11, respectively, from v_{12} to v_1. Note that $P_1 + 3C_{14}$ and $P_2 + 3C_{11}$ are two walks of lengths 45 and 44, respectively, from v_{12} to v_1. Then, $l(D) \leqslant 44$, a contradiction. If $(v_{13}, v_3) \in A(D)$ or $(v_{14}, v_4) \in A(D)$, a similar contradiction will be yielded.

If $(v_8, v_{12}) \in A(D)$, then there are two paths P_3 and P_4 of lengths 1 and 9, respectively, from v_{11} to v_{12}. Note that $P_3 + 3C_{14}$ and $P_4 + 3C_{11}$ are two walks of lengths 43 and 42, respectively, from v_{11} to v_{12}. Then, $l(D) \leqslant 42$, a contradiction. If $(v_9, v_{13}) \in A(D)$ or $(v_{10}, v_{14}) \in A(D)$, we can deduce a contradiction similarly.

Thus, $l(S) = 199$ implies that $S \cong S_{14,14,11}$. This completes the proof of this result. □

Lemma 3.9. *Let $n \geqslant 12$ be even and S be a signed digraph on n vertices. Suppose C_{n-3} and C_n are a distinguished cycle pair of S. Then, $l(S) \leqslant \frac{1}{2}\left(3n^2 - 15n + 20\right)$, where the equality holds if and only if $S \cong S_{14,14,11}$.*

Proof. Let $D_1 = (V, A)$ be the digraph, where $V = \{v_1, v_2, \ldots, v_n\}$ and $A = \{(v_i, v_{i+1}) : 1 \leqslant i \leqslant n-1\} \cup \{(v_{n-3}, v_1), (v_n, v_1)\}$. It is easy to see that D has D_1 as its subgraph, and there are two paths P_1 and P_2 of lengths 1 and 4, respectively, from v_{n-3} to v_1.

If $1 \leqslant g(D) \leqslant n-6$, since $n \geqslant 12$ is even, Lemmas 3.6–3.7 imply that $l(D) \leqslant \frac{(n-6)(n-5)}{2} + 1$. By Lemma 3.2 and $n \geqslant 12$,

$$l(S) \leqslant l(D) + 3 + n(n-3) \leqslant \frac{(n-6)(n-5)}{2} + 4 + n(n-3) < \frac{1}{2}\left(3n^2 - 15n + 20\right).$$

If $l(D) \leqslant n-1$, Lemma 3.2 implies that $l(S) \leqslant n-1+3+n(n-3) < \frac{1}{2}(3n^2 - 15n + 20)$.

Thus, we may suppose that $g(D) \geqslant n-5 \geqslant \left\lceil \frac{n+1}{2} \right\rceil$ and $l(D) \geqslant n$ in the following. There are three cases to be considered.

Case 1. $n \equiv 1 \pmod 3$.

Note that $P_1 + \frac{n-4}{3}C_{n-3}$ and $P_2 + \frac{n-7}{3}C_n$ are two walks of lengths $\frac{1}{3}(n-7)n+5$ and $\frac{1}{3}(n-7)n+4$, respectively, from v_{n-3} to v_1. Using Corollary 3.5 and $n \geqslant 13$, we have

$$l(S) \leqslant l(D) + n(n-3) \leqslant \frac{1}{3}(n-7)n + 4 + n(n-3) < \frac{1}{2}\left(3n^2 - 15n + 20\right).$$

Case 2. $n \equiv -1 \pmod 3$.

Note that $P_1 + \frac{n-2}{3}C_{n-3}$ and $P_2 + \frac{n-5}{3}C_n$ are two walks of lengths $\frac{1}{3}(n-5)n+3$ and $\frac{1}{3}(n-5)n+4$, respectively, from v_{n-3} to v_1. By Corollary 3.5 and $n \geqslant 14$

$$l(S) \leqslant l(D) + n(n-3) \leqslant \frac{1}{3}(n-5)n + 3 + n(n-3) \leqslant \frac{1}{2}\left(3n^2 - 15n + 20\right).$$

If $l(S) = \frac{1}{2}\left(3n^2 - 15n + 20\right)$, then $n = 14$ and $l(S) = \frac{1}{2}\left(3 \times 14^2 - 15 \times 14 + 20\right) = 199$. By Lemma 3.8, we can conclude that $S \cong S_{14,14,11}$. Conversely, if $S \cong S_{14,14,11}$, then $l(S) = 199$ by Lemma 3.8.

Case 3. $n \equiv 0 \pmod 3$.

Then, $\gcd(n, n-3) \geqslant 3$. Recall that D is primitive. The greatest common divisor of the lengths of all the cycles in D is 1. Thus, there exists some cycle C_p in D such that $p \neq n-3$ and $p \neq n$. Since $g(D) \geqslant n-5$, it follows that $p \geqslant n-5$.

If $p = n-5$, then $g(D) = n-5$. Since n is even, $sgn(C_n) = -1$ by Proposition 2.1. Note that $n-5$ is odd. Then, C_{n-5} and C_n are also a distinguished cycle pair of S by Proposition 2.1. Now, Lemma 3.7 and Corollary 3.5 imply that

$$l(S) \leqslant l(D) + n(n-5) \leqslant \frac{(n-5)(n-4)}{2} + 1 + n(n-5) < \frac{1}{2}\left(3n^2 - 15n + 20\right).$$

If $n-4 \leqslant p \leqslant n-1$, since $p \notin \{n-3, n\}$, we get $p \in \{n-4, n-2, n-1\}$. Thus, $l(D) \leqslant n-1$ by Lemma 3.1. Using Corollary 3.5 and $n \geqslant 12$, we have

$$l(S) \leqslant l(D) + n(n-3) \leqslant n - 1 + n(n-3) < \frac{1}{2}\left(3n^2 - 15n + 20\right).$$

This completes the proof of this result. □

Lemma 3.10. *Let S be a signed digraph on $n \geqslant 12$ vertices. Suppose C_{n-1} and C_{n-3} are a distinguished cycle pair of S. Then, $l(S) \leqslant \frac{1}{2}\left(3n^2 - 15n + 20\right)$, where the equality holds if and only if $S \cong S_{n,n-1,n-3}$.*

Proof. By Proposition 2.1, n is even.

If $1 \leqslant g(D) \leqslant n-4$, since $n \geqslant 12$ is even, by Lemmas 3.2, 3.6 and 3.7

$$l(S) \leqslant l(D) + 4 + (n-1)(n-3) \leqslant \frac{(n-4)(n-5)}{2} + 5 + (n-1)(n-3)$$
$$< \frac{3n^2 - 15n + 20}{2}.$$

If $l(D) \leqslant n-1$, by Lemma 3.2 we get $l(S) \leqslant n + 3 + (n-1)(n-3) < \frac{1}{2}\left(3n^2 - 15n + 20\right)$.

Thus, we suppose that $g(D) = n - 3 > \left\lceil \frac{n+1}{2} \right\rceil$ and $l(D) \geqslant n$ in the following. Now, Corollary 3.5 and Lemma 2.7 imply that

$$l(S) \leqslant l(D) + (n-1)(n-3) \leqslant \frac{n^2 - 7n + 14}{2} + (n-1)(n-3) = \frac{3n^2 - 15n + 20}{2}. \quad (3.1)$$

If $l(S) = \frac{3n^2-15n+20}{2}$, then $l(D) = \frac{n^2-7n+14}{2}$ and hence $S \cong S_{n,n-1,n-3}$ by inequality (3.1) and Lemma 2.7. Conversely, if $S \cong S_{n,n-1,n-3}$, then $l(S) = \frac{3n^2-15n+20}{2}$ by Corollary 2.8. □

Proof of Theorem 1.2. Note that S is primitive non-powerful. By Proposition 2.1, S has a distinguished cycle pair C_{p_1} and C_{p_2}, where $p_2 \geqslant p_1$. We consider the following two cases.

Case 1. Either $p_1 + p_2 \leqslant n$ or $l(D) \leqslant n-1$.

If $p_1 + p_2 \leqslant n$, since $g(D) \leqslant p_1 \leqslant \frac{n}{2}$ and $n \geqslant 7$, by Lemmas 3.2, 3.6 and 3.7

$$l(S) \leqslant l(D) + 2n - p_1 - p_2 + p_1p_2$$
$$\leqslant \frac{n(n-3)}{4} + 2n - 1 + (p_1 - 1)(p_2 - 1)$$
$$\leqslant \frac{n^2 + 5n - 4}{4} + \frac{1}{4}(p_1 + p_2 - 2)^2$$
$$\leqslant \frac{2n^2 + n}{4}.$$

Note that $\frac{2n^2+n}{4} < \frac{3n^2-15n+20}{2} < \frac{3n^2-9n+6}{2}$ by $n \geqslant 7$. Thus, the result follows. If $l(D) \leqslant n-1$, it can be proved similarly that the result holds.

Case 2. $p_1 + p_2 \geqslant n+1$ and $l(D) \geqslant n$.

Then, C_{p_1} and C_{p_2} have some common vertex. If $p_1 = p_2$, by Lemmas 2.7 and 3.3

$$l(S) < l(D) + 2n \leqslant \frac{n^2 - 5n + 6}{2} + 2n < \frac{3n^2 - 15n + 20}{2}.$$

The result already holds. Since $l(D) \geqslant n$, $g(D) \geqslant 4$ by Lemma 3.6. Thus, we may suppose that $p_2 > p_1 \geqslant g(D) \geqslant 4$ in the sequel. We divide the proof into the following five subcases.

Subcase 2.1. $4 \leqslant p_1 \leqslant n-5$.

Thus, $4 \leqslant g(D) \leqslant n-5$.

If n is odd, by Lemmas 3.2 and 3.7

$$l(S) \leqslant l(D) + 2n - 9 + p_1p_2 \leqslant \frac{(n-5)(n-3)}{2} + 2n - 9 + n(n-5) < \frac{3n^2 - 9n + 6}{2}.$$

If n is even, by Lemmas 3.2 and 3.7

$$l(S) \leqslant l(D) + 2n - 9 + p_1p_2 \leqslant \frac{(n-5)(n-4)}{2} + 2n - 8 + n(n-5) < \frac{3n^2 - 15n + 20}{2}.$$

Subcase 2.2. $p_1 = n-4$.

Now, $p_2 > p_1$ implies that $n-3 \leqslant p_2 \leqslant n$ and hence $4 \leqslant g(D) \leqslant n-4$.

If $n-3 \leqslant p_2 \leqslant n-1$, since $n \geqslant 8$, using Lemmas 3.2 and 3.7, we get

$$l(S) \leqslant l(D) + 7 + p_1p_2 \leqslant \frac{(n-4)(n-3)}{2} + 7 + (n-4)(n-1) < \frac{3n^2-15n+20}{2}.$$

If $p_2 = n$, by Proposition 2.1 we can conclude that n is odd because C_{n-4} and C_n are a distinguished cycle pair. From Lemmas 3.2 and 3.7, it follows that

$$l(S) \leqslant l(D) + 4 + p_1p_2 \leqslant \frac{(n-4)(n-3)}{2} + 4 + n(n-4) < \frac{3n^2-9n+6}{2}.$$

Subcase 2.3. $p_1 = n-3$.

Then, $n-2 \leqslant p_2 \leqslant n$.

If $p_2 = n-2$, it follows from Lemmas 3.1 and 3.2 that

$$l(S) \leqslant l(D) + 5 + (n-2)(n-3) \leqslant n-3+5+(n-2)(n-3) < \frac{3n^2-15n+20}{2}.$$

If $p_2 = n-1$, then n is even by Proposition 2.1. By Lemma 3.10, the result holds.

If $p_2 = n$, in view of Lemma 3.9 we may suppose that n is odd. Because $p_1 = n-3$, by Lemmas 2.7 and 3.2

$$l(S) \leqslant l(D) + 3 + n(n-3) \leqslant \frac{n^2-5n+6}{2} + 3 + n(n-3) < \frac{3n^2-9n+6}{2}.$$

Subcase 2.4. $p_1 = n-2$.

Then, $n-1 \leqslant p_2 \leqslant n$.

If $p_2 = n-1$, then Lemmas 3.1 and 3.2 imply that

$$l(S) \leqslant l(D) + 3 + (n-1)(n-2) \leqslant n-2+3+(n-1)(n-2) = n^2-2n+3. \tag{3.2}$$

If $n \in \{7, 9, 11\}$, the result follows from inequality (3.2). If $n \geqslant 12$, inequality (3.2) implies that $l(S) \leqslant n^2-2n+3 < \frac{3n^2-15n+20}{2}$, the result also holds.

If $p_2 = n$, then n is odd by Proposition 2.1. If $4 \leqslant g(D) \leqslant \left\lceil \frac{n+1}{2} \right\rceil - 1 \leqslant \frac{n}{2}$, it follows from Lemmas 3.2 and 3.7 that

$$l(S) \leqslant l(D) + 2 + n(n-2) \leqslant \frac{n(n-3)}{4} + 2 + n(n-2) < \frac{3n^2-9n+6}{2}.$$

Thus, we may suppose that $g(D) \geqslant \left\lceil \frac{n+1}{2} \right\rceil$ in the following. Note that $l(D) \geqslant n$. By Corollary 3.5 and Lemma 2.7,

$$l(S) \leqslant l(D) + n(n-2) \leqslant \frac{n^2-5n+6}{2} + n(n-2) = \frac{3n^2-9n+6}{2}. \tag{3.3}$$

If $l(S) = \frac{3n^2-9n+6}{2}$, then $l(D) = \frac{n^2-5n+6}{2}$ and hence $S \cong S_{n,n,n-2}$ by inequality (3.3) and Lemma 2.7. Conversely, if $S \cong S_{n,n,n-2}$, then $l(S) = \frac{3n^2-9n+6}{2}$ by Corollary 2.8.

Subcase 2.5. $p_1 = n-1$.

Then, $p_2 = n$, and hence D contains $D_{n,n,n-1}$ as its subgraph. By Corollary 2.6,

$$l(S) \leqslant l(S_{n,n,n-1}) = n^2-n+1. \tag{3.4}$$

If $n \in \{7, 9, 11\}$, the result follows from inequality (3.4). If $n \geqslant 12$, inequality (3.4) implies that $l(S) \leqslant n^2-n+1 < \frac{3n^2-15n+20}{2}$, the result also holds.

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Ordering the Zagreb Coindices of Connected Graphs [1]

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Abstract

In this paper, we give a simple approach to order the first Zagreb indices of connected graphs and the second Zagreb coindices of trees and unicyclic graphs, respectively. As an application of our new method, we determine the first eight smallest and the first three largest (respectively, first eight smallest and first three largest, first seven smallest and first two largest) values of the first Zagreb coindices in the class of trees (respectively, unicyclic graphs, bicyclic graphs) on n vertices, and we also determine the first eleven (respectively, thirteen) smallest values of the second Zagreb coindices in the class of trees (respectively, unicyclic graphs) on n vertices. Furthermore, we also identify the smallest value of the first Zagreb coindices in the class of chemical trees on $n \geq 8$ vertices, partially giving an answer to a question of Ashrafi, Došlić and Hamzeh.

1 Introduction

Throughout this paper, we only consider undirected simple graphs. Suppose G has n vertices and m edges. If $m = n + c - 1$, then G is called a c-cyclic graph. Specially, when m is equal to $n-1$, n and $n+1$, then G is called a tree, a unicyclic graph and a bicyclic

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graph, respectively. We use the notations $\mathbb{T}_n$ (respectively, $\mathbb{U}_n$ and $\mathbb{B}_n$) to denote the class of trees (respectively, unicyclic and bicyclic graphs) on n vertices.

Let $d(u)$ be the degree of u. Specially, $\Delta = \Delta(G)$ denotes the maximum degree of vertices of G. The sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v)$ holds for some $v \in V(G)$. In the sequel, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. Let $\pi(G)$ be the degree sequence of G, and let $\Gamma(\pi)$ define the class of connected simple graphs with degree sequence π.

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are two famous important topological indices, where $M_1(G)$ and $M_2(G)$ are defined as [11]:

$$M_1(G) = \sum_{v \in V(G)} d(v)^2, \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \tag{1}$$

Recent research showed that they have been closely correlated with many chemical and mathematical properties [3, 4, 9, 10, 16, 19, 20].

Recently, Došlić [5] defined two new graphical invariants $\overline{M_1(G)}$ and $\overline{M_2(G)}$, where

$$\overline{M_1} = \overline{M_1(G)} = \sum_{uv \notin E(G)} (d(u) + d(v)), \quad \overline{M_2} = \overline{M_2(G)} = \sum_{uv \notin E(G)} d(u)d(v). \tag{2}$$

One can easily discover that

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)).$$

Thus, Ashrafi et al. [1, 2] called $\overline{M_1}$ and $\overline{M_2}$ the first Zagreb coindex and second Zagreb coindex of G, respectively. These two new topological indices received much attention quickly [1, 2, 7, 17, 18].

In this paper, we give a simple approach to order the first Zagreb coindices of connected graphs (respectively, trees and unicyclic graphs). As an application of this new ordering method, we determine the first eight smallest and the first three largest (respectively, first eight smallest and first three largest, first seven smallest and first two largest) values of the first Zagreb coindices in the class of trees (respectively, unicyclic graphs, bicyclic graphs) on n vertices, and we also determine the first eleven (respectively, thirteen) smallest values of the second Zagreb coindices in the class of trees (respectively, unicyclic graphs) on n vertices. Furthermore, we also identify the smallest value of the first Zagreb coindices in the class of chemical trees on $n \geq 8$ vertices, partially giving an answer to a question of Ashrafi, Došlić and Hamzeh.

2 The main results

Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two different non-increasing graphic degree sequences, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is sometimes called *majorization* (see [8, 13]).

Recently, the following majorization theorems of the Zagreb indices were proved.

Lemma 2.1. [12] *Let $\pi = (d_1, d_2, \ldots, d_n)$ with $G \in \Gamma(\pi)$ and let $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $G' \in \Gamma(\pi')$. If $\pi \lhd \pi'$, then $M_1(G) < M_1(G')$.*

Lemma 2.2. [13, 15] *Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two degree sequences of trees (respectively, unicyclic graphs). Suppose G and G' have the largest second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd \pi'$, then $M_2(G) < M_2(G')$.*

For the relation between M_1 and $\overline{M_1}$ (respectively, M_2 and $\overline{M_2}$), it is well-known that

Lemma 2.3. [1] *Let G be a connected graph with n vertices and m edges. Then,*

$$(1)\ \overline{M_1(G)} = 2m(n-1) - M_1(G), \quad (2)\ \overline{M_2(G)} = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).$$

Remark 2.4. By (1) of Lemma 2.3, if G and G' are two graphs of $\Gamma(\pi)$, then $\overline{M_1(G)} = \overline{M_1(G')}$. By (2) of Lemma 2.3, G has the largest second Zagreb index in $\Gamma(\pi)$ if and only if G has the smallest second Zagreb coindex in $\Gamma(\pi)$.

Theorem 2.5. *Let $\pi = (d_1, d_2, \ldots, d_n)$ with $G \in \Gamma(\pi)$ and let $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $G' \in \Gamma(\pi')$. If $\pi \lhd \pi'$, then $\overline{M_1(G)} > \overline{M_1(G')}$.*

Proof. Since $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, G and G' contains exactly m edges and n vertices, respectively. So, the result clearly follows from Lemmas 2.1 and 2.3 (1). ■

With the similar reason, by Lemmas 2.1–2.2 and 2.3 (2), and Remark 2.4 we have

Theorem 2.6. *Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two degree sequences of trees (respectively, unicyclic graphs). Suppose G and G' have the smallest second Zagreb coindices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd \pi'$, then $\overline{M_2(G)} > \overline{M_2(G')}$.*

In [2], Ashrafi et al. determined the largest and smallest values of $\overline{M_1(G)}$ and $\overline{M_2(G)}$ in the class of trees on n vertices. In the following, as an application of the majorization theorems of the Zagreb coindices, we shall determine the first eight smallest and first three

largest (respectively, first eleven smallest) values of the first (respectively, second) Zagreb coindices in the class of trees on n vertices.

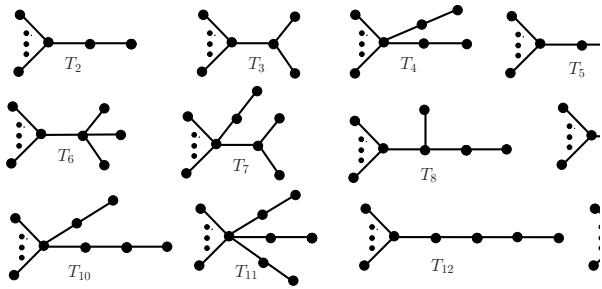


Figure 1: The trees $T_2, T_3, \ldots, T_{13}$.

Let T_1 be the star and $T_2, T_3, \ldots, T_{13}$ be the trees on n vertices as shown in Fig. 1.

Theorem 2.7. (1) *Suppose* $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_{13}\}$ *and* $n \geq 13$. *Then,* $\overline{M_1(T_1)} < \overline{M_1(T_2)} < \overline{M_1(T_3)} < \overline{M_1(T_4)} = \overline{M_1(T_5)} < \overline{M_1(T_6)} < \overline{M_1(T_7)} = \overline{M_1(T_8)} = \overline{M_1(T_9)} < \overline{M_1(T_{10})} = \overline{M_1(T_{11})} = \overline{M_1(T_{12})} < \overline{M_1(T_{13})} < \overline{M_1(T)}$;

(2) *Suppose* $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_8, T_{10}, T_{11}, T_{13}\}$ *and* $n \geq 22$. *Then,* $\overline{M_2(T_1)} < \overline{M_2(T_2)} < \overline{M_2(T_3)} < \overline{M_2(T_4)} < \overline{M_2(T_5)} < \overline{M_2(T_6)} < \overline{M_2(T_7)} < \overline{M_2(T_{11})} < \overline{M_2(T_8)} < \overline{M_2(T_{10})} < \overline{M_2(T_{13})} < \overline{M_2(T)}$.

Proof. Obviously, T_1 is the unique tree with $\Delta = n-1$, T_2 is the unique tree with $\Delta = n-2$, T_3, T_4, T_5 are all the trees with $\Delta = n-3$, $T_6, \ldots, T_{12}$ are all the trees with $\Delta = n-4$. Recall that $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_{13}\}$. So, $\Delta(T) \leq n-5$. Since $\pi(T_{13}) = (n-5, 5, 1, \ldots, 1)$ and $\Gamma(\pi(T_{13})) = \{T_{13}\}$, we have $\pi(T) \lhd \pi(T_{13})$. By Theorems 2.5–2.6, it follows that $\overline{M_1(T_{13})} < \overline{M_1(T)}$ and $\overline{M_2(T_{13})} < \overline{M_2(T)}$.

By an elementary computation, we have $\overline{M_1(T_5)} = n^2 + n - 12$, $\overline{M_1(T_6)} = n^2 + 3n - 28$, $\overline{M_1(T_{12})} = n^2 + 3n - 22$, $\overline{M_1(T_{13})} = n^2 + 5n - 46$, $\overline{M_2(T_4)} = \frac{1}{2}(n^2 + 5n - 24)$, $\overline{M_2(T_5)} = \frac{1}{2}(n^2 + 7n - 34)$, $\overline{M_2(T_6)} = \frac{1}{2}(n^2 + 9n - 58)$, $\overline{M_2(T_7)} = \frac{1}{2}(n^2 + 9n - 46)$, $\overline{M_2(T_8)} = \frac{1}{2}(n^2 + 11n - 60)$, $\overline{M_2(T_9)} = \frac{1}{2}(n^2 + 13n - 70)$, $\overline{M_2(T_{10})} = \frac{1}{2}(n^2 + 11n - 52)$, $\overline{M_2(T_{11})} = \frac{1}{2}(n^2 + 9n - 40)$, $\overline{M_2(T_{12})} = \frac{1}{2}(n^2 + 13n - 64)$, $\overline{M_2(T_{13})} = \frac{1}{2}(n^2 + 13n - 94)$.

Note that $\pi(T_5) = \pi(T_4) \lhd \pi(T_3) \lhd \pi(T_2) \lhd \pi(T_1)$. By the above values and Theorem 2.6, (2) follows when $n \geq 22$. Now, we turn to prove (1). It is easily checked that $\pi(T_{12}) = \pi(T_{11}) = \pi(T_{10}) \lhd \pi(T_9) = \pi(T_8) = \pi(T_7) \lhd \pi(T_6)$ and $\pi(T_5) = \pi(T_4) \lhd \pi(T_3) \lhd \pi(T_2) \lhd \pi(T_1)$. So, (1) follows from Theorem 2.5 and Lemma 2.3 (1). ■

Theorem 2.8. *In the class of trees on n vertices, the path has the largest first Zagreb coindex, the trees with degree sequence* $(3, 2, 2, \ldots, 2, 1, 1, 1)$ *have the second largest first Zagreb coindex, and the trees with degree sequence* $(3, 3, 2, \ldots, 2, 1, 1, 1, 1)$ *have the third largest first Zagreb coindex.*

Proof. Suppose $T \in \mathbb{T}(n)$. Let $\pi_1 = (2, 2, 2, \ldots, 2, 1, 1)$, $\pi_2 = (3, 2, 2, \ldots, 2, 1, 1, 1)$ and $\pi_3 = (3, 3, 2, \ldots, 2, 1, 1, 1, 1)$. Suppose $\pi(T) \notin \{\pi_1, \pi_2, \pi_3\}$. Then, $\pi_1 \lhd \pi_2 \lhd \pi_3 \lhd \pi(T)$. By Theorem 2.5, the result follows. ■

Ashrafi et al. [2] also determined the smallest and largest values of $\overline{M_1(G)}$ in the class of unicyclic graphs and bicyclic graphs on n vertices. In the following, we shall identify the first eight smallest and the first three largest (respectively, the first seven smallest and the first two largest) values of the first Zagreb coindices in the class of unicyclic (respectively, bicyclic) graphs on n vertices, and we also determine the first thirteen smallest values of the second Zagreb coindices in the class of unicyclic graphs on n vertices.

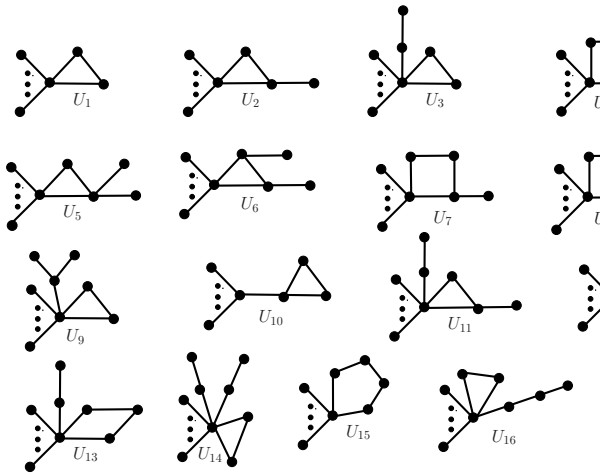


Figure 2: The unicyclic graphs U_1, U_2, ..., U_{17}.

Let $U_1, \ldots, U_{17}$ be the unicyclic graphs on n vertices as shown in Fig. 2.

Theorem 2.9. (1) *If $n \geq 12$ and $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_{17}\}$, then* $\overline{M_1(U_1)} < \overline{M_1(U_2)} < \overline{M_1(U_3)} = \overline{M_1(U_4)} < \overline{M_1(U_5)} < \overline{M_1(U_6)} < \overline{M_1(U_7)} = \overline{M_1(U_8)} = \overline{M_1(U_9)} = \overline{M_1(U_{10})} = \overline{M_1(U_{11})} = \overline{M_1(U_{12})} < \overline{M_1(U_{13})} = \overline{M_1(U_{14})} = \overline{M_1(U_{15})} = \overline{M_1(U_{16})} < \overline{M_1(U_{17})} < \overline{M_1(U)}$;

(2) *If* $n \geq 23$ *and* $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_7, U_9, U_{12}, U_{13}, U_{14}, U_{16}, U_{17}\}$, *then* $\overline{M_2(U_1)} < \overline{M_2(U_2)} < \overline{M_2(U_3)} < \overline{M_2(U_4)} < \overline{M_2(U_5)} < \overline{M_2(U_6)} < \overline{M_2(U_{11})} < \overline{M_2(U_9)} < \overline{M_2(U_{14})} < \overline{M_2(U_{12})} < \overline{M_2(U_7)} < \overline{M_2(U_{13})} = \overline{M_2(U_{16})} < \overline{M_2(U_{17})} < \overline{M_2(U)}$.

Proof. Clearly, U_1 is the unique unicyclic graph with $\Delta = n-1$, U_2, U_3, U_4 are all the unicyclic graphs with $\Delta = n-2$, and $U_5, U_6, \ldots, U_{16}$ are all the unicyclic graphs with $\Delta(G) = n-3$. If $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_{17}\}$, then $\Delta(G) \leq n-4$. Since $\Gamma(\pi(U_{17})) = \{U_{17}\}$, we have $\pi(U) \lhd \pi(U_{17})$. By Theorems 2.5–2.6, $\overline{M_1(U_{17})} < \overline{M_1(U)}$ and $\overline{M_2(U_{17})} < \overline{M_2(U)}$.

By an elementary computation, we have $\overline{M_1(U_4)} = n^2 + n - 12$, $\overline{M_1(U_5)} = n^2 + 3n - 26$, $\overline{M_1(U_{16})} = n^2 + 3n - 20$, $\overline{M_1(U_{17})} = n^2 + 5n - 42$, $\overline{M_2(U_3)} = \frac{1}{2}(n^2 + 5n - 20)$, $\overline{M_2(U_4)} = \frac{1}{2}(n^2 + 7n - 28)$, $\overline{M_2(U_5)} = \frac{1}{2}(n^2 + 9n - 52)$, $\overline{M_2(U_6)} = \frac{1}{2}(n^2 + 9n - 48)$, $\overline{M_2(U_7)} = \frac{1}{2}(n^2 + 11n - 48)$, $\overline{M_2(U_8)} = \frac{1}{2}(n^2 + 13n - 58)$, $\overline{M_2(U_9)} = \frac{1}{2}(n^2 + 9n - 36)$, $\overline{M_2(U_{10})} = \frac{1}{2}(n^2 + 13n - 60)$, $\overline{M_2(U_{11})} = \frac{1}{2}(n^2 + 9n - 38)$, $\overline{M_2(U_{12})} = \frac{1}{2}(n^2 + 11n - 50)$, $\overline{M_2(U_{13})} = \frac{1}{2}(n^2 + 11n - 40)$, $\overline{M_2(U_{14})} = \frac{1}{2}(n^2 + 9n - 30)$, $\overline{M_2(U_{15})} = \frac{1}{2}(n^2 + 13n - 50)$, $\overline{M_2(U_{16})} = \frac{1}{2}(n^2 + 11n - 40)$, $\overline{M_2(U_{17})} = \frac{1}{2}(n^2 + 13n - 84)$.

Note that $\pi(U_4) = \pi(U_3) \lhd \pi(U_2) \lhd \pi(U_1)$. By the above values and Theorem 2.6, (2) follows when $n \geq 23$. Now, we turn to prove (1). It is easy to see that $\pi(U_{16}) = \pi(U_{15}) = \pi(U_{14}) = \pi(U_{13}) \lhd \pi(U_{12}) = \pi(U_{11}) = \pi(U_{10}) = \pi(U_9) = \pi(U_8) = \pi(U_7) \lhd \pi(U_6) \lhd \pi(U_5)$ and $\pi(U_4) = \pi(U_3) \lhd \pi(U_2) \lhd \pi(U_1)$. Therefore, (1) follows from Theorem 2.5 and Lemma 2.3 (1). ■

With the similar reason as Theorem 2.8, it follows that

Theorem 2.10. *In the class of unicyclic graphs on n vertices, the cycle has the largest first Zagreb coindex, the unicyclic graphs with degree sequence* (3, 2, 2, . . . , 2, 1) *have the second largest first Zagreb coindex, and the unicyclic graphs with degree sequence* (3, 3, 2, . . . , 2, 1, 1) *have the third largest first Zagreb coindex.*

Theorem 2.11. *Suppose* $n \geq 11$ *and* $B \in \mathbb{B}(n) \setminus \{B_1, \ldots, B_{12}\}$, *where* $B_1, \ldots, B_{12}$ *are the bicyclic graphs on n vertices as shown in Fig.* 3. *Then,* $\overline{M_1(B_1)} < \overline{M_1(B_2)} < \overline{M_1(B_3)} < \overline{M_1(B_4)} = \overline{M_1(B_5)} < \overline{M_1(B_6)} = \overline{M_1(B_7)} = \overline{M_1(B_8)} = \overline{M_1(B_9)} < \overline{M_1(B_{10})} = \overline{M_1(B_{11})} < \overline{M_1(B_{12})} < \overline{M_1(B)}$.

Proof. It is easy to check that B_1, B_2 are all the bicyclic graphs with $\Delta = n-1$, $B_3, \ldots, B_{11}$ are all the bicyclic graphs with $\Delta = n-2$. Since $B \in \mathbb{B}(n) \setminus \{B_1, \ldots, B_{12}\}$, $\Delta(G) \leq n-3$. Note that $\pi(B_{12}) = (n-3, 5, 2, 2, 1, ..., 1)$ and $\Gamma(\pi(B_{12})) = \{B_{12}\}$. Then, $\pi(B) \lhd \pi(B_{12})$, which implies that $\overline{M_1(B_{12})} < \overline{M_1(B)}$ by Theorem 2.5.

It is easily checked that $\pi(B_{11}) = \pi(B_{10}) \lhd \pi(B_9) = \pi(B_8) = \pi(B_7) = \pi(B_6) \lhd \pi(B_5) = \pi(B_4) \lhd \pi(B_3)$ and $\pi(B_2) \lhd \pi(B_1)$. Furthermore, by an elementary computation, we have $\overline{M_1(B_2)} = n^2 + n - 14 < n^2 + 3n - 26 = \overline{M_1(B_3)}$, and $\overline{M_1(B_{11})} = n^2 + 3n - 20 < n^2 + 5n - 40 = \overline{M_1(B_{12})}$. Thus, by Theorem 2.5 and Lemma 2.3 (1), the result follows. ■

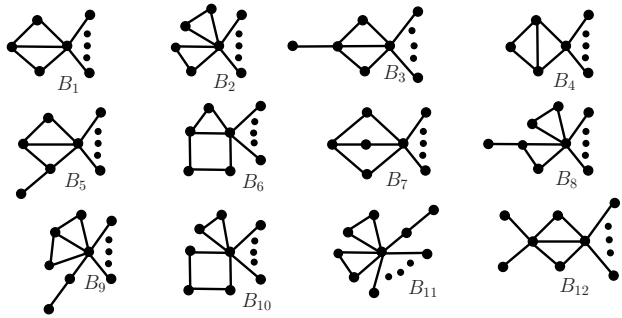


Figure 3: The bicyclic graphs B_1, B_2, ..., B_{12}.

Theorem 2.12. *In the class of bicyclic graphs on n vertices, the bicyclic graphs with degree sequence* $(3, 3, 2, 2, \ldots, 2)$ *have the largest first Zagreb coindex, and the bicyclic graphs with degree sequence* $(3, 3, 3, 2, \ldots, 2, 1)$ *or* $(4, 2, 2, \ldots, 2)$ *have the second largest first Zagreb coindex.*

Proof. Suppose $B \in \mathbb{B}(n)$. Let $\pi_1 = (3, 3, 2, 2, \ldots, 2)$, $\pi_2 = (3, 3, 3, 2, \ldots, 2, 1)$, and $\pi_3 = (4, 2, 2, \ldots, 2)$. Since $B \in \mathbb{B}(n)$, $\Delta(B) \geq 3$. If $\Delta(B) = 3$, $\pi_1 \lhd \pi_2 \lhd \pi(B)$. If $\Delta(B) \geq 4$, $\pi_1 \lhd \pi_3 \lhd \pi(B)$.

Suppose $G_i \in \Gamma(\pi_i)$, where $i = 1, 2, 3$. Since $M_1(G_2) = 4n+12 = M_1(G_3)$, by Theorem 2.5 and Lemma 2.3 (1), we have $\overline{M_1(G_1)} > \overline{M_1(G_2)} = \overline{M_1(G_3)} > \overline{M_1(B)}$. ■

For integers n, c, k with $c \geq 0$ and $0 \leq k \leq n - 2c - 1$, let $\mathcal{G}_n(c, k)$ be the class of connected c-cyclic graphs with n vertices and k pendant vertices.

Theorem 2.13. *In the class of $\mathcal{G}_n(c, k)$, where $c \geq 0$ and $1 \leq k \leq n - 2c - 1$, the graphs with degree sequence* $(2c+k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k})$ *have the largest first Zagreb coindices.*

Proof. Let $\pi_1 = (2c + k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k})$. Suppose $G \in \mathcal{G}_n(c, k)$ with $\pi(G) = (d_1, d_2, \ldots, d_n)$. If $\pi(G) \neq \pi_1$, then $d_{n-k+1} = d_{n-k+2} = \cdots = d_n = 1$ and $d_2 \geq d_3 \geq \cdots \geq d_{n-k} \geq 2$. Thus, $\pi(G) \lhd \pi_1$.

Now, the result follows from Theorem 2.5 and Lemma 2.3 (1). ■

3 Concluding remarks

In this note, we prove that the majorization theorem also holds for the first Zagreb coindices of connected graphs and the second Zagreb coindices of trees and unicyclic graphs, namely, Theorems 2.5–2.6. The proofs are based on the corresponding majorization theorems of the first Zagreb index and the second Zagreb index, i.e., Lemmas 2.1–2.2. Actually, if the majorization theorem also holds for the second Zagreb index of the other c-cyclic graphs, then it also holds to the second Zagreb coindex.

As shown in [6, 12, 14] and also illustrated in the former section, the majorization theorem is a good tool to deal with the ordering of (signless Laplacian) spectral radii and/or the topological indices. But the majorization theorem cannot hold to all the topological indices [13]. Thus, it is a good question to find out which topological index also obey the majorization theorem (The known results show that such topological index are always closely related with the degree sequence of the graph).

In the end of this paper, we shall apply Theorem 2.5 to determine the smallest value of the first Zagreb coindices over chemical trees on n vertices, which partially answers an open problem asked in [2].

Theorem 3.1. *In the class of chemical trees on $n \geq 8$ vertices, the trees with degree sequence π_0 have the smallest first Zagreb coindices, where π_0 is defined as follows:*

(1) *If $n \equiv 0 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 2, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n}{3}$,*

(2) *If $n \equiv 1 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 3, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n+1}{3}$,*

(3) *If $n \equiv 2 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n+2}{3}$.*

Proof. Let $\pi_1 = (4, \ldots, 4, 1, \ldots, 1)$, $\pi_2 = (4, \ldots, 4, 3, 1, \ldots, 1)$ and $\pi_3 = (4, \ldots, 4, 2, 1, \ldots, 1)$. Suppose T is a chemical tree on n vertices. Here we only prove the case of $n \equiv 0 \pmod 3$, since the other cases can be shown by using the similar argument.

Suppose that $n \equiv 0 \pmod 3$. If $\pi(T) = \pi_1$, we assume that the cardinality of 4 in $\pi(T)$ is x. Then, $4x + n - x = 2(n-1)$, which contradicts $n \equiv 0 \pmod 3$. So, $\pi(T) \neq \pi_1$. Similarly, $\pi(T) \neq \pi_2$. If $\pi(T) \neq \pi_3$, since $\Delta(T) \leq 4$, we have $\pi(T) \lhd \pi_3$.

Now, the result follows from Theorem 2.5 and Lemma 2.3 (1). ■

Remark 3.2. In [2], Ashrafi et al. also asked the smallest value of the second Zagreb coindices over chemical trees on n vertices. By Theorem 2.6 and the proof of Theorem 3.1, we can conclude that the smallest value of the second Zagreb coindices among $\Gamma(\pi_0)$, where π_0 is denoted as in Theorem 3.1, is also the smallest value of the second Zagreb coindices over chemical trees on $n \geq 8$ vertices.

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Maximal Lanzhou index of trees and unicyclic graphs with prescribed diameter

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ABSTRACT

Given a connected graph G, its Lanzhou index is $Lz(G) = \sum_{v\in V(G)} d(v)^2\,[n-1-d(v)]$, where n is the order and $d(v)$ is the degree of $v \in G$. As usual with topological indices and their meaning in Chemical Graph Theory, we are interested in determining the graphs maximizing or minimizing the considered index. We show that by applying the majorization method, we identify all unified extremal trees with maximum Lanzhou index among the trees of order n and diameter $d \geq 8$. Using the same method, we identify the unified extremal unicyclic graphs with maximum Lanzhou index among the unicyclic graphs of order n and diameter $d \geq 9$ with $n \geq 3d - 8$.

1. Introduction

As usual with topological indices, we consider simple and connected graphs. By $G = (V(G), E(G))$ we denote a graph whose vertex set is $V(G)$ and whose edge set is $E(G)$: the order is $|V(G)|$ and the size is $|E(G)|$, in such a case we say that G is a n-graph. For connected graph of order n and size m, the number $c = m - n + 1$ denotes the cyclomatic numer, and we say that G is a c-cyclic graph. For small values of c, the graph G is called a tree ($c = 0$), unicyclic graph ($c = 1$), bicyclic graph ($c = 2$), or a tricyclic graph ($c = 3$). Let $d(u)$ and $N(u)$ denote, respectively, the degree and neighbor set of the vertex $u \in G$, in particular let $\Delta(G) = \max\{d(u), u \in G\}$ and $\delta(G) = \min\{d(u), u \in G\}$. A vertex with degree equals 1 is said to be a pendant vertex. A graph G is a chemical graph if it is connected graph and $\Delta(G) = 4$. We will list the vertices according to the magnitude of their degrees, hence if G has order n the vertex set is $V(G) = \{v_1, v_2, \ldots, v_n\}$, so that $\Delta = d(v_1) = d_1 \geq d(v_2) = d_2 \geq \ldots \geq d(v_n) = d_n = \delta$. The n-tuple with non-increasing entries $\pi(G) = (\Delta = d_1, d_2, \ldots, \delta = d_n)$ is the degree sequence of G. In case of repeated entries in the degree sequences, the term $a^{(b)}$ indicates that the integer a is repeated b times in the sequence. Sometimes, we write $d_i(G)$ in place of d_i to distinguish among degree sequences of other graphs. For a connected graph G, the following relation between the order n, the size m, the cyclomatic number c and the degrees $\pi = (d_1, d_2, \ldots, d_n)$ is well-known:

$$\sum_{i=1}^{n} d_i = 2m = 2(n + c - 1). \tag{1.1}$$

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Two vertices u and v have distance $\mathrm{dist}(u,v) = d_{u,v}$ if $d_{u,v}$ equals the number of edges in some shortest path joining u and v. The maximal distance among all pairs of vertices in a connected graph G is the diameter $\mathrm{diam}(G)$. For a real number r, by $\lfloor r \rfloor$ (resp., $\lceil r \rceil$) we denote the largest (resp., smallest) integer not greater (resp., larger) than r.

It is well known that molecules can be represented by graphs in which vertices correspond to the atoms while edges represent the covalent bonds between atoms [6,14]. Predicting physicochemical properties of molecules is considered to be a fascinating issue in theoretical chemistry. Many predictive methods have been developed for correlating molecular structures with their physicochemical properties. One of the simplest such methods involves topological indices [3]. Topological indices are numerical quantities of a graph which are invariant under graph isomorphism. For a graph G, two important topological indices are the first Zagreb index $M_1(G)$ and the forgotten index $F(G)$. They are, respectively, defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \text{ and } F(G) = \sum_{v \in V(G)} d(v)^3.$$

The first Zagreb index has been defined by Gutman and Trinajstić in [9], while the forgotten index was reintroduced by Furtula and Gutman in [7]. The properties of the first Zagreb index have been studied from a chemical and mathematical viewpoint in [8,19,20].

In 2018, Vukičević, Li, Sedlar and Doslić, proposed a new topological index, that is, the Lanzhou index $Lz(G)$. For a (chemical) n-graph G [16], the Lanzhou index is defined as

$$Lz(G) = (n-1)M_1(G) - F(G) = \sum_{v \in V(G)} d(v)^2 [n - 1 - d(v)]. \tag{1.2}$$

In [16], the authors showed that from a chemical viewpoint the Lanzhou index has interesting properties and it behaves better, with respect to other indices, in predicting some chemically relevant properties. The careful reader might haven noticed that the Lanzhou index is a linear combination of Zagreb and forgotten indices [1].

Determining the extreme values or the extremal graphs for different topological indices in prescribed graph classes is a relevant research topic in Chemical Graph Theory. In this line, the extremal (that is, minimal and maximal) Lanzhou indices among all connected n-graphs were determined by Vukičević et al. [16]. In the same paper, Vukičević et al. determined the minimum and maximum Lanzhou indices in the class of all n-trees [16]. Later, Liu et al. [13] determined the extremal Lanzhou indices in the class of unicyclic n-graphs and chemical n-graphs, respectively; Liu [12] determined the extremal Lanzhou indices, respectively, among bicyclic n-graphs. Recently, Cui and Zhao [4,5] identified the extremal Lanzhou indices among tricyclic n-graphs and unicyclic graphs with fixed maximum degree, respectively.

By establishing an upper bound to the Lanzhou index for trees on n vertices and fixed maximum degree, Li et al. [11] also deduced the extremal Lanzhou indices of unicyclic n-graphs, and they also determined the maximum Lanzhou index for chemical n-trees. Recently, Albalahi et al. [2] also determined the maximum Lanzhou index of the chemical graphs on n vertices and m edges. Generalizing the corresponding results of [4,11–13], two of the present authors and Chen [10] identified the unique extremal graph with respect to the maximum Lanzhou index among all c-cyclic n-graphs for $3 \le c \le n/13$, and they also determined the minimum Lanzhou index among all c-cyclic n-graphs for $n \ge 3c+4$. Here, we determine all unified extremal trees with the maximum Lanzhou index in the class of n-trees with diameter $d \ge 8$, and the unicyclic n-graphs with diameter $d \ge 9$, where $n \ge 3d-8$.

Here is the first of our main results:

Theorem 1.1. *Let G be a maximal graph with respect to the Lanzhou index among the n-trees with diameter $d \ge 8$.*

(i) If $8 \le d \le (n+10)/3$, then $\pi(G) = (\lceil (n+3-d)/2 \rceil, \lfloor (n+3-d)/2 \rfloor, 2^{(d-3)}, 1^{(n+1-d)})$,
(ii) If $d = (n+11)/3$, then $\pi(G) = (d_1, n+3-d-d_1, 2^{(d-3)}, 1^{(n+1-d)})$,
(iii) If $(n+12)/3 \le d \le n-1$, then $\pi(G) = (n+1-d, 2^{(d-2)}, 1^{(n+1-d)})$.

Note that the diameter d is an integer. Hence, the above theorem cover all case of $8 \le d \le n-1$. Let C_k and P_k be, respectively, the cycle and the path on k vertices. For $1 \le j \le d-2$, let $C_3(n,d,j)$ be the graph consisting of the triangle $C_3 = z_1z_2z_3z_1$ by appending at z_1 the path P_j and $\lceil (n-2-d)/2 \rceil$ isolated vertices, and then appending at z_2 the path P_{d-j-1} and $\lfloor (n-2-d)/2 \rfloor$ isolated vertices. For $1 \le j \le d-3$, let $C_4(n,d,j)$ be the unicyclic graph consisting of the quadrangle $C_4 = z_1z_2z_3z_4z_1$ by appending at z_1 the path P_j and $\lceil (n-2-d)/2 \rceil$ isolated vertices, and then appending at z_3 the path P_{d-j-2} and $\lfloor (n-d-2)/2 \rfloor$ isolated vertices.

Under the above notation, here is our second and last main result of this paper:

Theorem 1.2. *Let G be a maximal graph with respect to the Lanzhou index among the unicyclic n-graphs with diameter d. If $9 \le d \le (n+8)/3$, then $G \in \{C_3(n,d,1), C_3(n,d,2), \ldots, C_3(n,d,d-2), C_4(n,d,1), C_4(n,d,2), \ldots, C_4(n,d,d-3)\}$.*

We outline the remainder of the paper. In Section 2, we recall the Majorization Theorem and some inequalities useful to prove the main results of this paper. In Section 3 and Section 4, we respectively prove our main results, that are, Theorem 1.1 and Theorem 1.2. The paper ends with Section 5, where we derive the conclusions of this research.

2. Preliminary results

We first recall the 'Majorization Theorem'. The majorization theorem is a very useful tool when dealing with extremal problems related to the graph spectrum and the topological index theory (see, for example, [17,18]).

Definition 2.1. A p-tuple $(a_1, a_2, \dots, a_p)$ of real numbers is called a p-sequence if $a_i \in \mathbb{R}_0^+$ and $a_i \geq a_j$ for $i < j$.

Definition 2.2. Let $\pi = (a_1, a_2, \dots, a_p)$ and $\pi' = (a'_1, a'_2, \dots, a'_p)$ be two p-sequences. We write $\pi \trianglelefteq \pi'$ and we call this a 'majorization' if and only if $\sum_{i=1}^{p} a_i = \sum_{i=1}^{p} a'_i$, and $\sum_{i=1}^{j} a_i \leq \sum_{i=1}^{j} a'_i$ for all $j = 1, 2, \dots, p$. Furthermore, we use the symbol $\pi \triangleleft \pi'$ to indicate that $\pi \trianglelefteq \pi'$ with $\pi \neq \pi'$.

A function $f(x) : D \to \mathbb{R}$, where D is a convex set, is said to be strictly convex if

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda) f(y)$$

holds for all $x, y \in D$ and for any $\lambda \in (0,1)$. The subsequent result for strictly convex functions has been discovered long time ago (cf. [15]).

Lemma 2.1 *(Majorization Theorem). Let $\pi = (a_1, a_2, \dots, a_p)$ and $\pi' = (a'_1, a'_2, \dots, a'_p)$ be two p-sequences and let $f(x)$ be a strictly convex function. If $\pi \trianglelefteq \pi'$, then $\sum_{i=1}^{p} f(a_i) \leq \sum_{i=1}^{p} f(a'_i)$, where equality occurs if and only if $\pi = \pi'$.*

To make effectively use of the majorization theorem, we define the following function

$$\varphi(x) = x^2(n-1-x).$$

In view of Equation (1.2), we now get the subsequent expression for the Lanzhou index:

$$Lz(G) = \sum_{v \in V(G)} \varphi(d(v)). \tag{2.1}$$

Let a n-sequence π be the degree sequence for some class of connected graphs, and let $\Gamma(\pi)$ be such class. The following corollary derives from Lemma 2.1.

Corollary 2.2. *Let π and π' be two degree n-sequences such that $\pi \triangleleft \pi'$. For any $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, we have:*

(i) If $\Delta(G') \leq (n-1)/3$, then $Lz(G) < Lz(G')$,
(ii) If $\delta(G') \geq (n-1)/3$, then $Lz(G) > Lz(G')$.

Proof. Consider first (i). Since $\Delta(G') \leq (n-1)/3$ and $\pi \triangleleft \pi'$, we have $\Delta(G) \leq \Delta(G') \leq (n-1)/3$ by Definition 2.2. Since $\varphi''(x) = 2(n-1-3x) \geq 0$ for $x \leq (n-1)/3$, $\varphi(x)$ is a strictly convex function for $x \leq (n-1)/3$. Thus, we have $Lz(G) < Lz(G')$ by Lemma 2.1.

We now prove (ii). Let G be a c-cyclic graph, $\pi = (d_1, d_2, \dots, d_n)$ and $\pi' = (d'_1, d'_2, \dots, d'_n)$. From $\pi \triangleleft \pi'$, we have $\sum_{i=1}^{n-1} d_i \leq \sum_{i=1}^{n-1} d'_i$, and thus $d_n \geq d'_n \geq (n-1)/3$ by (1.1). Note that $-\varphi''(x) = 2(3x-n+1) \geq 0$ for $x \geq (n-1)/3$, so $-\varphi(x)$ is a strictly convex function for $x \geq (n-1)/3$. From $\pi \triangleleft \pi'$, in view of Lemma 2.1 and Equation (2.1), we have $Lz(G) > Lz(G')$. □

In what follows, let

$$\begin{aligned}
f_1(x) &= \varphi(x) + \varphi(\lceil (2n+16-3d-3x)/3 \rceil) + \varphi(\lfloor (n-1)/3 \rfloor) + (d-4)\varphi(2) \\
&\quad + (n-d+1)\varphi(1), \\
f_2(x) &= \varphi(x) + \varphi(n+3-d-x) + (d-3)\varphi(2) + (n-d+1)\varphi(1), \\
f_3(x) &= \varphi(x) + \varphi(\lfloor (n-1)/3 \rfloor) + \varphi(\lceil (2n+19-3d-3x)/3 \rceil) + (d-3)\varphi(2) \\
&\quad + (n-d)\varphi(1), \text{ and} \\
f_4(x) &= \varphi(x) + \varphi(n+4-d-x) + (d-2)\varphi(2) + (n-d)\varphi(1),
\end{aligned}$$

where $x, n, d \in \mathbb{N}^*$.

Lemma 2.3. *If $d \geq 8$ then $f_1(\lceil (2n+10-3d)/3 \rceil) = f_2(\lceil (2n+10-3d)/3 \rceil)$. Furthermore, we have:*

(i) If $x > \lfloor (n-1)/3 \rfloor$, then $f'_1(x) > 0$,
(ii) If $n > 3d-11$ and $x > (2n+10-3d)/3$, then $f'_2(x) < 0$,

(*iii*) *If* $n \le 3d-12$ *and* $x \ge \lfloor (n+2)/3 \rfloor$, *then* $f_2'(x) > 0$,
(*iv*) *If* $n \le 3d-13$ *and* $x \ge \lfloor (n-1)/3 \rfloor$, *then* $f_2'(x) \ge 0$.

Proof. It is easy to check that $f_1(\lceil (2n+10-3d)/3 \rceil) = f_2(\lceil (2n+10-3d)/3 \rceil)$.

We first show (*i*). Let $(n-1) \equiv 0 \pmod 3$, then $\lfloor (n-1)/3 \rfloor = (n-1)/3$. Since $d \ge 8$, we have $f_1''(x) = 6(d-6) > 0$. Hence, we have $f_1'(x) > f_1'(\lfloor (n-1)/3 \rfloor) = 3(d-6)^2 > 0$, as $d \ge 8$. Let $(n-1) \equiv 1 \pmod 3$. Then, $\lfloor (n-1)/3 \rfloor = (n-2)/3$. Since $f_1''(x) = 2(3d-19) > 0$ for $d \ge 8$, we have $f_1'(x) > f_1'(\lfloor (n-1)/3 \rfloor) = (d-7)(3d-19) > 0$. Finally, let $(n-1) \equiv 2 \pmod 3$. Then, $\lfloor (n-1)/3 \rfloor = (n-3)/3$. Since $f_1''(x) = 2(3d-20) > 0$ for $d \ge 8$, we have $f_1'(x) > f_1'(\lfloor (n-1)/3 \rfloor) = (d-8)(3d-20) \ge 0$. This confirms (*i*).

Next we prove (*ii*). Since $n > 3d-11$, we have $f_2''(x) = 2(3d-n-11) < 0$. Note that $x > (2n+10-3d)/3$. Thus, $3f_2'(x) < 3f_2'((2n+10-3d)/3) = -(n+11-3d)^2 < 0$, so (*ii*) holds.

Now, we show (*iii*). Since $n \le 3d-12$, we have $f_2''(x) = 2(3d-n-11) > 0$. Combining this with $x \ge \lfloor (n+2)/3 \rfloor$ and $n \le 3d-12$, we have $3f_2'(x) \ge 3f_2'(\lfloor (n+2)/3 \rfloor) \ge 3f_2'(n/3) = (n+11-3d)(n+9-3d) > 0$. Thus, (*iii*) holds.

Finally, we prove (*iv*). Let $n \le 3d-15$ and $x \ge \lfloor (n-1)/3 \rfloor$. Then, we have $3f_2'(x) \ge 3f_2'(\lfloor (n-1)/3 \rfloor) \ge 3f_2'((n-3)/3) = (n+15-3d)(n+11-3d) \ge 0$. If $n = 3d-13$, then $(n-1) \equiv 1 \pmod 3$. Thus, $3f_2'(x) \ge 3f_2'(\lfloor (n-1)/3 \rfloor) = 3f_2'((n-2)/3) = (n+13-3d)(n+11-3d) = 0$. Finally, if $n = 3d-14$, then $(n-1) \equiv 0 \pmod 3$. Thus, $3f_2'(x) \ge 3f_2'(\lfloor (n-1)/3 \rfloor) = 3f_2'((n-1)/3) = (n+11-3d)^2 > 0$. Hence, (*iv*) holds.

This completes the proof. □

Lemma 2.4. *If* $d \ge 9$, *then* $f_3(\lceil (2n+13-3d)/3 \rceil) = f_4(\lceil (2n+13-3d)/3 \rceil)$. *Furthermore, we have:*

(*i*) *If* $x > \lfloor (n-1)/3 \rfloor$, *then* $f_3'(x) > 0$,
(*ii*) *If* $n \ge 3d-8$ *and* $x \ge \lceil (2n+13-3d)/3 \rceil$, *then* $f_4'(x) < 0$.

Proof. The equality $f_3(\lceil (2n+13-3d)/3 \rceil) = f_4(\lceil (2n+13-3d)/3 \rceil)$ can be easily verified.

Now we prove (*i*). If $(n-1) \equiv 0 \pmod 3$, then $\lfloor (n-1)/3 \rfloor = (n-1)/3$. Note that $f_3''(x) = 6(d-7) > 0$ for $d \ge 9$. Hence, we have $f_3'(x) > f_3'(\lfloor (n-1)/3 \rfloor) = 3(d-7)^2 > 0$ for $d \ge 9$. If $(n-1) \equiv 1 \pmod 3$, then $\lfloor (n-1)/3 \rfloor = (n-2)/3$. Note that $f_3''(x) = 2(3d-22) > 0$ by $d \ge 9$. Hence, we have $f_3'(x) > f_3'(\lfloor (n-1)/3 \rfloor) = (3d-22)(d-8) > 0$ for $d \ge 9$. Finally, if $(n-1) \equiv 2 \pmod 3$, then $\lfloor (n-1)/3 \rfloor = (n-3)/3$. Note that $f_3''(x) = 2(3d-23) > 0$ for $d \ge 9$. Hence, we have $f_3'(x) > f_3'(\lfloor (n-1)/3 \rfloor) = (d-9)(3d-23) \ge 0$ for $d \ge 9$, and (*i*) is proved.

We next prove (*ii*). Observe that $f_4''(x) = 2(3d-n-14) < 0$ for $n \ge 3d-8$. Hence, we have $3f_4'(x) \le 3f_4'(\lceil (2n+13-3d)/3 \rceil) \le 3f_4'((2n+13-3d)/3) = -(n+14-3d)^2 < 0$ for $n \ge 3d-8$. The latter confirms (*ii*).

This completes the proof. □

3. The proof of Theorem 1.1

In this section we consider our main result related to trees, that is Theorem 1.1. Prior to that, we need some additional notations and results.

We now list some relevant degree sequences:

$$\pi_1 = \left(\lfloor (n-1)/3 \rfloor, \lfloor (n-1)/3 \rfloor, n+5-d-2\lfloor (n-1)/3 \rfloor, 2^{(d-4)}, 1^{(n+1-d)}\right),$$

$$\pi_2 = \left(\lceil (n+3-d)/2 \rceil, \lfloor (n+3-d)/2 \rfloor, 2^{(d-3)}, 1^{(n+1-d)}\right),$$

$$\pi_3 = \left(d_1, \lfloor (n-1)/3 \rfloor, \lceil 2(n+8)/3 \rceil - d - d_1, 2^{(d-4)}, 1^{(n+1-d)}\right),$$

$$\pi_4 = \left(d_1, n+3-d-d_1, 2^{(d-3)}, 1^{(n-d+1)}\right),$$

$$\pi_5 = \left(\lceil (d_1+d_2)/2 \rceil, \lfloor (d_1+d_2)/2 \rfloor, d_3, \ldots, d_n\right),$$

$$\pi_6 = \left(\lceil (d_1+d_2)/2 \rceil, \lfloor (d_1+d_2)/2 \rfloor, n+5-d-(d_1+d_2), 2^{(d-4)}, 1^{(n+1-d)}\right),$$

$$\pi_7 = (\lfloor (n-1)/3 \rfloor, \lceil (2n+10-3d)/3 \rceil, 2^{(d-3)}, 1^{(n+1-d)}), \text{ and}$$

$$\pi_8 = (n+1-d, 2^{(d-2)}, 1^{(n+1-d)}).$$

Let $\mathcal{T}_{n,d}$ be the class of n-trees with diameter d. For a graph $G \in \mathcal{T}_{n,d}$, let x_0 and x_d be two vertices of G at diametral distance d and let $\overline{P} = x_0x_1 \ldots x_d \cong P_{d+1}$ be the (unique) path from x_0 to x_d. If $d_1 \ge d_2 \ge \cdots \ge d_{d-1} \ge 2$ and $d_d = d_{d+1} = \cdots = d_n = 1$, then let $\overline{T}$ be the tree obtained from $\overline{P}$ by attaching $d_1-2, d_2-2, \ldots, d_{d-1}-2$ isolated vertices to $x_1, x_2, \ldots, x_{d-1}$, respectively (cf. Fig. 3.1). This implies that $\overline{T}$ is a tree of $\mathcal{T}_{n,d}$ with $\pi(\overline{T}) = (d_1, d_2, \ldots, d_n)$. From this fact, let G_i with $G_i \in \mathcal{T}_{n,d}$ the tree corresponding to $\overline{T}$ such that $\pi(G_i) = \pi_i$, where $1 \le i \le 8$ and $i \ne 5$.

For the remainder of this section, let G be a graph with maximum Lanzhou index among all trees in $\mathcal{T}_{n,d}$, and let $\pi(G) = (d_1, d_2, \ldots, d_n)$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $d(v_i) = d_i = d_i(G)$ for $1 \le i \le n$.

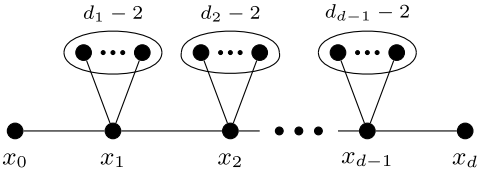


Fig. 3.1. The graph $\overline{T}$.

Lemma 3.1. *If $d \geq 8$, $n \geq 3d-12$ and $2 \leq \Delta(G) \leq (n-1)/3$, then $\pi(G) = \pi_1$.*

Proof. We first show that

$$2 \leq n+5-d-2\lfloor (n-1)/3 \rfloor \leq \lfloor (n-1)/3 \rfloor. \tag{3.1}$$

Observe that $(n-3)/3 \leq \lfloor (n-1)/3 \rfloor \leq (n-1)/3$ for $n \in \mathbb{N}^*$. If $d \geq 8$ and $n \geq 3d-11$, then $n+5-d-2\lfloor (n-1)/3 \rfloor - \lfloor (n-1)/3 \rfloor \leq n+5-d-3((n-3)/3) = 8-d \leq 0$ and $n+5-d-2\lfloor (n-1)/3 \rfloor - 2 \geq n+3-d-2((n-1)/3) = (n-3d+11)/3 \geq 0$. Thus, Equation (3.1) holds. Assume next that $n = 3d-12$, and so $\lfloor (n-1)/3 \rfloor = d-5 = (n-3)/3$. Since $n+5-d-2\lfloor (n-1)/3 \rfloor - \lfloor (n-1)/3 \rfloor = n+5-d-3((n-3)/3) = 8-d \leq 0$ and $n+5-d-2\lfloor (n-1)/3 \rfloor - 2 = n+3-d-2((n-3)/3) = 1 > 0$, as $d \geq 8$ and $n = 3d-12$. Thus, Equation (3.1) again holds.

Consider $\pi_1 = (d_1', d_2', \ldots, d_n')$ and let $\pi(G) \neq \pi_1$. By Lemma 2.1 and Corollary 2.2, it suffices to show that $\pi(G) \lhd \pi_1$. In view of Definition 2.2, assume to the contrary that there exists j_0 with $1 \leq j_0 \leq n$ such that $\sum_{i=1}^{j_0} d_i' < \sum_{i=1}^{j_0} d_i$. Since $\operatorname{diam}(G) = d$, G contains a path of length d, which implies that $d_1 \geq d_2 \geq \cdots \geq d_{d-1} \geq 2$.

For $4 \leq j \leq d-1$, we have $\sum_{i=1}^{j} d_i \leq 2(n-1) - (n-d+1) - 2(d-j-1) = n-d+2j-1 = \sum_{i=1}^{j} d_i'$. For $d \leq j \leq n$, we have $\sum_{i=1}^{j} d_i \leq 2(n-1) - (n-j) = n+j-2 = \sum_{i=1}^{j} d_i'$. Thus, by the choice of j_0, we have $1 \leq j_0 \leq 3$. Combining this with $\Delta(G) \leq (n-1)/3$, we have $j_0 = 3$ and so $\sum_{i=1}^{3} d_i' < \sum_{i=1}^{3} d_i$. Recall that $d_1 \geq d_2 \geq \cdots \geq d_{d-1} \geq 2$. Thus, $\sum_{i=1}^{n} d_i > \sum_{i=1}^{3} d_i' + 2(d-4) + (n-d+1) = 2(n-1)$, a contradiction. □

Lemma 3.2. *If $d \geq 8$, $3d/2 - 2 \leq n \leq 3d-13$ and $2 \leq \Delta(G) \leq (n-1)/3$, then $\pi(G) = \pi_7$.*

Proof. Since $d_{d-1} \geq 2$ and $\Delta(G) \leq (n-1)/3$, it suffices to show that

$$2 \leq \lceil (2n+10-3d)/3 \rceil \leq \lfloor (n-1)/3 \rfloor. \tag{3.2}$$

Since $3d/2 - 2 \leq n$, we have $\lceil (2n+10-3d)/3 \rceil - 2 \geq \lceil (3d-4+10-3d-6)/3 \rceil = 0$, and so the left inequality of (3.2) holds. If $n \leq 3d-15$, then $\lceil (2n+10-3d)/3 \rceil - \lfloor (n-1)/3 \rfloor \leq (2n+12-3d)/3 - (n-3)/3 = (n+15-3d)/3 \leq 0$. If $3d-14 \leq n \leq 3d-13$, then we have $\lceil (2n+10-3d)/3 \rceil - \lfloor (n-1)/3 \rfloor \leq d-5-(d-5) = 0$. Now, we can conclude that (3.2) holds, implying that $\pi(G) = \pi_7$. □

Lemma 3.3. *If $d \geq 8$, $n \geq 3d-9$ and $\Delta(G) > (n-1)/3$, then $\pi(G) = \pi_2$.*

Proof. Denote by $\pi_2 = (d_1', d_2', \ldots, d_n')$. Recall that $\pi(G) = (d_1, d_2, \ldots, d_n)$. Since $d_1 \geq d_2 \geq d_3 \geq \cdots \geq d_{d-1} \geq 2$ and $d_d \geq d_{d+1} \geq \cdots \geq d_n \geq 1$, we have $d_1 \leq n-d+1$. We first show that

$$d_3 < \lfloor (n-1)/3 \rfloor \leq (n-1)/3 \leq \lfloor (n-d+3)/2 \rfloor. \tag{3.3}$$

First, we assume that $d_3 \geq \lfloor (n-1)/3 \rfloor \geq (n-3)/3$. Since $\Delta(G) > (n-1)/3$ and $d \geq 8$, it follows that

$$2(n-1) > (n-1)/3 + 2 \times (n-3)/3 + 2(d-4) + n + 1 - d > 2n + d - 10 \geq 2(n-1),$$

a contradiction. This implies that $d_3 < \lfloor (n-1)/3 \rfloor$. Secondly, we will show that $\lfloor (n-d+3)/2 \rfloor \geq (n-1)/3$. If $n \geq 3d-8$, then $(n-d+3)/2 \geq (n-d+2)/2 \geq (n-1)/3$. Otherwise, $n = 3d-9$. In this case, $\lfloor (n-d+3)/2 \rfloor = d-3 > (n-1)/3$, and thus (3.3) holds.

Case 1. $d_1 > (n-1)/3$ and $d_2 \leq (n-1)/3$. Then, $d_2 \leq \lfloor (n-1)/3 \rfloor$. Since $\lceil (2n+10-3d)/3 \rceil - (n-1)/3 \geq (2n+10-3d)/3 - (n-1)/3 = (n+11-3d)/3 \geq \frac{2}{3} > 0$, we have $(n-1)/3 < \lceil (2n+10-3d)/3 \rceil$.

Subcase 1.1. $d_1 \leq \lceil (2n+10-3d)/3 \rceil$.

We claim that $\pi(G) \trianglelefteq \pi_3$. Since $d_1 \geq d_2 \geq d_3 \geq \cdots \geq d_{d-1} \geq 2$ and $d_2 \leq \lfloor (n-1)/3 \rfloor$, it suffices to show that

$$2 \leq \lceil 2(n+8)/3 \rceil - d - d_1 < \lfloor (n-1)/3 \rfloor. \tag{3.4}$$

Since $\lceil 2(n+8)/3 \rceil \leq 2(n+9)/3$ and $\lfloor (n-1)/3 \rfloor \geq (n-3)/3$, we have $\lfloor (n-1)/3 \rfloor - (\lceil 2(n+8)/3 \rceil - d - d_1) \geq (n-3)/3 + d + d_1 - 2(n+9)/3 = (3d+3d_1-n-21)/3 > (3d-22)/3 > 0$, as $d \geq 8$. Thus, the upper bound of (3.4) holds. Since $d_1 \leq \lceil (2n+10-3d)/3 \rceil$, we have $\lceil 2(n+8)/3 \rceil - d - d_1 - 2 \geq \lceil 2(n+8)/3 \rceil - d - \lceil (2n+10-3d)/3 \rceil - 2 = 0$. This implies that (3.4) holds and so $\pi(G) \trianglelefteq \pi_3$.

Since $\pi(G) \trianglelefteq \pi_3$, we have $(d_2, d_3, \dots, d_n) \trianglelefteq (\lfloor (n-1)/3 \rfloor, \lceil 2(n+8)/3 \rceil - d - d_1, 2^{(d-4)}, 1^{(n+1-d)})$. By Lemma 2.1 and $d_2 \le \lfloor (n-1)/3 \rfloor$, we have $Lz(G) \le Lz(G_3) = f_1(d_1)$. Since $(n-1)/3 < d_1 \le \lceil (2n+10-3d)/3 \rceil$, we further have $Lz(G) \le Lz(G_3) = f_1(d_1) \le f_1(\lceil (2n+10-3d)/3 \rceil)$ by Lemma 2.3 (i). Next, we will show that

$$Lz(G_2) \ge f_1(\lceil (2n+10-3d)/3 \rceil) \ge Lz(G_3) \ge Lz(G). \tag{3.5}$$

Since $\pi(G_2) = \pi_2$ and $\varphi(x) = x^2(n-1-x)$, we have $Lz(G_2) - f_1(\lceil (2n+10-3d)/3 \rceil) = \varphi(\lceil (n+3-d)/2 \rceil) + \varphi(\lfloor (n+3-d)/2 \rfloor) - \varphi(\lceil (2n+10-3d)/3 \rceil) - \varphi(\lfloor (n-1)/3 \rfloor)$. If $n = 3d-9$, then we have $Lz(G_2) - f_1(\lceil (2n+10-3d)/3 \rceil) = 2\varphi(d-3) - \varphi(d-2) - \varphi(d-4) = 2 > 0$. It suffices to consider the case of $n \ge 3d-8$.

Since $\lceil (n+3-d)/2 \rceil + \lfloor (n+3-d)/2 \rfloor = n+3-d = (n-d+4)/2 + (n-d+2)/2$, we have $(\lceil (n+3-d)/2 \rceil, \lfloor (n+3-d)/2 \rfloor) \trianglelefteq ((n+4-d)/2, (n+2-d)/2)$ by Definition 2.2. Note that $n \ge 3d-8$. Thus, $\lfloor (n+3-d)/2 \rfloor \ge (n+2-d)/2 \ge (n-1)/3$. By Lemma 2.1, we have $Lz(G_2) - f_1(\lceil (2n+10-3d)/3 \rceil) \ge \varphi((n+4-d)/2) + \varphi((n+2-d)/2) - \varphi(\lceil (2n+10-3d)/3 \rceil) - \varphi(\lfloor (n-1)/3 \rfloor) = \psi_1(n)$.

If $(n-1) \equiv 0 \pmod 3$, then $\psi_1(n) = \varphi((n-d+4)/2) + \varphi((n-d+2)/2) - \varphi((2n+10-3d)/3) - \varphi((n-1)/3)$. Since $6\psi_1''(n) = n+11-3d > 0$ and $2\psi_1'(n) \ge 2\psi_1'(3d-8) = 1 > 0$, we have $\psi_1(n) \ge \psi_1(3d-8) = 0$. By the choice of G, we have $\psi_1(n) = 0$ and so $n = 3d-8$. This implies that $\pi_2 = \pi_3$.

If $(n-1) \equiv 1 \pmod 3$, then $\psi_1(n) = \varphi((n-d+4)/2) + \varphi((n-d+2)/2) - \varphi((2n+11-3d)/3) - \varphi((n-2)/3)$. Since $18\psi_1''(n) = 3n - 9d + 37 > 0$ and $18\psi_1'(n) \ge 18\psi_1'(3d-8) = 23 > 0$, we have $3\psi_1(n) \ge 3\psi_1(3d-8) = 4 > 0$. If $(n-1) \equiv 2 \pmod 3$, then we have $\psi_1(n) = \varphi((n-d+4)/2) + \varphi((n-d+2)/2) - \varphi((2n+12-3d)/3) - \varphi((n-3)/3)$. Since $18\psi_1''(n) = 3n - 9d + 41 > 0$ and $18\psi_1'(n) \ge 18\psi_1'(3d-8) = 41 > 0$, we have $3\psi_1(n) \ge 3\psi_1(3d-8) = 10 > 0$. This implies that (3.5) holds.

Subcase 1.2 $\lceil (2n+10-3d)/3 \rceil < d_1 \le n+1-d$.

Since $\lceil (2n+10-3d)/3 \rceil < d_1 \le n-d+1$, we have $2 \le n+3-d-d_1 < n+3-d-\lceil (2n+10-3d)/3 \rceil = \lfloor (n-1)/3 \rfloor < d_1$. Combining this with $d_1 \ge d_2 \ge d_3 \ge \cdots \ge d_{d-1} \ge 2$, we have $\pi(G) \trianglelefteq \pi_4$. This implies that $(d_2, d_3, \dots, d_n) \trianglelefteq (n+3-d-d_1, 2^{(d-3)}, 1^{(n-d+1)})$. Since $n+3-d-d_1 < \lfloor (n-1)/3 \rfloor$, we have $Lz(G) \le Lz(G_4) = f_2(d_1)$, where $\pi(G_4) = \pi_4$.

Since $\lceil (2n+10-3d)/3 \rceil < d_1 \le n-d+1$, we have

$$Lz(G) \le Lz(G_4) = f_2(d_1) < f_2(\lceil (2n+10-3d)/3 \rceil)$$

by Lemma 2.3 (ii). By Lemma 2.3 and (3.5), we have

$$Lz(G) \le Lz(G_4) < f_2(\lceil (2n+10-3d)/3 \rceil) = f_1(\lceil (2n+10-3d)/3 \rceil) \le Lz(G_2). \tag{3.6}$$

Case 2. $d_1 \ge d_2 > (n-1)/3$. If $d_1 + d_2 > n+3-d$, then $2(n-1) > n+3-d+2(d-3)+(n-d+1) = 2(n-1)$ (as $d_1 \ge d_2 \ge \cdots \ge d_{d-1} \ge 2$), a contradiction. Thus, $d_1 + d_2 \le n+3-d$.

Note that $d_1 \ge \lceil (d_1+d_2)/2 \rceil \ge \lfloor (d_1+d_2)/2 \rfloor \ge d_2$ and $\lceil (d_1+d_2)/2 \rceil + \lfloor (d_1+d_2)/2 \rfloor = d_1 + d_2$. Since $(n-1)/3 < d_1$ and $d \ge 8$, we have $2 \le n+5-d-(d_1+d_2) < n+5-d-2((n-1)/3) < (n-1)/3 < d_2$. Now, we can conclude that $\pi_5 \trianglelefteq \pi_6$ and $\pi_5 \trianglelefteq \pi(G)$, as $d_{d-1} \ge 2$. Since $d_{d-1} \ge 2$, we can construct the corresponding G_5 with $\pi(G_5) = \pi_5$.

Since $(\lceil (d_1+d_2)/2 \rceil, \lfloor (d_1+d_2)/2 \rfloor) \trianglelefteq (d_1, d_2)$ and $d_1 + d_2 = \lceil (d_1+d_2)/2 \rceil + \lfloor (d_1+d_2)/2 \rfloor$, we have

$$(d_3, d_4, \dots, d_n) \trianglelefteq (n+5-d-(d_1+d_2), 2^{(d-4)}, 1^{(n-d+1)}).$$

Note that $\lceil (d_1+d_2)/2 \rceil \ge \lfloor (d_1+d_2)/2 \rfloor \ge d_2 > (n-1)/3$ and $n+5-d-(d_1+d_2) \le \lfloor (n-1)/3 \rfloor$. Thus, $Lz(G) \le Lz(G_5) \le Lz(G_6)$ by Lemma 2.1.

Let $d_1 + d_2 = x$. Then, $x > 2(n-1)/3$. If $d_1 + d_2$ is even, then $Lz(G_6) = 2\varphi(x/2) + \varphi(n+5-d-x) + (d-4)\varphi(2) + (n-d+1)\varphi(1) = g_1(x)$. If $d_1 + d_2$ is odd, then $Lz(G_6) = \varphi((x+1)/2) + \varphi((x-1)/2) + \varphi(n+5-d-x) + (d-4)\varphi(2) + (n-d+1)\varphi(1) = g_2(x)$.

Since $d \ge 8$ and $x > 2(n-1)/3$, we have $2g_1''(x) = 2g_2''(x) = 3(4d-2n+3x-22) > 12(d-6) > 0$. Hence, $g_1'(x) > g_1'(2(n-1)/3) = 3(d-6)^2 > 0$ and $4g_2'(x) > 4g_2'(2(n-1)/3) = 3(2d-11)(2d-13) > 0$. Combining this with $d_1 + d_2 \le n+3-d$, it follows that $Lz(G_2) - Lz(G_6) \ge Lz(G_2) - g_1(n+3-d) = 0$ if $d_1 + d_2$ is even and $Lz(G_2) - Lz(G_6) \ge Lz(G_2) - g_2(n+3-d) = 0$ if $d_1 + d_2$ is odd, with equality if and only if $\pi_2 = \pi_6$. □

Lemma 3.4. *If $d \ge 8$, $n \le 3d-10$ and $\Delta(G) > (n-1)/3$, then $\pi(G) = \pi_4$.*

Proof. Since $d_{d-1} \ge 2$ and $d_1 > (n-1)/3$, it suffices to show that $2 \le n+3-d-d_1 < \lfloor (n-1)/3 \rfloor$ by Lemma 2.1. Since $d_1 \le n-d+1$, we have $n+3-d-d_1 \ge n+3-d-(n-d+1) = 2$. Note that $d_1 > (n-1)/3$. Thus, $n+3-d-d_1 - \lfloor (n-1)/3 \rfloor < n+3-d-(n-1)/3-(n-3)/3 = (n+13-3d)/3 \le 1$, as $n \le 3d-10$. This implies that $n+3-d-d_1 \le \lfloor (n-1)/3 \rfloor$. Now, we have $\pi(G) \trianglelefteq \pi_4$. □

Proof of Theorem 1.1. We divide the proof into the following three cases:

Case 1. $8 \le d \le (n+10)/3$. If $d_1 \le (n-1)/3$, then by Lemma 3.1, we have $Lz(G) \le Lz(G_1) = f_1(\lfloor (n-1)/3 \rfloor)$. Since $f_1'(x) > 0$ holds for $x > \lfloor (n-1)/3 \rfloor$ by Lemma 2.3 (i) and $\lfloor (n-1)/3 \rfloor < \lceil (2n+10-3d)/3 \rceil$, we have $Lz(G) \le Lz(G_1) = f_1(\lfloor (n-1)/3 \rfloor) < f_1(\lceil (2n+10-3d)/3 \rceil) = f_2(\lceil (2n+10-3d)/3 \rceil) \le Lz(G_2)$ by Lemma 2.3 and (3.6).

Next, we consider the case of $d_1 > (n-1)/3$. By Lemma 3.3, the result already holds for $n \ge 3d-9$. For $n = 3d-10$, by Lemma 3.4, we have $Lz(G) \le Lz(G_4)$. Since $\lfloor (n-1)/3 \rfloor = (n-2)/3 = d-4$, we have $d_1 \ge d-3$. Note that $f_2''(d_1) = 2(3d-n-11) < 0$ for $n = 3d-10$. Thus, $f_2'(d_1) \le f_2'(d-3) = (n+11-3d)(n+9-3d) < 0$, as $d_1 \ge d-3$. Since $\lceil (n-d+3)/2 \rceil = d-3$, it follows that $Lz(G_2) - Lz(G_4) = f_2(d-3) - f_2(d_1) \ge 0$, where equality occurs iff $\pi(G) = \pi_2$.

Case 2. $(n+11)/3 \le d < 2(n+2)/3$. If $n = 3d-11$, then by Lemmas 3.1 and 3.4, we have $Lz(G) \le Lz(G_1) = f_1(\lfloor (n-1)/3 \rfloor) = Lz(G_4)$ (Here, π_1 is a special case of π_7). Next, we consider the case of $(n+12)/3 \le d < 2(n+2)/3$.

We first suppose that $\Delta(G) > (n-1)/3$. By Lemma 3.4, we have $Lz(G) \le Lz(G_4)$. It suffices to show that

$$Lz(G_4) \le Lz(G_8), \tag{3.7}$$

with equality if and only if $\pi_4 = \pi_8$. By Lemma 2.3 (*iii*), we have $f_2(d_1) \le f_2(n-d+1) = Lz(G_8)$ for $\lfloor (n-1)/3 \rfloor + 1 \le d_1 \le n-d+1$. This means that $Lz(G_8) - Lz(G_4) = f_2(n-d+1) - f_2(d_1) \ge 0$, with equality if and only if $d_1 = n-d+1$, that is, with equality if and only if $\pi_4 = \pi_8$. Thus, (3.7) holds.

Next, we suppose that $\Delta(G) \le (n-1)/3$. If $n = 3d-12$, then $\lfloor (n-1)/3 \rfloor = d-5$. Since $d \ge 8$, we have $Lz(G_1) - Lz(G_8) = 2\varphi(\lfloor (n-1)/3 \rfloor) + \varphi(n+5-d-2\lfloor (n-1)/3 \rfloor) - \varphi(n-d+1) - 2\varphi(2) = 2\varphi(d-5) + \varphi(3) - \varphi(2d-11) - 2\varphi(2) = -2(2d-13)(d-7) < 0$. Combining this with Lemma 3.1, we have $Lz(G) \le Lz(G_1) < Lz(G_8)$. Otherwise, $(n+13)/3 \le d < 2(n+2)/3$. Since $f_2'(x) \ge 0$ holds for $x \ge \lfloor (n-1)/3 \rfloor$ by Lemma 2.3 (*iv*) and $\lfloor (n-1)/3 \rfloor < n-d+1$, we have $Lz(G) \le Lz(G_7) = f_2(\lfloor (n-1)/3 \rfloor) < f_2(n-d+1) = Lz(G_8)$ by Lemma 3.2.

Case 3. $2(n+2)/3 \le d \le n-1$. Note that $n-d+1-(n-1)/3 = (2n+4-3d)/3 \le 0$, as $2(n+2)/3 \le d$. Thus, $n-d+1 \le (n-1)/3$.

Suppose that $\pi_8 = (d_1', d_2', \dots, d_n')$ and $\pi_8 \ne \pi(G)$. Since $d_1 \le n-d+1 \le (n-1)/3$, by Lemma 2.1 and Corollary 2.2, it suffices to show that $\pi(G) \lhd \pi_8$. By Definition 2.2, assume to the contrary, that there exists j_0 with $1 \le j_0 \le n$ such that $\sum_{i=1}^{j_0} d_i' < \sum_{i=1}^{j_0} d_i$.

For $2 \le j \le d-1$, we have $\sum_{i=1}^{j} d_i \le 2(n-1) - (n-d+1) - 2(d-j-1) = n-d+2j-1 = \sum_{i=1}^{j} d_i'$. For $d \le j \le n$, we have $\sum_{i=1}^{j} d_i \le 2(n-1) - (n-j) = n+j-2 = \sum_{i=1}^{j} d_i'$. Thus, by the choice of j_0, we have $j_0 = 1$, that is, $d_1 > d_1'$. Recall that $n-d+1 = d_1' \ge d_2' \ge \cdots \ge d_{d-1}' \ge 2$. Thus, we have $\sum_{i=1}^{n} d_i > d_1' + 2(d-2) + (n-d+1) = 2(n-1)$, a contradiction. □

4. The proof of Theorem 1.2

In this section we focus on unicyclic n-graphs with diameter d. Similarly to the previous section, we denote by $\mathcal{U}_{n,d}$ the class of such graphs. Let $G \in \mathcal{U}_{n,d}$ and let $P_{d+1} = x_0x_1 \cdots x_d$ be a shortest path of length d from x_0 to x_d and $N_{P_{d+1}}$ be the set of vertices of $V(P_{d+1})$ whose degree is at least 2 in G. It is not hard to see that

$$d-1 \le \left| N_{P_{d+1}} \right| \le d+1. \tag{4.1}$$

Let $p(G)$ be the number of pendant vertices of G. From ([17], Lemma 5.3), we can deduce the following useful lemma.

Lemma 4.1 *([17]). If $G \in \mathcal{U}_{n,d}$ and C_g is the unique cycle of G, then $p(G) \le n-d$, and the equality occurs when x_0 and x_d have both degree 1, $g \in \{3,4\}$ and $\left| V(P_{d+1}) \cap V(C_g) \right| = g-1$.*

Lemma 4.2. *Let $\pi = (d_1, d_2, \dots, d_n)$ a unicyclic degree sequence. If $d_1 \ge d_2 \ge 3$ and $d_3 \ge \cdots \ge d_d \ge 2 > 1 = d_{d+1} = \cdots = d_n$, then there exists a unicyclic graph $\overline{U}$ with $\pi(\overline{U}) = \pi$ and $\mathrm{diam}(\overline{U}) = d$, where $d \ge 4$.*

Proof. Let $P_{d+1} = x_0x_1 \dots x_d$ be the path of length d. Firstly, we construct U^* from P_{d+1} by adding one new vertex z and two edges zx_1 and zx_2. Next, we define $\overline{U}$ as the unicyclic graph obtained from U^* by attaching d_1-3, d_2-3, and d_d-2 isolated vertices to x_1, x_2 and z, respectively, and then attaching d_j-2 vertices to x_j for $3 \le j \le d-1$ (cf. Fig. 4.1). Now, one can easily check that $\overline{U}$ is a unicyclic graph as required. □

For the remainder of this section, we assume that G is a unicyclic graph with maximum Lanzhou index among all unicyclic graphs in $\mathcal{U}_{n,d}$, and let $\pi(G) = (d_1, d_2, \dots, d_n)$, where $V(G) = \{v_1, v_2, \dots, v_n\}$ and $d(v_i) = d_i = d_i(G)$ for $1 \le i \le n$. In the sequel we consider the subsequent degree sequences:

$$\begin{aligned}
\pi_9 &= \left(\lfloor (n-1)/3 \rfloor, \lfloor (n-1)/3 \rfloor, n+6-d-2\lfloor (n-1)/3 \rfloor, 2^{(d-3)}, 1^{(n-d)}\right),\\
\pi_{10} &= \left(\lceil (n+4-d)/2 \rceil, \lfloor (n+4-d)/2 \rfloor, 2^{(d-2)}, 1^{(n-d)}\right),\\
\pi_{11} &= \left(d_1, \lfloor (n-1)/3 \rfloor, \lceil (2n+19-3d-3d_1)/3 \rceil, 2^{(d-3)}, 1^{(n-d)}\right),\\
\pi_{12} &= \left(d_1, n+4-d-d_1, 2^{(d-2)}, 1^{(n-d)}\right),\\
\pi_{13} &= \left(\lceil (d_1+d_2)/2 \rceil, \lfloor (d_1+d_2)/2 \rfloor, d_3, \dots, d_n\right), \text{ and}\\
\pi_{14} &= \left(\lceil (d_1+d_2)/2 \rceil, \lfloor (d_1+d_2)/2 \rfloor, n+6-d-d_1-d_2, 2^{(d-3)}, 1^{(n-d)}\right).
\end{aligned}$$

Since G is a graph of $\mathcal{U}_{n,d}$ with degree sequence $(d_1, d_2, \dots, d_n)$, we have $p(G) \le n-d$ by Lemma 4.1. We claim that $d_1 \le n-d+1$. Otherwise, by contradiction, assume that $d_1 \ge n-d+2$. Since $p(G) \le n-d$, we have $d_2 \ge d_3 \ge \cdots \ge d_d \ge 2$. Combining this with $d_1 \ge n-d+2$, it follows that $2n \ge n-d+2(d-1)+2-d+n = 2n$ by (1.1), and thus $p(G) = n-d$. Since $p(G) = n-d$, we have $d_1 \ge d_2 \ge 3$ by Lemma 4.1. Thus, from (1.1), we can deduce that $2n \ge n-d+2+3+2(-2+d)-d+n = 2n+1$, a contradiction. Now, we can conclude that

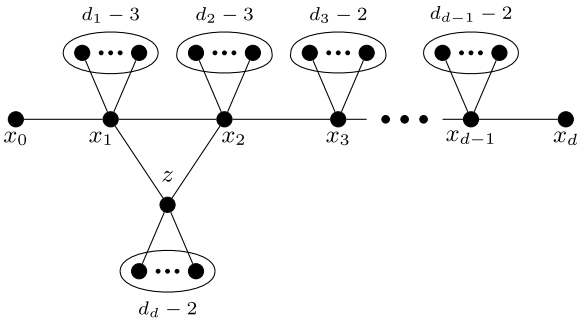


Fig. 4.1. The graph $\overline{U}$.

$$p(G) \le n-d \text{ and } d_1 \le n+1-d. \tag{4.2}$$

From Lemma 4.2 and Equation (4.2), if $d \ge 9$ and $n \ge 3d-8$, then let G_i be the unicyclic graph corresponding to $\overline{U}$ such that $\pi(G_i) = \pi_i$ and $\mathrm{diam}(G_i) = d$, where $9 \le i \le 12$.

Lemma 4.3. *If $d \ge 9$, $n \ge 3d-8$ and $2 \le \Delta(G) \le (n-1)/3$, then $\pi(G) = \pi_9$.*

Proof. We claim that

$$2 \le n+6-d-2\lfloor (n-1)/3 \rfloor \le \lfloor (n-1)/3 \rfloor. \tag{4.3}$$

Note that $(n-3)/3 \le \lfloor (n-1)/3 \rfloor \le (n-1)/3$, as $n \in \mathbb{N}^*$. If $d \ge 9$ and $n \ge 3d-8$, then $n+6-d-2\lfloor (n-1)/3 \rfloor - \lfloor (n-1)/3 \rfloor \le n+6-d-3((n-3)/3) = 9-d \le 0$ and $n+6-d-2\lfloor (n-1)/3 \rfloor - 2 \ge n+4-d-2((n-1)/3) = (n+14-3d)/3 > 0$. Thus, (4.3) holds.

Suppose that $\pi_9 = (d_1', d_2', \ldots, d_n')$ with $\pi_9 \ne \pi(G)$. By Lemma 2.1 and Corollary 2.2, it suffices to show that $\pi(G) \lhd \pi_9$. Assume to the conversely, that there exists j_0 with $1 \le j_0 \le n$ such that $\sum_{i=1}^{j_0} d_i' < \sum_{i=1}^{j_0} d_i$.

For $4 \le j \le d$, we have $\sum_{i=1}^{j} d_i \le 2n-(n-d)-2(d-j) = n-d+2j = \sum_{i=1}^{j} d_i'$. For $d+1 \le j \le n$, we have $\sum_{i=1}^{j} d_i \le 2n-(n-j) = n+j = \sum_{i=1}^{j} d_i'$. Thus, by the choice of j_0, we have $1 \le j_0 \le 3$. Combining this with $\Delta(G) \le (n-1)/3$, we have $j_0 = 3$ and so $\sum_{i=1}^{3} d_i' < \sum_{i=1}^{3} d_i$. On the other hand, since $d_1 \ge d_2 \ge \cdots \ge d_d \ge 2$ by (4.2), we have $\sum_{i=1}^{n} d_i > \sum_{i=1}^{3} d_i' + 2(d-3) + (n-d) = 2n$, a contradiction. □

Lemma 4.4. *If $d \ge 9$, $n \ge 3d-8$ and $\Delta(G) > (n-1)/3$, then $\pi(G) = \pi_{10}$*

Proof. We first show that

$$d_3 < \lfloor (n-1)/3 \rfloor \le (n-1)/3 \le \lfloor (n-d+4)/2 \rfloor. \tag{4.4}$$

Since $n \ge 3d-8$, we have $\lfloor (n-d+4)/2 \rfloor \ge (n-d+2)/2 \ge (n-1)/3$. Thus, to show (4.4), it suffices to show $d_3 < \lfloor (n-1)/3 \rfloor$. By contradiction, assume that $d_3 \ge \lfloor (n-1)/3 \rfloor \ge (n-3)/3$. By (4.2), we have $p(G) \le n-d$, and thus $d_2 \ge d_3 \ge \cdots \ge d_d \ge 2$. Since $\Delta(G) > (n-1)/3$ and $d \ge 9$, it follows that

$$2n > (n-1)/3 + 2 \times ((n-3)/3) + 2(d-3) + n - d > 2n + d - 9 \ge 2n,$$

a contradiction. This implies that $d_3 < \lfloor (n-1)/3 \rfloor$. Thus (4.4) holds.

Case 1. $d_1 > (n-1)/3$ and $d_2 \le (n-1)/3$. Then, $d_2 \le \lfloor (n-1)/3 \rfloor$. Recall that $d_1 \le n+1-d$ by (4.2), we consider the following two cases.

Subcase 1.1. $d_1 \le \lceil (2n+13-3d)/3 \rceil$.

Since $\lceil (2n+13-3d)/3 \rceil - (n-1)/3 \ge (2n+13-3d)/3 - (n-1)/3 = (n-3d+14)/3 \ge 2 > 0$, we have $(n-1)/3 < \lceil (2n+13-3d)/3 \rceil$.

We claim that $\pi \trianglelefteq \pi_{11}$. Since $d_1 \ge d_2 \ge d_3 \ge \cdots \ge d_d \ge 2$ by (4.2) and $d_2 \le \lfloor (n-1)/3 \rfloor$, it suffices to show that

$$2 \le \lceil (2n+19-3d-3d_1)/3 \rceil < \lfloor (n-1)/3 \rfloor. \tag{4.5}$$

Since $\lceil (2n+19)/3 \rceil \le (2n+21)/3$ and $\lfloor (n-1)/3 \rfloor \ge (n-3)/3$, we have $\lfloor (n-1)/3 \rfloor - (\lceil (2n+19-3d-3d_1)/3 \rceil) \ge (n-3)/3 + d + d_1 - (2n+21)/3 = (3d+3d_1-n-24)/3 > (3d-25)/3 > 0$, as $d \ge 9$. Since $d_1 \le \lceil (2n+13-3d)/3 \rceil$, we have $\lceil (2n+19-3d-3d_1)/3 \rceil - 2 \ge \lceil (2n+19-3d)/3 \rceil - \lceil (2n+13-3d)/3 \rceil - 2 = 0$. This implies that (4.5) holds and so $\pi \trianglelefteq \pi_{11}$.

Since $\pi \trianglelefteq \pi_{11}$, we have $(d_2, d_3, \ldots, d_n) \trianglelefteq (\lfloor (n-1)/3 \rfloor, \lceil (2n+19-3d-3d_1)/3 \rceil, 2^{(d-3)}, 1^{(n-d)})$. Note that $(n-1)/3 < d_1 \le \lceil (2n+13-3d)/3 \rceil$. Thus, $f_3(\lceil (2n+13-3d)/3 \rceil) \ge f_3(d_1)$ by Lemma 2.4 (i). Considering this together with Lemma 2.1, we have $Lz(G) \le Lz(G_{11}) = f_3(d_1) \le f_3(\lceil (2n+13-3d)/3 \rceil)$.

Next, we will show that

$$Lz(G_{10}) \geq f_3(\lceil (2n+13-3d)/3 \rceil) \geq Lz(G_{11}) \geq Lz(G). \tag{4.6}$$

By an elementary computation, we have

$$Lz(G_{10}) - f_3(\lceil (2n+13-3d)/3 \rceil) = \varphi(\lceil (n-d+4)/2 \rceil) + \varphi(\lfloor (n-d+4)/2 \rfloor) - (\varphi(\lceil (2n+13-3d)/3 \rceil) + \varphi(\lfloor (n-1)/3 \rfloor)),$$

where $\varphi(x) = x^2(n-1-x)$. Note that $\lceil (n+4-d)/2 \rceil + \lfloor (n+4-d)/2 \rfloor = n+4-d = (n+6-d)/2 + (n+2-d)/2$ and $\lfloor (n+4-d)/2 \rfloor \geq (n+2-d)/2 \geq (n-1)/3$, we have $(\lceil (n+4-d)/2 \rceil, \lfloor (n+4-d)/2 \rfloor) \trianglelefteq ((n+6-d)/2, (n+2-d)/2)$ by Definition 2.2. Now, by Lemma 2.1, we have $Lz(G_{10}) - f_3(\lceil (2n+10-3d)/3 \rceil) \geq \varphi((n+6-d)/2) + \varphi((n+2-d)/2) - (\varphi(\lceil (2n+13-3d)/3 \rceil) + \varphi(\lfloor (n-1)/3 \rfloor)) = \psi_2(n)$.

If $(n-1) \equiv 0 \pmod 3$, then we have $\psi_2(n) = \varphi((n+6-d)/2) + \varphi((n+2-d)/2) - \varphi((2n+13-3d)/3) - \varphi((n-1)/3)$. Since $6\psi_2''(n) = n+14-3d > 0$ and $\psi_2'(n) \geq \psi_2'(3d-8) = 2 > 0$, we have $\psi_2(n) \geq \psi_2(3d-8) = 0$. By the choice of G, we have $\psi_2(n) = 0$ and so $n = 3d-8$. This implies that $\pi_{10} = \pi_{11}$. If $(n-1) \equiv 1 \pmod 3$, then we have $\psi_2(n) = \varphi((n+6-d)/2) + \varphi((n+2-d)/2) - \varphi((2n+14-3d)/3) - \varphi((n-2)/3)$. Since $18\psi_2''(n) = 3n-9d+46 > 0$ and $9\psi_2'(n) \geq 9\psi_2'(3d-8) = 31 > 0$, we have $3\psi_2(n) \geq 3\psi_2(3d-8) = 14 > 0$. If $(n-1) \equiv 2 \pmod 3$, then we have $\psi_2(n) = \varphi((n+6-d)/2) + \varphi((n+2-d)/2) - \varphi((2n+15-3d)/3) - \varphi((n-3)/3)$. Since $18\psi_2''(n) = 3n-9d+50 > 0$ and $9\psi_2'(n) \geq 9\psi_2'(3d-8) = 46 > 0$, we have $3\psi_2(n) \geq 3\psi_2(3d-8) = 32 > 0$. This implies that (4.6) holds.

Case 2. $d_1 \geq d_2 > (n-1)/3$.

If $d_1 + d_2 > n+4-d$, then $2n > n+4-d+2(d-2)+(n-d) = 2n$ (as $d_1 \geq d_2 \geq \cdots \geq d_d \geq 2$), a contradiction. Thus, $d_1 + d_2 \leq n+4-d$.

Note that $d_1 \geq \lceil (d_1+d_2)/2 \rceil \geq \lfloor (d_1+d_2)/2 \rfloor \geq d_2$ and $\lceil (d_1+d_2)/2 \rceil + \lfloor (d_1+d_2)/2 \rfloor = d_1 + d_2$. Since $d_1 > (n-1)/3$ and $d \geq 9$, we have $2 = n+6-d-(n+4-d) \leq n+6-d-(d_1+d_2) < n+6-d-2((n-1)/3) = (n-1)/3+7-d < (n-1)/3-1 < \lfloor (n-1)/3 \rfloor < d_2$. Now, we have $\pi_{13} \trianglelefteq \pi(G)$ and $\pi_{13} \trianglelefteq \pi_{14}$. Since $d_1 \geq d_2 > (n-1)/3 \geq 6$, by Lemma 4.2 and (4.2), we can construct the corresponding graph G_i such that $\pi(G_i) = \pi_i$ for $13 \leq i \leq 14$ (Here, maybe G_{13} does not exist, but the proof also holds).

Since $d_1 \geq \lceil (d_1+d_2)/2 \rceil \geq \lfloor (d_1+d_2)/2 \rfloor \geq d_2$ and $\lceil (d_1+d_2)/2 \rceil + \lfloor (d_1+d_2)/2 \rfloor = d_1 + d_2$, we have $(d_3, d_4, \ldots, d_n) \trianglelefteq (n+6-d-(d_1+d_2), 2^{(d-3)}, 1^{(n-d)})$. Note that $\lceil (d_1+d_2)/2 \rceil \geq \lfloor (d_1+d_2)/2 \rfloor \geq (n-1)/3$ and $n+6-d-(d_1+d_2) \leq \lfloor (n-1)/3 \rfloor$. Thus, $Lz(G) \leq Lz(G_{13}) \leq Lz(G_{14})$ by Lemma 2.1.

Let $d_1 + d_2 = x$. Then, $x > 2(n-1)/3$. If $d_1 + d_2$ is even, then $Lz(G_{14}) = 2\varphi(x/2) + \varphi(n+6-d-x) + (d-3)\varphi(2) + (n-d)\varphi(1) = h_1(x)$. If $d_1 + d_2$ is odd, then $Lz(G_{14}) = \varphi((x+1)/2) + \varphi((x-1)/2) + \varphi(n+6-d-x) + (d-3)\varphi(2) + (n-d)\varphi(1) = h_2(x)$.

Since $d \geq 9$ and $x > 2(n-1)/3$, we have $2h_1''(x) = 2h_2''(x) = 3(4d-2n+3x-26) > 12(d-7) > 0$. Hence, we have $h_1'(x) > h_1'(2(n-1)/3) = 3(d-7)^2 > 0$ and $4h_2'(x) > 4h_2'(2(n-1)/3) = 3(2d-13)(2d-15) > 0$ by $d \geq 9$. Therefore, we have $Lz(G_{10}) - Lz(G_{14}) \geq Lz(G_{10}) - h_1(n+4-d) = 0$ if $d_1 + d_2$ is even and $Lz(G_{10}) - Lz(G_{14}) \geq Lz(G_{10}) - h_2(n+4-d) = 0$ if $d_1 + d_2$ is odd, with equality if and only if $\pi_{10} = \pi_{14}$. □

Proof of Theorem 1.2. We claim that $\pi(G) = \pi_{10}$. If $\Delta(G) > (n-1)/3$, then the result is a consequence of Lemma 4.4. We now consider the case of $\Delta(G) \leq (n-1)/3$. By Lemma 4.3, we have $Lz(G) \leq Lz(G_9) = f_3(\lfloor (n-1)/3 \rfloor)$. From $\lfloor (n-1)/3 \rfloor \leq (n-1)/3 < (2n+13-3d)/3 \leq \lceil (2n+13-3d)/3 \rceil$, we get that $Lz(G) \leq Lz(G_9) = f_3(\lfloor (n-1)/3 \rfloor) < f_3(\lceil (2n+13-3d)/3 \rceil) \leq Lz(G_{10})$ by Lemma 2.4 (i) and (4.6), that is contrary to the choice of G. This proves the claim that $\pi(G) = \pi_{10}$.

For $1 \leq i \leq d-2$ and $1 \leq j \leq d-3$, one can easily check that $C_3(n,d,i)$, $C_4(n,d,j) \in \mathcal{U}_{n,d}$ and $\pi(C_3(n,d,i)) = \pi(C_4(n,d,j)) = \pi_{10}$. Thus, it suffices to show that

$$G \in \{C_3(n,d,1), C_3(n,d,2), \ldots, C_3(n,d,d-2), C_4(n,d,1), C_4(n,d,2), \ldots, C_4(n,d,d-3)\}.$$

By the definition of π_{10} and Lemma 4.1, x_0 and x_d are pendant vertices, $g \in \{3,4\}$ and $\left|V_{P_{d+1}} \cap V(C_g)\right| = g-1$. Here, we only present the proof of $g = 3$, as the case of $g = 4$ can be shown by a similar method.

Let z_1z_2 be the sub-path of P_{d+1} intersecting with C_3, where $C_3 = z_1z_2z_3z_1$. As P_{d+1} is a shortest path between x_0 and x_d, we have $d(z_1) \geq 3$ and $d(z_2) \geq 3$. By the definition of π_{10}, it is $d_3 = 2$, and we may assume that $d(z_1) = \lceil (n+4-d)/2 \rceil$ and $d(z_2) = \lfloor (n+4-d)/2 \rfloor$. Note that x_0 and x_d are pendant vertices (in G). Thus, G consists of a C_3 by appending at z_1 a path P_k and $\lceil (n-2-d)/2 \rceil$ isolated vertices, and by appending at z_2 another path P_{d-k-1} and $\lfloor (n-2-d)/2 \rfloor$ isolated vertices, where $1 \leq k \leq d-2$. Therefore, we conclude that $G = C_3(n,d,i)$ for some i, where $1 \leq i \leq d-2$. □

5. Conclusions

In this paper we have applied the Majorization Theorem to derive the maximal graphs with respect to the Lanzhou index for the classes of trees and unicyclic graphs of prescribed order and diameter. Once again, this analytical tool has proved to be effective in the search of extremal graphs with respect to a topological index. This method can be further employed to solve similar cases as, for example, bicyclic graphs with prescribed order and diameter.

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Data availability

No data was used for the research described in the article.

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Note

Note on Sombor index of connected graphs with given degree sequence☆

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ABSTRACT

For a simple connected graph $G = (V, E)$, let $d(u)$ be the degree of the vertex u of G. The general Sombor index of G is defined as

$$SO_\alpha(G) = \sum_{uv \in E} \left[d(u)^2 + d(v)^2\right]^\alpha$$

where $SO(G) = SO_{0.5}(G)$ is the recently invented Sombor index. In this paper, we show that in the class of connected graphs with a fixed degree sequence (for which the minimum degree being equal to one), there exists a special extremal *BFS*-graph with minimum general Sombor index for $0 < \alpha < 1$ (resp. maximum general Sombor index for either $\alpha > 1$ or $\alpha < 0$). Moreover, for any given tree, unicyclic, and bicyclic degree sequences with minimum degree 1, there exists a unique extremal *BFS*-graph with minimum general Sombor index for $0 < \alpha < 1$ and maximum general Sombor index for either $\alpha > 1$ or $\alpha < 0$.

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1. Introduction

Throughout this paper we consider undirected simple connected graphs. Let G be such a graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Let $d(u) = d_G(u)$ and $N(u) = N_G(u)$ denote, respectively, the degree and neighbor set of the vertex $u \in V(G)$. If $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d(v_i)$, $1 \le i \le n$, then $\pi = (d_1, d_2, \ldots, d_n)$ is said to be the degree sequence of G. In what follows, we always suppose that $d_1 \ge d_2 \ge \cdots \ge d_n$ and denote by $\Gamma(\pi)$ the class of connected graphs with degree sequence π. A connected graph with n vertices and $n + c - 1$ edges will be referred as a c- cyclic graph. In particular, when $c = 0$, 1, and 2, a c-cyclic graph is also called a tree, unicyclic graph, and bicyclic graph, respectively.

Recently, Gutman proposed a geometric approach for interpreting degree-based graph invariants [7], and according to this approach, he introduced the so-called Sombor index, defined as,

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{(d(u)^2 + d(v)^2)}\,. \tag{1}$$

Eventually, this graph invariant attracted much attention, and in a series of researches its main mathematical properties have been determined; see, for instance [1,3–6,8,16,17,20] and the review [11].

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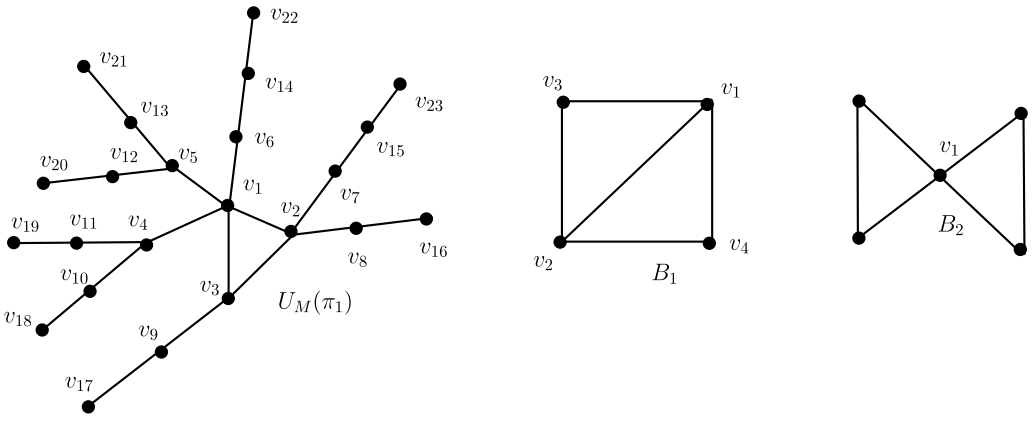


Fig. 1. The graphs $U_M(\pi_1)$, B_1 and B_2.

One of the several modifications of the original Sombor index, Eq. (1), is the general Sombor index [9,15], defined as

$$SO_\alpha = SO_\alpha(G) = \sum_{uv \in \mathbf{E}(G)} \left[d(u)^2 + d(v)^2\right]^\alpha$$

where $\alpha \neq 0$ is a real number. Evidently, $SO_{0.5}(G) = SO(G)$.

It is of evident interest to determine the elements of $\Gamma(\pi)$, extremal w.r.t. a certain graph invariant. Several such researches have been published [2,10,12,13,18]. Among these results, in many cases the extremal graphs are *BFS*-type (*BFS* = breadth first search).

Definition 1. Let G be a connected graph. We say that G is a *BFS*-graph if there exists a vertex ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $\mathbf{V}(G)$ satisfying: (*i*) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1; (*ii*) let $v \in N(u)\backslash N(w)$ and $z \in N(w)\backslash N(u)$ such that $h(v) = h(u) + 1$ and $h(z) = h(w) + 1$. If $u \prec w$, then $v \prec z$.

Definition 2 (*[13]*)**.** For a c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$ and $n \geq 3$, if G is a *BFS*-graph such that $\{v_1, v_2, v_3\}$ forms a triangle of G when $c \geq 1$, then G is called a special extremal *BFS*-graph.

Recently, Gutman posed the problem of determining extremal graphs with minimum or maximum Sombor index among the class of connected graphs with given degree sequence (via private communication). In this paper, we settle the minimum case. Actually, we can go further by showing the following

Theorem 3. *For any given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, there exists a special extremal BFS-graph with minimum $SO_\alpha(G)$ in the class of $\Gamma(\pi)$ for $0 < \alpha < 1$, and there also exists a special extremal BFS-graph with maximum $SO_\alpha(G)$ in the class of $\Gamma(\pi)$ for either $\alpha > 1$ or $\alpha < 0$.*

Hereafter, we use the symbol $p^{(q)}$ to define q copies of the real number p. In [21] the authors show that for any tree degree sequence π there exists a unique *BFS*-tree, here denoted by $T_M(\pi)$. The *BFS*-trees are also called greedy trees in the literature, e.g. [10,18]. In fact, we can also construct a unique unicyclic *BFS*-graph $U_M(\pi)$ by the following breadth-first-search method for any unicyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$ [13]: The unique cycle of $U_M(\pi)$ is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Select the vertex v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices v_2, v_3, v_4, v_5,..., v_{d_1+1} as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$. Let $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$ and $N(v_3) = \{v_1, v_2, v_{d_1+d_2}, \ldots, v_{d_1+d_2+d_3-3}\}$. Then, append $d_4 - 1$ vertices to v_4 such that $N(v_4) = \{v_1, v_{d_1+d_2+d_3-2}, \ldots, v_{d_1+d_2+d_3+d_4-4}\}$, and so on. Informally, the *BFS*-unicyclic graph is constructed from a *BFS*-tree by adding an edge between v_2 and v_3. As an example, considering the unicyclic degree sequence $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, $U_M(\pi_1)$ is depicted in Fig. 1.

Denote by $\mathcal{R}(G)$ the reduced graph obtained from G by recursively deleting pendent vertices to the resultant graph until no pendent vertices remain. If $c \geq 1$ and G is a c-cyclic graph, then $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a c-cyclic graph.

Some paths P_{l_1}, P_{l_2}, ..., P_{l_k} are said to have almost equal lengths if their lengths pairwise differ at most by 1, that is, $|l_i - l_j| \leq 1$ for $1 \leq i < j \leq k$. Let B_1 and B_2 be the two bicyclic graphs depicted in Fig. 1. If $\pi = (d_1, d_2, \ldots, d_n)$ is a

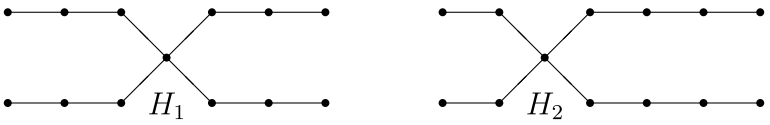


Fig. 2. The trees H_1 and H_2.

bicyclic degree sequence with $d_n = 1$, then $\sum_{i=1}^{n} d_i = 2n + 2$, which implies that π should be one of the following two cases. When $d_n = 1$, we construct a unique bicyclic graph $B_M(\pi)$ of $\Gamma(\pi)$ as follows:

(*i*) If $d_n = 1$ and $d_1 \geq d_2 \geq 3$, then let $B_M(\pi)$ be a *BFS*-graph such that $\mathcal{R}(B_M(\pi)) = B_1$ and the remaining vertices appear in a *BFS*-ordering.

(*ii*) If $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$, then let $B_M(\pi)$ be the bicyclic graph with n vertices obtained from B_2 by attaching $d_1 - 4$ paths of almost equal lengths to the v_1 of B_2 (see Fig. 1).

Definition 4. For a given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, we say that G is a precisely extremal graph of $\Gamma(\pi)$, if G has minimum $SO_\alpha(G)$ among all graphs of $\Gamma(\pi)$ for $0 < \alpha < 1$ and G has maximum $SO_\alpha(G)$ among all graphs of $\Gamma(\pi)$ for either $\alpha > 1$ or $\alpha < 0$.

Theorem 5. *For any c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, then*

(*i*) *$T_M(\pi)$ is a precisely extremal graph for $c = 0$;*

(*ii*) *$U_M(\pi)$ is a precisely extremal graph for $c = 1$;*

(*iii*) *$B_M(\pi)$ is a precisely extremal graph for $c = 2$.*

In Theorems 3 and 5, we can only confirm that there exists a (precisely) extremal *BFS*-graph, as the extremal graphs of $\Gamma(\pi)$ are always not uniquely. For instance, let $\pi_2 = (4, 2^{(8)}, 1^{(4)})$ and let H_1 and H_2 be the two trees as shown in Fig. 2. It is easy to see that H_1 is the unique *BFS*-tree of $\Gamma(\pi_2)$ and $SO_\alpha(H_1) = SO_\alpha(H_2)$ for any $\alpha \neq 0$.

The research of extremal graph in the class of connected graphs with given degree sequence has close relation with the Majorization theorem. Now, we introduce the notation of Majorization.

Definition 6 ([14])**.** Let $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ be two different non-increasing sequences of real numbers. We write $(x) \lhd (y)$ if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, \ldots, n$. The ordering $\pi \lhd \pi'$ is said to be a majorization.

Theorem 7. *Let π and π' be two c-cyclic degree sequences and let G and G' be a maximum extremal graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $c \in \{0, 1, 2\}$ and $\pi \lhd \pi'$, then $SO_\alpha(G) < SO_\alpha(G')$ for $\alpha > 1$.*

2. Proof of Theorems 3 and 5

This section is dedicated to the proofs of Theorems 3 and 5. We need to introduce more notations. A symmetric bivariate function $f(x, y)$ defined on positive real numbers is called escalating (resp. de-escalating) if

$$f(x_1, x_2) + f(y_1, y_2) \geq \ (\text{resp.}, \leq)\ f(y_1, x_2) + f(x_1, y_2) \tag{2}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (2) is strict if $x_1 > y_1$ and $x_2 > y_2$.

Further, Wang [19] defined the connectivity function of a connected graph G associated with a symmetric bivariate function $f(x, y)$ to be

$$M_f(G) = \sum_{uv \in \mathbf{E}(G)} f(d(u), d(v)).$$

It is easily to see that $SO_\alpha(G)$ is just a special case of $M_f(G)$.

The proofs of Theorems 3 and 5 rely on the following two lemmas:

Lemma 8 ([13])**.** *For any given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, there exists a special extremal BFS-graph G such that $M_f(G)$ is maximized in $\Gamma(\pi)$ when $f(x, y)$ is escalating and $M_f(G)$ is minimized in $\Gamma(\pi)$ when $f(x, y)$ is de-escalating.*

Lemma 9 ([13]). *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a given c-cyclic degree sequence with $d_n = 1$. In the class of $\Gamma(\pi)$,*

(i) if $c = 0$, then $T_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $T_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;

(ii) if $c = 1$, then $U_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $U_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;

(iii) if $c = 2$, then $B_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $B_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;

Throughout this paper, denote by $h(x, y) = \left(x^2 + y^2\right)^{\alpha}$, where $\min\{x, y\} > 0$. From Lemmas 8–9, to show Theorems 3 and 5, it suffices to show that the following proposition holds.

Proposition 10. *$SO_\alpha(G)$ is escalating for either $\alpha > 1$ or $\alpha < 0$, and $SO_\alpha(G)$ is de-escalating for $0 < \alpha < 1$.*

Proof. In what follows, we suppose that $x_1 \geq y_1 \geq 1$ and $x_2 \geq y_2 \geq 0$. It suffices to show that $h(x, y)$ satisfies (2). Since the equality holds in (2) for either $x_1 = y_1$ or $x_2 = y_2$, we may suppose that $x_1 > y_1$ and $x_2 > y_2$.

One can easily check that

$$h(x_1, x_2) + h(y_1, y_2) - h(y_1, x_2) - h(x_1, y_2) = \int_{y_1}^{x_1} 2t\alpha(t^2 + x_2^2)^{\alpha-1}dt - \int_{y_1}^{x_1} 2t\alpha(t^2 + y_2^2)^{\alpha-1}dt. \tag{3}$$

Case 1. $0 < \alpha < 1$. Since $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 0$ and $2t\alpha(t^2 + y_2^2)^{\alpha-1} > 0$ for $t \geq y_1 > 0$, we have

$$2t\alpha(t^2 + x_2^2)^{\alpha-1} < 2t\alpha(t^2 + y_2^2)^{\alpha-1}, \tag{4}$$

as $x_2 > y_2 > 0$ and $0 < \alpha < 1$. Combining (4) with $x_1 > y_1 > 0$, we can conclude that $h(x_1, x_2) + h(y_1, y_2) < h(y_1, x_2) + h(x_1, y_2)$ by (3). Thus, $SO_\alpha(G)$ is de-escalating for $0 < \alpha < 1$.

Case 2. $\alpha < 0$ **or** $\alpha > 1$. If $\alpha > 1$, then $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 2t\alpha(t^2 + y_2^2)^{\alpha-1}$ for $t \geq y_1 > 0$ and $x_2 > y_2$. Combining this with $x_1 > y_1 > 0$, we can conclude that $h(x_1, x_2) + h(y_1, y_2) > h(y_1, x_2) + h(x_1, y_2)$ by (3), which implies that $SO_\alpha(G)$ is escalating for $\alpha > 1$.

Otherwise, $\alpha < 0$. Since $2t\alpha(t^2 + x_2^2)^{\alpha-1} < 0$ and $2t\alpha(t^2 + y_2^2)^{\alpha-1} < 0$, we have $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 2t\alpha(t^2 + y_2^2)^{\alpha-1}$ for $t \geq y_1 > 0$ and $x_2 > y_2 > 0$. Taking this with $x_1 > y_1 > 0$ into consideration, we also deduce that $SO_\alpha(G)$ is escalating for $\alpha < 0$. □

3. Proof of Theorem 7

The following definition will play a crucial role in the proof of Theorem 7.

Definition 11 ([12]). A non-negative escalating function $f(x, y)$ is called a good escalating function, if $f(x, y)$ satisfies $\frac{\partial f(x,y)}{\partial x} > 0$, $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$, and

$$f(x_1 + 1, x_2) + f(x_1 + 1, y_2) + f(x_1 + 1, y_1 - 1) > f(x_1, x_2) + f(y_1, y_2) + f(x_1, y_1)$$

holds for any $x_1 \geq y_1 \geq 2$ and $x_2 \geq y_2 \geq 1$.

Lemma 12 ([12]). *Let π and π' be two c-cyclic degree sequences with $\pi \lhd \pi'$ and $c \in \{0, 1, 2\}$. Let G and G' have maximum $M_f(G)$ and $M_f(G')$ in the class of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is good escalating, then $M_f(G) < M_f(G')$.*

Proof of Theorem 7. By Lemma 12, to complete the proof of Theorem 7, it suffices to show that $h(x, y)$ is a good escalating function for $\alpha > 1$. We already know that $h(x, y)$ is a non-negative escalating function for $\alpha > 1$ by Proposition 10.

Since $\alpha > 1$, we have

$$\frac{\partial h(x, y)}{\partial x} = 2x\alpha(x^2 + y^2)^{\alpha-1} > 0 \text{ and } \frac{\partial^2 h(x, y)}{\partial x^2} = 2\alpha(x^2 + y^2)^{\alpha-2}\left[(x^2 + y^2) + 2x^2(\alpha - 1)\right] > 0.$$

Since $h(x, y)$ is a strictly increasing function on x, we have $h(x_1 + 1, x_2) > h(x_1, x_2)$ and $h(x_1 + 1, y_2) > h(y_1, y_2)$, as $x_1 \geq y_1$.

Since $\left[(x_1 + 1)^2 + (y_1 - 1)^2\right] - \left[x_1^2 + y_1^2\right] = 2(x_1 - y_1 + 1) > 0$ for $x_1 \geq y_1$, we have

$$h(x_1 + 1, y_1 - 1) - h(x_1, y_1) = \left[(x_1 + 1)^2 + (y_1 - 1)^2\right]^{\alpha} - \left(x_1^2 + y_1^2\right)^{\alpha} > 0$$

for $\alpha > 1$. Now, we can see that $h(x, y)$ is a good escalating function for $\alpha > 1$. □

Data availability

No data was used for the research described in the article.

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Extremal augmented Zagreb index of trees with given numbers of vertices and leaves

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ABSTRACT

The augmented Zagreb index $AZI(G)$ of a connected graph G is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3,$$

where $d(u)$ and $d(v)$ are the degrees of the end-vertices of an edge uv, respectively. We determine the unique tree with given numbers of vertices and leaves that minimizes augmented Zagreb index, and characterize the unique graph with minimum augmented Zagreb index in the class of connected graphs with given numbers of vertices and pendent vertices. Furthermore, we also determine the maximum augmented Zagreb index with the extremal trees characterized in the class of all trees with given numbers of vertices and leaves.

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1. Introduction

Throughout the paper, we consider only simple connected graphs. Let $d_G(u)$, or $d(u)$ if no confusion occurs, be the degree of vertex u of G. A **k-vertex** is a vertex of degree k. A k-vertex is referred as a **pendent vertex** if $k = 1$ and **non-pendent vertex** if $k \geq 2$. An edge incident to a pendent vertex will be referred to a **pendent edge**. A pendent vertex of a tree is also called a **leaf**. Let $\Delta := \Delta(G)$ be the maximum degree of G. As usual, let K_n, P_n and C_n be the complete graph, path and cycle on n vertices, respectively.

The **atom-bond connectivity index** $ABC(G)$, or for short ABC-index, of a connected graph G is defined as

$$ABC(G) = \sum \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}},$$

where the sum is over all edges $uv \in E(G)$.

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The ABC index is one of the most important topological indices and was first introduced by Estrada et al. [5] in 1998. It was then extended by Furtula et al. [7] to the **general atom-bond connectivity index** $ABC_\alpha(G)$ for any nonzero real number α, where

$$ABC_\alpha(G) = \sum_{uv\in E(G)} \left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^\alpha. \tag{1.1}$$

Clearly, when $\alpha = 1/2$, it is the ABC index. When $\alpha = -3$, it is called the **augmented Zagreb index** (shortly AZI) $AZI(G)$ of G [7]. That is,

$$AZI(G) = ABC_{-3}(G) = \sum_{uv\in E(G)} \Phi(d(u), d(v)), \text{ where } \Phi(x, y) = \left(\frac{xy}{x+y-2}\right)^3.$$

Both the ABC index and AZI have various applications in chemistry [5,10].

The research of extremal values for the ABC index and AZI received much attention in recent years [1–3,6–9,11,13,15,17,18,21,22]. As early as in 2009, Furtula, Graovac and Vukičević have shown that the star has maximum ABC index among all trees with n vertices in [6]. However, the problem of charactering trees with the minimum ABC index is much more complicated. Until most recently, it was resolved by Hosseini, Mohar and Ahmadi [11] with a precise description of ABC minimum trees with sufficiently many vertices. In recent years, much work focuses on the question that which trees with t leaves attain the minimum ABC index has been studied extensively in [8,9,15,17,18], among others. Such trees are called t-optimal trees. Characterization of t-optimal trees was discovered by [9] for $t \le 53$ and improved by [15] for $t \le 219$. In [15], Lin et al. put forward a conjecture on the order of t-optimal trees. However, their conjecture was disproved by Mohar [18], who characterized the unique t-optimal tree for every $t \ge 1195$.

Let $\mathbb{T}_k^n$ be the family of trees on n vertices with k leaves and let $\mathbb{T}_k$ be the family of trees with k leaves. For the AZI, it has been shown by Furtula, Graovac and Vukičević [7] that the star uniquely minimizes AZI among all trees with n vertices. In the same paper [7], they posted an open question to characterize tree(s) on n vertices with maximum AZI. The question was recently solved in [16] and [19]. In [16], Lin, Dimitrov and Škrekovski further proposed the following open problem.

Problem 1 *([16]).* Characterize trees with the maximum or minimum AZI in the class of $\mathbb{T}_k$.

We first give a very short answer to Problem 1. In fact, by Lemmas 2.2(i) and 2.6 in the next section, we can easily see that the star $K_{1,k}$ uniquely attains the minimum AZI among all trees with k leaves. However, there is no tree can attain the maximum AZI among all trees with k leaves, as we can always add an edge between an isolated vertex and a leaf of any tree to get a tree with a larger AZI value.

Motivated by the above work, it is natural to consider the following problem.

Problem 2. Characterize trees with maximum or minimum AZI in the class of $\mathbb{T}_k^n$.

For a graph family $\mathcal{G}$ and $G \in \mathcal{G}$, if $AZI(G)$ is minimum among all graphs of $\mathcal{G}$, then G is called an **AZI-minimum** (or simply, minimum) graph of $\mathcal{G}$. Similarly, we can also define the AZI-**maximum** graph of $\mathcal{G}$.

Let $F^n_{x,k-x}$ be the tree on n vertices obtained from a path P_{n-k} by attaching $k-x$ and x leaves to the two leaves of P_{n-k}, respectively. Since the star is the unique tree with n vertices and $n-1$ leaves, we may always assume that $k \le n-2$ in the sequel.

Theorem 1.1. *If $2 \le k \le n-2$, then F_0 is the unique AZI-minimum tree of $\mathbb{T}_k^n$, where*

$$F_0 = \begin{cases} F^n_{\lfloor \frac{k}{2}\rfloor, \lceil \frac{k}{2}\rceil} & \text{if } n-k \ge 3, \\ F^n_{1,k-1} & \text{if } n-k = 2. \end{cases}$$

By the definition of AZI and Theorem 1.1, the minimum AZI of $\mathbb{T}_k^n$ is equal to $AZI(F_0)$, where

$$AZI(F_0) = \begin{cases} \frac{\left(\lfloor \frac{k}{2}\rfloor+1\right)^3}{\left(\lfloor \frac{k}{2}\rfloor\right)^2} + \frac{\left(\lceil \frac{k}{2}\rceil+1\right)^3}{\left(\lceil \frac{k}{2}\rceil\right)^2} + 8(n-k-1) & \text{if } n-k \ge 3, \\ \frac{(n-2)^3}{(n-3)^2} + 16 & \text{if } n-k = 2. \end{cases}$$

The maximum AZI of $\mathbb{T}_k^n$ seems much more difficult. To solve this problem, we need to introduce more notations. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be a degree sequence of a tree and let $\mathscr{T}(\pi)$ be the set of all trees with degree sequence π.

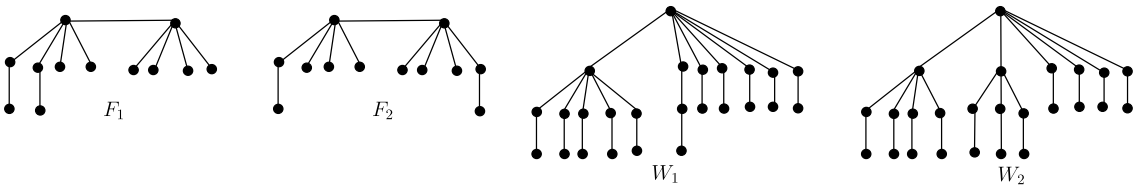


Fig. 1.1. The four trees F_1, F_2, W_1 and W_2.

Definition 1.2. Let T be a tree. If there exists an ordering $v_0 \prec v_1 \prec \cdots \prec v_{n-1}$ of $V(T)$ satisfying the following (i) and (ii), then T is called a **greedy tree** by [14] or a BFS**-tree** by [20]:
(i) $d(v_0) \geq d(v_1) \geq \cdots \geq d(v_{n-1})$ and $h(v_0) \leq h(v_1) \leq \cdots \leq h(v_{n-1})$, where $h(v)$ is the distance between v and v_0 of T.
(ii) let $v \in N(u)\backslash N(w)$, $z \in N(w)\backslash N(u)$ such that $h(u) = h(w) = h(v) - 1 = h(z) - 1$, if $u \prec w$, then $v \prec z$.

It is well-known that the greedy tree is unique for any given tree degree sequence π from [20]. The following theorem shows that the unique greedy tree is an AZI-maximum tree of $\mathscr{T}(\pi)$. Generally, the AZI-maximum trees of $\mathscr{T}(\pi)$ are not unique [14] (see F_1 and F_2 in Fig. 1.1).

Theorem 1.3 *([14]). For any tree degree sequence π, the unique greedy tree is an AZI-maximum tree among all trees of $\mathscr{T}(\pi)$.*

Let $q^{(s)}$ be the s-tuple $(q, q, \ldots, q)$. Throughout the paper, let

$$\pi_0 = \left(\left\lceil \frac{k}{2} \right\rceil + 1, \left\lfloor \frac{k}{2} \right\rfloor + 1, 2^{(n-k-2)}, 1^{(k)}\right)$$

and let $\mathbb{T}_0$ be the set of trees of $\mathscr{T}(\pi_0)$ such that
(i) if $0 \leq n-k-2 < k$ and k is odd, then $\mathbb{T}_0$ contains a unique tree, which is the unique greedy tree of $\mathscr{T}(\pi_0)$;
(ii) if $0 \leq n-k-2 < k$ and k is even, then $\mathbb{T}_0 \subseteq \mathscr{T}(\pi_0)$ and for each tree T_0 of $\mathbb{T}_0$, v_0 is adjacent to v_1, and $N(v_0) \cup N(v_1)$ contains exactly $n-k-2$ vertices of degree two, where v_0 and v_1 are vertices of T_0 with the largest degree and the second largest degree;
(iii) if $n-k-2 \geq k$, then $\mathbb{T}_0 \subseteq \mathscr{T}(\pi_0)$ and for each tree T_0 of $\mathbb{T}_0$, v_0 is adjacent to v_1 and $\left\lceil \frac{k}{2} \right\rceil$ vertices of degree two, and v_1 is adjacent to $\left\lfloor \frac{k}{2} \right\rfloor$ vertices of degree two, where v_0 and v_1 are vertices of T_0 with the largest degree and the second largest degree.

Theorem 1.4. *If $12 \leq k \leq n-2$ and $T \in \mathbb{T}_k^n$, then $AZI(T) \leq f(n,k)$ with equality if and only if $T \in \mathbb{T}_0$, where*
(i) $f(n,k) = \Phi(\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1) + \lfloor \frac{k}{2} \rfloor \Phi(\lfloor \frac{k}{2} \rfloor + 1, 1) + (\lceil \frac{k}{2} \rceil + k + 2 - n)\Phi(\lceil \frac{k}{2} \rceil + 1, 1) + 16(n-k-2)$, *if* $0 \leq n-k-2 \leq \lceil \frac{k}{2} \rceil$;
(ii) $f(n,k) = \Phi(\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1) + (2k+2-n)\Phi(\lfloor \frac{k}{2} \rfloor + 1, 1) + 16(n-k-2)$, *if* $\lceil \frac{k}{2} \rceil \leq n-k-2 < k$;
(iii) $f(n,k) = \Phi(\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1) + 8(n-2)$, *if* $n-k-2 \geq k$.

Based on Theorem 1.1, we also identify the unique AZI-minimum graph in the class of connected graphs with n vertices and k pendent vertices. Let $\mathbb{G}_k^n$ be the set of connected graphs with n vertices and k pendent vertices. Denote by U_k^n the unicyclic graph on n vertices obtained from a cycle C_{n-k} by attaching k pendent vertices to one vertex of C_{n-k}.

Theorem 1.5. *If $1 \leq k \leq n-2$, then G_0 is the unique AZI-minimum graph of $\mathbb{G}_k^n$, where*

$$G_0 = \begin{cases} F_{1,k-1}^n & \text{if } n-k=2, \\ F_{\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil}^n & \text{if } n-k \geq 3 \text{ and } k \geq 4, \\ U_k^n & \text{if } n-k \geq 3 \text{ and } 1 \leq k \leq 3. \end{cases}$$

2. Preliminaries

In this section, we list some useful preliminaries. Denote by $\psi(x,y) = \Phi(x,y) - \Phi(x-1,y)$, where $x \geq 2$, $y \geq 1$ and $x+y \geq 4$. The following lemma comes from Lemma 6 of [14], where (iii) has been slightly modified with a similar proof.

Lemma 2.1 *([14]). For $x \geq 2$ and $y \geq 1$,*
(i) $\psi(x,1)$ (<0) *strictly increases with $x \geq 3$.*
(ii) $\psi(x,2) = 0$ *for $x \geq 3$.*
(iii) *If $y \geq 3$ is fixed, then $\psi(x,y)$ (>0) strictly increases with $2 \leq x \leq y-1$, and strictly decreases with $x \geq y-1$.*

Lemma 2.2 *([12]). Let x and y be two real numbers, where $\min\{x, y\} \geq 1$. Then,*
(i) $\Phi(1, y)$ is decreasing for $y \geq 2$.
(ii) $\Phi(2, y) = 8$ for any real number y.
(iii) If $y \geq 3$ is fixed, then $\Phi(x, y) > 8$ is increasing for $x \geq 3$.

Lemma 2.3 *([4]). Let G be a connected graph with two non-adjacent vertices u and v. If $\alpha \leq \frac{1}{2}$ and $\alpha \neq 0$, then $ABC_\alpha(G + uv) > ABC_\alpha(G)$.*

Lemma 2.4. *Let $\Phi_1(x) = \Phi(p + 2x + 2, 1) - \Phi(p + 2x, 1)$, where $p \geq 2$. Then $\Phi_1(x)$ is a strictly increasing function for $x \geq 0$.*

Proof. Since $\Phi_1(x) = \Phi(p + 2x + 2, 1) - \Phi(p + 2x, 1) = \Psi(p + 2x + 2, 1) + \Psi(p + 2x + 1, 1)$, by Lemma 2.1 (i), it is easy to see that $\Phi_1(x)$ is a strictly increasing function for $x \geq 0$. □

Lemma 2.5. *Let $\Phi_3(x) = x\Phi(x + 1, 1) + (z - x)\Phi(z - x + 1, 1)$, where $\min\{x, z\} > 0$. Then $\Phi_3(x)$ is strictly decreasing on $\left(0, \frac{z}{2}\right]$ and strictly increasing on $\left[\frac{z}{2}, z\right)$.*

Proof. By definition,

$$\Phi_3(x) = x\left(\frac{x+1}{x}\right)^3 + (z - x)\left(\frac{z-x+1}{z-x}\right)^3.$$

Thus,

$$\begin{aligned}\Phi_3'(x) &= \left(1 + \frac{1}{x}\right)^3 - 3x\left(1 + \frac{1}{x}\right)^2 \frac{1}{x^2} - \left(1 + \frac{1}{z-x}\right)^3 + 3(z - x)\left(1 + \frac{1}{z-x}\right)^2 \frac{1}{(z-x)^2} \\ &= \Phi_4(x) - \Phi_4(z - x),\end{aligned}$$

where $\Phi_4(x) = \left(1 + \frac{1}{x}\right)^3 - 3x\left(1 + \frac{1}{x}\right)^2 \frac{1}{x^2}$. It follows that

$$\Phi_4'(x) = \frac{6(x+1)}{x^4} > 0.$$

Thus, $\Phi_3(x)$ is strictly decreasing on $\left(0, \frac{z}{2}\right]$ and strictly increasing on $\left[\frac{z}{2}, z\right)$. □

A connected graph with n vertices and $n + c - 1$ edges is called a ***c*-cyclic graph**.

Lemma 2.6. *If G is a c-cyclic graph with exactly k pendent vertices, then $\Delta \leq k + 2c$.*

Proof. Since $2(n - 1 + c) = \sum_{v \in G} d(v) \geq 2(n - k - 1) + \Delta + k$, $\Delta \leq k + 2c$. □

If $n - k \geq 3$, then by the definitions of $F^n_{x,k-x}$ and U^n_k, we have

$$AZI(F^n_{x,k-x}) = 8(n - k - 1) + x\Phi(x + 1, 1) + (k - x)\Phi(k - x + 1, 1), \tag{2.1}$$

$$AZI\left(F^n_{\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil}\right) = 8(n - k - 1) + \frac{\left(\lceil \frac{k}{2} \rceil + 1\right)^3}{\left(\lceil \frac{k}{2} \rceil\right)^2} + \frac{\left(\lfloor \frac{k}{2} \rfloor + 1\right)^3}{\left(\lfloor \frac{k}{2} \rfloor\right)^2}, \tag{2.2}$$

$$AZI(U^n_k) = 8(n - k) + k\Phi(k + 2, 1). \tag{2.3}$$

3. The proof of Theorem 1.1

This section is dedicated to the proof of Theorem 1.1. We first introduce the following definition.

Definition 3.1. A vertex u is called a **quasi-pendent vertex** of G if it is a pendent vertex of $\mathcal{R}(G)$, while u is called a **quasi-vertex** of G if it is adjacent to at least one pendent vertex of G.

By Definition 3.1, any quasi-vertex of G must be a non-pendent vertex of G, and any quasi-pendent vertex of G is also a quasi-vertex of G, but not vice versa.

Denote by $\mathcal{R}(G)$ the graph obtained from G by deleting all its pendent vertices (and the incident edges accordingly). Throughout this section, let F_0 be an AZI-minimum tree of $\mathbb{T}_k^n$. Since F_0 is a tree and we always suppose that $k \le n-2$, $\mathcal{R}(F_0)$ is also a tree and thus contains at least two pendent vertices. This implies that F_0 contains at least two quasi-pendent vertices. Thus, we can define that u_0 and v_0 are two quasi-pendent vertices of F_0 such that the degrees of u_0 and v_0 in F_0 are largest and second largest among all quasi-pendent vertices of F_0, where $d_{F_0}(u_0) = d_{F_0}(v_0)$ is allowed. In the rest of this section, we suppose that u_0 and v_0 are adjacent to exactly n_{u_0} and n_{v_0} leaves in F_0, respectively. The following lemma indicates that the maximum degree of F_0 is less than $k-n_{v_0}+1$ if F_0 contains at least three quasi-pendent vertices.

Lemma 3.2. *If F_0 contains at least three quasi-pendent vertices, then $\Delta(F_0) < k - n_{v_0} + 1$.*

Proof. By contradiction, we assume that $\Delta = \Delta(F_0) \ge k - n_{v_0} + 1$.

If $n_{u_0} = 1$, then $n_{v_0} = 1$ by the choice of u_0 and v_0. Since F_0 contains at least three quasi-pendent vertices, we have $k \ge 3$. Since $\mathcal{R}(F_0)$ is a tree with $n-k$ vertices, $\mathcal{R}(F_0)$ contains exactly $n-k-1$ edges, each of which contributes at least 8 to $AZI(F_0)$. Combining this with $\Delta \le k$ by Lemma 2.6, from Lemma 2.2(i) and (2.1), it follows that

$$\begin{aligned} AZI(F_0) - AZI(F_{1,k-1}^n) &\ge \big(16 + (k-2)\Phi(\Delta, 1)\big) - \big(8 + (k-1)\Phi(k,1)\big) \\ &\ge 8 - \Phi(k,1) > 0, \end{aligned}$$

contrary to the choice of F_0. Thus, $n_{u_0} > 1$.

Since F_0 contains at least three quasi-pendent vertices, we have $n_{u_0} + n_{v_0} < k$, and thus $n_{v_0} + 1 \le n_{u_0} + 1 < k - n_{v_0} + 1 \le \Delta$, implying that neither u_0 nor v_0 is the vertex with maximum degree of F_0. In view of F_0 being a tree, F_0 has at least $\Delta + \big(n_{u_0} - 1\big) + \big(n_{v_0} - 1\big)$ pendent vertices, showing that

$$\Delta + \big(n_{u_0} - 1\big) + \big(n_{v_0} - 1\big) \ge k + n_{u_0} - 1 > k,$$

a contradiction. □

Lemma 3.3. *If $n - k \ge 2$, then $F_0 = F_{x,k-x}^n$, where $1 \le x \le \lfloor \frac{k}{2} \rfloor$.*

Proof. It is easily checked that the result holds for $n - k = 2$. Thus, we may suppose that $n - k \ge 3$ in the following. Let $Q(F_0)$ be the set of quasi-vertices of F_0. Then $\{u_0, v_0\} \subseteq Q(F_0)$. We claim that $Q(F_0) = \{u_0, v_0\}$.

By contradiction, we assume that $Q(F_0) = \{u_0, v_0, w_1, \ldots, w_p\}$, where $p \ge 1$. Suppose that w_i is adjacent to exactly s_i pendent vertices of F_0 for $1 \le i \le p$. Then,

$$n_{u_0} + n_{v_0} + s_1 + \cdots + s_p = k, \quad \text{where } \max\{s_1, s_2, \ldots, s_p\} \ge 1. \tag{3.1}$$

Let $\Delta = \Delta(F_0)$ and $T^* = F_{n_{v_0}, k-n_{v_0}}$. Since $\mathcal{R}(F_0)$ contains exactly $n-1-k$ edges, each of which contributes at least 8 to $AZI(F_0)$. By Lemma 2.2(i), Lemma 3.2 and (3.1),

$$\begin{aligned} &AZI(F_0) - AZI(T^*) \\ &\ge n_{u_0}\Phi(n_{u_0}+1, 1) + \sum_{1 \le i \le p} s_i \Phi(d(w_i), 1) - (k - n_{v_0})\Phi(k - n_{v_0} + 1, 1) \\ &\ge (n_{u_0} + s_1 + \cdots + s_p)\Phi(\Delta, 1) - (k - n_{v_0})\Phi(k - n_{v_0} + 1, 1) \\ &= (k - n_{v_0})\big(\Phi(\Delta, 1) - \Phi(k - n_{v_0} + 1, 1)\big) > 0, \end{aligned}$$

contrary to the choice of F_0. Thus, $Q(F_0) = \{u_0, v_0\}$ as claimed.

As $Q(F_0) = \{u_0, v_0\}$, each of the other $n-k-2$ non-pendent vertices of F_0 is not adjacent to any leaf. Since F_0 is a tree, we can deduce that each of the other $n-k-2$ non-pendent vertices of F_0 is a 2-vertex of F_0. This implies that $F_0 = F_{x,k-x}^n$, where $1 \le x \le \lfloor \frac{k}{2} \rfloor$. □

Proof of Theorem 1.1. By Lemma 3.3, $F_0 = F_{x,k-x}^n$. Since $n - k \ge 2$, we have the following two cases.

Case 1. $n - k \ge 3$. In view of (2.1), by setting $z = k$ in Lemma 2.5, we can deduce that $AZI(F_{x,k-x}^n) \ge AZI\big(F_{\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil}^n\big)$ with equality if and only if $x = \lfloor \frac{k}{2} \rfloor$. This implies that $F_0 = F_{\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil}^n$.

Case 2. $n - k = 2$. Since $F_0 = F_{x,k-x}^n$, we have $F_0 = F_{1,1}^4$ if $k = 2$, and $F_0 = F_{1,2}^5$ if $k = 3$. Thus, the result holds for $2 \le k \le 3$. In what follows, we suppose that $k \ge 4$.

If $x=2$, then

$$\begin{aligned}&AZI(F^n_{2,k-2})-AZI(F^n_{1,k-1})\\&=2\Phi(3,1)+\Phi(3,k-1)+(k-2)\Phi(k-1,1)-16-(k-1)\Phi(k,1)\\&=\frac{(k-3)^2(67k^5-324k^4+604k^3-556k^2+256k-48)}{4k^3(k-1)^2(k-2)^2}>0\ \big(\text{as } k\geq 4\big),\end{aligned}$$

a contradiction.

If $3\leq x\leq \lfloor\frac{k}{2}\rfloor$, then by Lemma 2.2(i),

$$\begin{aligned}&AZI(F^n_{x,k-x})-AZI(F^n_{1,k-1})\\&=x\Phi(x+1,1)+\Phi(x+1,k-x+1)+(k-x)\Phi(k-x+1,1)-16-(k-1)\Phi(k,1)\\&>k\Phi(k,1)+\Phi(x+1,k-x+1)-16-(k-1)\Phi(k,1)\\&>\Phi(x+1,k-x+1)-16\\&=\left(\frac{(x+1)(k-x+1)}{k}\right)^3-16=\left(\frac{-x^2+kx+k+1}{k}\right)^3-16\\&\geq 64\left(\frac{k-2}{k}\right)^3-16\geq 64\left(\frac{2}{3}\right)^3-16>2.96>0,\end{aligned}$$

a contradiction. Thus, $x=1$ and so $F_0=F^n_{1,k-1}$. This completes the proof. □

4. The proof of Theorem 1.5

Let $\mathbb{C}^n_k$ be the family of connected graphs on n vertices with k pendent vertices that contain at least one cycle. Obviously, $\mathbb{G}^n_k=\mathbb{C}^n_k\cup\mathbb{T}^n_k$. Since every graph of $\mathbb{C}^n_k$ contains at least one cycle, the number of pendent vertices is at most $n-3$. Thus we only need to consider the case of $k\leq n-3$ for $\mathbb{C}^n_k$.

Lemma 4.1. *For any graph $G\in\mathbb{C}^n_k$ and $k\geq 1$, we have $AZI(G)\geq AZI(U^n_k)$, with equality if and only if $G=U^n_k$.*

Proof. Suppose that G is a c-cyclic graph with maximum degree Δ.

Case 1. $c\geq 2$. All edges of $\mathcal{R}(G)$ contribute at least $8(n+c-k-1)$ to $AZI(G)$, and all k pendent edges of G contribute at least $k\Phi(\Delta,1)$ to $AZI(G)$. By Lemma 2.2(i), Lemma 2.4, Lemma 2.6 and (2.3),

$$\begin{aligned}AZI(G)-AZI(U^n_k)&\geq 8(c-1)+k\Phi(\Delta,1)-k\Phi(k+2,1)\\&\geq 8(c-1)+k\big(\Phi(k+2c,1)-\Phi(k+2,1)\big)\\&=8(c-1)+k\sum_{1\leq i\leq c-1}\big(\Phi(k+2i+2,1)-\Phi(k+2i,1)\big)\\&\geq 8(c-1)+k(c-1)\big(\Phi(k+4,1)-\Phi(k+2,1)\big)\\&=2(c-1)\frac{4k^6+45k^5+198k^4+439k^3+534k^2+356k+108}{(k+1)^3(k+3)^3}\\&>0.\end{aligned}$$

Case 2. $c=1$. All edges of $\mathcal{R}(G)$ contribute at least $8(n-k)$ to $AZI(G)$, and all k pendent edges of G contribute at least $k\Phi(\Delta,1)$ to $AZI(G)$. By Lemma 2.2(i), Lemma 2.6 and (2.3),

$$AZI(G)-AZI(U^n_k)\geq k\Phi(\Delta,1)-k\Phi(k+2,1)\geq 0. \tag{4.1}$$

If the equality holds in (4.1), then each of the quasi-vertices of G is a $(k+2)$-vertex by (4.1). Suppose that G contains exactly q quasi-vertices. Then

$$2n\geq 2(n-k-q)+q(k+2)+k=2n+(q-1)k,$$

and thus $q=1$. This implies that G contains exactly one quasi-vertex, which is a $(k+2)$-vertex. Now, we can deduce that $G=U^n_k$. □

Proof of Theorem 1.5. By Theorem 1.1 and Lemma 4.1, to determine the AZI-minimum graph of $\mathbb{G}_k^n$, it suffices to compare $AZI(F_0)$ (defined in Theorem 1.1) and $AZI(U_k^n)$. If $n-k=2$, then $\mathbb{G}_k^n=\mathbb{T}_k^n$, as every cycle contains at least three vertices. By Theorem 1.1, we have $G_0=F_0=F_{1,k-1}^n$. Thus, we may assume that $n-k\geq 3$ in the following.

If $k=1$, then $\mathbb{G}_k^n=\mathbb{C}_k^n$, since any tree contains at least two pendent vertices. By Lemma 4.1, we have $G_0=U_k^n$.

If $k=2$, then $AZI(U_2^n)-AZI(F_{1,1}^n)=2\Phi(4,1)-8<-3.25<0$ by (2.1) and (2.3), and thus $G_0=U_2^n$ by Theorem 1.1 and Lemma 4.1.

If $k=3$, then $AZI(U_3^n)-AZI(F_{1,2}^n)=3\Phi(5,1)-2\Phi(3,1)<-0.89<0$ by (2.1) and (2.3), and thus $G_0=U_3^n$.

If $k\geq 4$ and k is even, then

$$\begin{aligned}AZI(U_k^n)-AZI\left(F^n_{\frac{k}{2},\frac{k}{2}}\right)&=8+k\Phi(k+2,1)-k\left(\frac{k+2}{k}\right)^3 \ \text{(by (2.2) and (2.3))}\\&=8+k\left(\frac{k+2}{k+1}\right)^3-k\left(\frac{k+2}{k}\right)^3\\&=\frac{5k^5+3k^4-31k^3-58k^2-36k-8}{k^2(k+1)^3}>0,\end{aligned}$$

and hence $G_0=F^n_{\frac{k}{2},\frac{k}{2}}$ by Theorem 1.1 and Lemma 4.1.

If $k\geq 5$ and k is odd, then

$$\begin{aligned}&AZI(U_k^n)-AZI\left(F^n_{\frac{k-1}{2},\frac{k+1}{2}}\right)\\&=8+k\Phi(k+2,1)-\frac{k-1}{2}\left(\frac{k+1}{k-1}\right)^3-\frac{k+1}{2}\left(\frac{k+3}{k+1}\right)^3 \ \text{(by (2.2) and (2.3))}\\&=8+k\left(\frac{k+2}{k+1}\right)^3-\frac{k-1}{2}\left(\frac{k+1}{k-1}\right)^3-\frac{k+1}{2}\left(\frac{k+3}{k+1}\right)^3\\&=\frac{5k^5-7k^4-32k^3-5k^2+13k-6}{(k-1)^2(k+1)^3}>0,\end{aligned}$$

and thus $G_0=F^n_{\frac{k-1}{2},\frac{k+1}{2}}$, completing the proof. □

5. The proof of Theorem 1.4

This section is dedicated to the proof of Theorem 1.4. Since the path is the unique tree with n vertices and two pendent vertices, we shall suppose that $3\leq k\leq n-2$ and thus $\Delta\geq 3$ in the following.

Lemma 5.1 *([14]). If $x\geq 2$, $y\geq 1$ and $x+y\geq 4$, then $\psi(x,y+1)>\psi(x,y)$.*

Lemma 5.2 *([16]). Let $x\geq 3$ and $f(x)=(x-2)\psi(x,1)+\Phi(x,1)$. Then $f(x)$ strictly increases with x, and $-1.25\leq f(x)<1$.*

Lemma 5.3 *([16]). If $y\geq 3$, then $y\psi(y+1,y-1)\geq(y-3)\psi(y-1,y)$, with equality if and only if $y=3$.*

Lemma 5.4. *If $y\geq 7$, and $y\geq x\geq 3$, then*

$$\big(\Phi(y+1,y)-\Phi(y,y-1)\big)+\big(\Phi(y+1,x-2)-\Phi(y,x)\big)>0.$$

Proof. It is easily checked that

$$\begin{aligned}f(x,y)=&\big(\Phi(y+1,y)-\Phi(y,y-1)\big)+\big(\Phi(y+1,x-2)-\Phi(y,x)\big)\\=&\Phi(y+1,y)-\Phi(y,y)+\Phi(y,y)-\Phi(y,y-1)+\Phi(y+1,x-2)\\&-\Phi(y,x-2)+\Phi(y,x-2)-\Phi(y,x-1)+\Phi(y,x-1)-\Phi(y,x)\\=&\psi(y+1,y)+\psi(y,y)+\psi(y+1,x-2)-\psi(x-1,y)-\psi(x,y).\end{aligned}$$

Case 1. $x=y$. Then,

$$\begin{aligned} f(x,y) &= \psi(y+1,y)+\psi(y+1,y-2)-\psi(y-1,y)\\ &= \frac{\psi_1(y)}{8(2y-1)^3(2y-3)^3(y-1)^3}, \end{aligned}$$

where $\psi_1(y) = 96y^{11}-1056y^{10}+4232y^9-8028y^8+6864y^7-315y^6-3816y^5+2064y^4+744y^3-1200y^2+480y-64>0$, as $y\geq 5$.

Case 2. $x = y-1$. Then,

$$\begin{aligned} f(x,y) =&\psi(y+1,y)+\psi(y,y)+\psi(y+1,y-3)-\psi(y-2,y)-\psi(y-1,y)\\ =&\frac{\psi_2(y)}{8(2y-1)^3(2y-3)^3(y-2)^3}, \end{aligned}$$

where $\psi_2(y) = 96y^{11}-1536y^{10}+9416y^9-28668y^8+44712y^7-28409y^6-8874y^5+19797y^4-3004y^3-7047y^2+4374y-729>0$, as $y\geq 7$.

Case 3. $x = y-2$. Then,

$$\begin{aligned} f(x,y) =&\psi(y+1,y)+\psi(y,y)+\psi(y+1,y-4)-\psi(y-3,y)-\psi(y-2,y)\\ =&\frac{\psi_3(y)}{8(2y-1)^3(2y-3)^3(2y-5)^3}, \end{aligned}$$

where $\psi_3(y) = 768y^{11}-14976y^{10}+112768y^9-416736y^8+784032y^7-650520y^6-14040y^5+336942y^4-86137y^3-114336y^2+79488y-13824>0$, as $y\geq 7$.

Case 4. $x = 3$. Then,

$$\begin{aligned} f(x,y) =&\psi(y+1,y)+\psi(y,y)+\psi(y+1,1)-\psi(2,y)-\psi(3,y)\\ =&\frac{\psi_4(y)}{y^3(2y-1)^3(2y-3)^3(y+1)^3}, \end{aligned}$$

where $\psi_4(y) = 24y^{14}-24y^{13}-1782y^{12}+10410y^{11}-24840y^{10}+29332y^9-17478y^8+6162y^7-2086y^6-630y^5+729y^4+316y^3-207y^2-54y+27>0$, as $y\geq 6$.

Case 5. $4\leq x\leq y-3$. By Lemma 2.1, we have

$$\begin{aligned} f(x,y) =&\psi(y+1,y)+\psi(y,y)+\psi(y+1,x-2)-\psi(x-1,y)-\psi(x,y)\\ \geq&\psi(y+1,y)+\psi(y,y)-\psi(x-1,y)-\psi(x,y)\\ \geq&\psi(y+1,y)+\psi(y,y)-\psi(y-4,y)-\psi(y-3,y)\\ =&\frac{16y^3(y-2)^2\psi_5(y)}{(2y-1)^3(2y-3)^3(2y-5)^3(2y-7)^3}, \end{aligned}$$

where $\psi_5(y) = 960y^6-11520y^5+51856y^4-107648y^3+96324y^2-15632y-16073>0$, as $y\geq 5$. □

In the following, let T_0 be an AZI-maximum tree of $\mathbb{T}_k^n$, and we suppose that the degree sequence of T_0 is

$$\pi = \left(d_0, d_1, d_2, \ldots, d_t, 2^{(n-k-t-1)}, 1^{(k)}\right), \text{where } \Delta(T_0) = \Delta = d_0 \geq d_1 \geq d_2 \geq \cdots \geq d_t \geq 3. \tag{5.1}$$

By Theorem 1.3, the unique greedy tree is an AZI-maximum tree of $\mathscr{T}(\pi)$. Thus, we may further suppose that T_0 is the unique greedy tree of $\mathscr{T}(\pi)$ with $V(T_0) = \{v_0, v_1, \ldots, v_{n-1}\}$ and $d(v_k) = d_k$, where $0\leq k\leq n-1$. If $\{u,v\}\subseteq V(T_0)$ with $h(u) = h(v)-1$ and $uv\in E(T_0)$, then u is called the **parent** of v. From our hypothesis, T_0 is an AZI-maximum tree of $\mathbb{T}_k^n$. If we can find another tree $T\in\mathbb{T}_k^n$ with the property $AZI(T_0) < AZI(T)$, then we will get a contradiction to the choice of T_0. We will always employ this fact straightly in the following discussion.

Lemma 5.5. *If $5\leq k\leq n-2$, then $t\geq 1$.*

Proof. By contradiction, suppose $t = 0$. Then, v_0 is the unique vertex of T_0 with degree at least three. This implies that $k = \Delta = d_0$. For convenience, let $z = d_0$ and $\{w_1, w_2, \ldots, w_z\}$ be the children of v_0, we have $z = k\geq 5$ and $2 = d(w_1)\geq d(w_2)\geq\cdots\geq d(w_z)\geq 1$ since $n-k\geq 2$. Let u be the child of w_1 and let $T_0^* = T_0 - v_0w_2 + w_1w_2$. Then, $T_0^*\in\mathbb{T}_n^k$ and

$$\begin{aligned} AZI(T_0^*) - AZI(T_0) =&\Phi(z-1,3)-\Phi(z,2)-\sum_{i=3}^{z}\psi(z,d(w_i))\\ &+\Phi(3,d(u))-\Phi(2,d(u))+\Phi(d(w_2),3)-\Phi(d(w_2),z). \end{aligned}$$

Since $2 = d(w_1) \geq d(w_2) \geq \cdots \geq d(w_z) \geq 1$, we have $\psi(z, d(w_i)) \leq 0$ by Lemma 2.1(i) and (ii). Note that $d(u) \in \{1, 2\}$, $d(w_2) \in \{1, 2\}$ and $z \geq 5$. Thus, by Lemma 2.2,

$$AZI(T_0^*) - AZI(T_0) \geq \Phi(z-1, 3) - 8 + \Phi(3, 1) - 8 \geq \Phi(4, 3) + \Phi(3, 1) - 16 > 1.19 > 0,$$

a contradiction. □

The following Lemmas 5.6 and 5.7 are respectively the counterparts of Lemmas 3.2 and 3.3 in [16], and can be proven analogously. Though the extremal trees among $\mathbb{T}_k^n$ may contain vertices of degree 2, different from those among $\mathbb{T}^n$ (the set of trees with n vertices), noting that $\Phi(x, 2) = 8$ is constant for any $x \geq 1$, the same techniques used in the proofs of Lemmas 3.2 and 3.3 in [16] are directly applicable to show our Lemmas 5.6 and 5.7 and thus we omit the proofs here.

Lemma 5.6. *If $t \geq 2$, $1 \leq q \leq t-1$, and v_p is the parent of v_q, then $d_q \geq d_p - 1$.*

Lemma 5.7. *If $\Delta \geq 3$, then $t \leq \Delta$.*

Lemma 5.8. $k = d_0 + \sum_{i=1}^{t}(d_i - 2)$.

Proof. Since $k = 2|E(T_0)| - d_0 - d_1 - \cdots - d_t - 2(n - t - k - 1)$, $k = d_0 + \sum_{i=1}^{t}(d_i - 2)$. □

Lemma 5.9. *Let $z = d_0$, $x = d_q$, $\{w_1, w_2, \ldots, w_z\}$ be the children of v_0, and $\{u_1, u_2, \ldots, u_{x-1}\}$ be the children of v_q, where $d(u_{x-1}) \leq \cdots \leq d(u_2) \leq d(u_1)$. If $t \geq 2$ and $1 \leq q \leq t$, then*

$$\sum_{i=q+1}^{z} \psi(z+1, d(w_i)) - \sum_{i=2}^{x-1} \psi(x, d(u_i)) + \Phi(z+1, d(u_1)) - \Phi(x, d(u_1)) \geq 0.$$

Proof. Since $t < \Delta = d_0$ by Lemma 5.7, we have $d(u_1) \leq 2$. We consider the following two cases.
Case 1. $d(u_1) = 2$. Then, $d(w_1) \geq d(w_2) \geq \cdots \geq d(w_z) \geq 2$. By Lemma 2.1,

$$\begin{aligned}
&\sum_{i=q+1}^{z} \psi(z+1, d(w_i)) - \sum_{i=2}^{x-1} \psi(x, d(u_i)) + \Phi(z+1, d(u_1)) - \Phi(x, d(u_1)) \\
\geq &\sum_{i=q+1}^{z} \psi(z+1, 2) - \sum_{i=2}^{x-1} \psi(x, 2) + \Phi(z+1, 2) - \Phi(x, 2) = 0.
\end{aligned}$$

Case 2. $d(u_1) = 1$. Then $d(u_2) = d(u_3) = \cdots = d(u_{x-1}) = 1$. By Lemma 2.1,

$$\begin{aligned}
&\sum_{i=q+1}^{z} \psi(z+1, d(w_i)) - \sum_{i=2}^{x-1} \psi(x, d(u_i)) + \Phi(z+1, d(u_1)) - \Phi(x, d(u_1)) \\
\geq &\sum_{i=q+1}^{z} \psi(z+1, 1) - \sum_{i=2}^{x-1} \psi(x, 1) + \Phi(z+1, 1) - \Phi(x, 1) \\
= &(z-q)\psi(z+1, 1) + \Phi(z+1, 1) - (x-2)\psi(x, 1) - \Phi(x, 1) \\
= &((z-1)\psi(z+1, 1) + \Phi(z+1, 1)) - ((x-2)\psi(x, 1) + \Phi(x, 1)) - (q-1)\psi(z+1, 1) \\
> &0 \quad \text{(by Lemma 5.2, as } x - 2 < z - 1).
\end{aligned}$$

This completes the proof of the lemma. □

Lemma 5.10. *If $x \geq 2$, then $h(x) = \psi(x, x)$ strictly increases.*

Proof. Since $x > 0$,

$$h'(x) = \frac{3x^2(16x^7 - 144x^6 + 536x^5 - 1047x^4 + 1134x^3 - 664x^2 + 192x - 24)}{8(2x-3)^4(x-1)^4} > 0,$$

and thus $h(x) = \psi(x, x)$ strictly increases with $x \geq 2$. □

Corollary 5.11. *If $z \geq 3$ and $z-1 \leq y \leq z$, then $\Phi(z+1, y+1) - \Phi(z, y) \geq \Phi(z+1, z) - \Phi(z, z-1)$.*

Proof. Since $\big(\Phi(z+1, z+1) - \Phi(z, z)\big) - \big(\Phi(z+1, z) - \Phi(z, z-1)\big) = \psi(z+1, z+1) - \psi(z, z) > 0$ by Lemma 5.10, we have $\Phi(z+1, y+1) - \Phi(z, y) \geq \Phi(z+1, z) - \Phi(z, z-1)$, as $z-1 \leq y \leq z$. □

Lemma 5.12. *If $12 \leq k \leq n-2$ and T_0 is an AZI-maximum tree of $\mathbb{T}_k^n$, then $T_0 \in \mathscr{T}(\pi)$.*

Proof. Let W_0 be the greedy tree of π_0, where $\pi_0 = (7^{(2)}, 2^{(n-14)}, 1^{(12)})$. By an elementary computation, we have

$$AZI(W_0) = \begin{cases} \Phi(7,7) + 8(n-2), & \text{if } n \geq 26; \\ \Phi(7,7) + (26-n)\Phi(7,1) + 16(n-14), & \text{if } 14 \leq n \leq 25. \end{cases} \tag{5.2}$$

For convenience, let $z = d_0$, $y = d_1$, $x = d_2$ and $b = d_3$. Let $\{w_1, w_2, \ldots, w_z\}$ be the children of v_0, $\{u_1, u_2, \ldots, u_{y-1}\}$ be the children of v_1, $\{s_1, s_2, \ldots, s_{x-1}\}$ be the children of v_2 and $\{h_1, h_2, \ldots, h_{b-1}\}$ be the children of v_3. Then, $v_1 = w_1$, $v_2 = w_2$ and $v_3 = w_3$, as $\Delta \geq 3$. Since $t \leq \Delta$ by Lemma 5.7, we have

$$d(h_{b-1}) \leq \cdots \leq d(h_1) \leq d(s_{x-1}) \leq \cdots \leq d(s_1) \leq d(u_{y-1}) \leq \cdots \leq d(u_2) \leq d(u_1) \leq 2. \tag{5.3}$$

As referred before, we suppose that T_0 is the greedy tree of $\mathscr{T}(\pi)$, where π is as described in (5.1). By contradiction, we assume that

$$\pi \neq \left(\left\lceil \frac{k}{2} \right\rceil + 1, \left\lfloor \frac{k}{2} \right\rfloor + 1, 2^{(n-k-2)}, 1^{(k)}\right). \tag{5.4}$$

Next, we will show the existence of another tree T_0^* of $\mathbb{T}_n^k$ with $AZI(T_0^*) > AZI(T_0)$ to get a contradiction. By Lemma 5.5, we have $t \geq 1$ if $k \geq 5$. Thus, we consider the following cases.

Case 1. $\Delta \geq 7$ **and** $t = 1$. By (5.4), we have $z \geq y+2$, as $y+z = 2(n-1) - 2(n-k-2) - k = k+2$. Let $T_0^* = T_0 - v_0w_2 + v_1w_2$. Then, $T_0^* \in \mathbb{T}_n^k$. Since $d(w_z) \leq d(w_{z-1}) \leq \cdots \leq d(w_2) = x \leq 2$ and $\Phi(y+1, 1) > \Phi(z, 1)$ by Lemma 2.2(i), it follows from Lemma 2.1 that

$$\begin{aligned}
&AZI(T_0^*) - AZI(T_0) \\
=&\Phi(z-1, y+1) + \sum_{i=3}^{z} \Phi(z-1, d(w_i)) + \sum_{i=1}^{y-1} \Phi(y+1, d(u_i)) \\
&+ \Phi(y+1, x) - \Phi(z, y) - \sum_{i=2}^{z} \Phi(z, d(w_i)) - \sum_{i=1}^{y-1} \Phi(y, d(u_i)) \\
=&\big(\Phi(z-1, y+1) - \Phi(z, y)\big) - \sum_{i=3}^{z} \psi(z, d(w_i)) + \sum_{i=1}^{y-1} \psi(y+1, d(u_i)) + \big(\Phi(y+1, x) - \Phi(z, x)\big) \\
\geq&\big(\Phi(z-1, y+1) - \Phi(z, y)\big) - \sum_{i=3}^{z} \psi(z, 2) + \sum_{i=1}^{y-1} \psi(y+1, 1) + \Phi(y+1, 2) - \Phi(z, 2) \\
=&\Phi(z-1, y+1) - \Phi(z, y) + (y-1)\psi(y+1, 1) \\
=&\psi(y+1, z-1) - \psi(z, y) + (y-1)\psi(y+1, 1) \\
\geq&\psi(y+1, y+1) - \psi(y+2, y) + (y-1)\psi(y+1, 1) \quad \text{(by Lemmas 5.1 and 2.1(iii), as } z \geq y+2) \\
=&\frac{3y^6 + 6y^5 - 30y^4 - 12y^3 + 28y^2 + 4y - 7}{8y^3(y-1)^2} > 0 \quad (\text{as } y \geq 3),
\end{aligned}$$

a contradiction.

Case 2. $\Delta \geq 7$, $t \geq 2$ **and** $d_2 \geq 4$. Let $T_0^* = T_0 - v_2s_1 - v_2s_2 + v_0s_1 + v_1s_2$ and let $\psi_6(z, x) = \Phi(z+1, z) - \Phi(z, z-1) + \Phi(z+1, x-2) - \Phi(z, x)$. Then, $T_0^* \in \mathbb{T}_n^k$ and $\psi_6(z, x) > 0$ by Lemma 5.4. Note that $z \geq y \geq x \geq 4$ and $y \geq z-1$ by Lemma 5.6. Thus, $\Phi(z+1, y+1) - \Phi(z, y) + \Phi(z+1, x-2) - \Phi(z, x) \geq \psi_6(z, x) > 0$ by Corollary 5.11. We have

$$\begin{aligned}
&AZI(T_0^*) - AZI(T_0) \\
=&\Phi(z+1, y+1) + \Phi(z+1, x-2) + \Phi(z+1, d(s_1)) + \Phi(y+1, d(s_2))
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{i=3}^{z}\Phi(z+1,d(w_i))+\sum_{i=1}^{y-1}\Phi(y+1,d(u_i))+\sum_{i=3}^{x-1}\Phi(x-2,d(s_i))\\
&-\sum_{i=1}^{z}\Phi(z,d(w_i))-\sum_{i=1}^{y-1}\Phi(y,d(u_i))-\sum_{i=1}^{x-1}\Phi(x,d(s_i))\\
=&\big(\Phi(z+1,y+1)-\Phi(z,y)\big)+\big(\Phi(z+1,x-2)-\Phi(z,x)\big)\\
&+\sum_{i=3}^{z}\psi(z+1,d(w_i))+\sum_{i=1}^{y-1}\psi(y+1,d(u_i))+\sum_{i=3}^{x-1}\big(\Phi(x-2,d(s_i))-\Phi(x,d(s_i))\big)\\
&+\big(\Phi(z+1,d(s_1))-\Phi(x,d(s_1))\big)+\big(\Phi(y+1,d(s_2))-\Phi(x,d(s_2))\big)\\
\geq&\sum_{i=3}^{z}\psi(z+1,d(w_i))+\sum_{i=1}^{y-1}\psi(y+1,d(u_i))-\sum_{i=3}^{x-1}\big(\psi(x,d(s_i))+\psi(x-1,d(s_i))\big)\\
&+\big(\Phi(z+1,d(s_1))-\Phi(x,d(s_1))\big)+\big(\Phi(y+1,d(s_2))-\Phi(x,d(s_2))\big)+\psi_6(z,x).
\end{aligned}
$$

Since $d(s_1)\leq d(u_1)\leq 2$ by (5.3), we consider the following three subcases.

Subcase 2.1. $d(s_1)=2$ **and** $d(s_2)=1$. Then, $d(w_1)\geq d(w_2)\geq\cdots\geq d(w_z)\geq 2$, $d(u_1)=d(u_2)=\cdots=d(u_{y-1})=2$ by (5.3), and $d(s_2)=d(s_3)=\cdots=d(s_{x-1})=1$. Since $\psi(z+1,d(w_i))\geq\psi(z+1,2)$ by Lemma 2.1, we have

$$
\begin{aligned}
AZI(T_0^*)-AZI(T_0)\geq&\sum_{i=3}^{z}\psi(z+1,2)+\sum_{i=1}^{y-1}\psi(y+1,2)-\sum_{i=3}^{x-1}\big(\psi(x,1)+\psi(x-1,1)\big)\\
&+\big(\Phi(z+1,2)-\Phi(x,2)\big)+\big(\Phi(y+1,1)-\Phi(x,1)\big)+\psi_6(z,x)\\
\geq&-(x-3)\big(\psi(x,1)+\psi(x-1,1)\big)+\big(\Phi(y+1,1)-\Phi(x,1)\big)+\psi_6(z,x)\\
=&-(x-2)\psi(x,1)-(x-3)\psi(x-1,1)-\Phi(x-1,1)+\Phi(y+1,1)+\psi_6(z,x)\\
>&-1-1+\Phi(x,1)+\Phi(y+1,1)+\psi_6(z,x)\qquad\text{(by Lemma 5.2, as } x\geq 4)\\
>&\psi_6(z,x)>0.
\end{aligned}
$$

Subcase 2.2. $d(s_1)=2$ **and** $d(s_2)=2$. Then, $d(w_1)\geq d(w_2)\geq\cdots\geq d(w_z)\geq 2$, and $d(u_1)=d(u_2)=\cdots=d(u_{y-1})=2$ by (5.3). By Lemma 2.1(i) and (ii),

$$
\begin{aligned}
AZI(T_0^*)-AZI(T_0)\geq&\sum_{i=3}^{z}\psi(z+1,2)+\sum_{i=1}^{y-1}\psi(y+1,2)-\sum_{i=3}^{x-1}\big(\psi(x,2)+\psi(x-1,2)\big)\\
&+\big(\Phi(z+1,2)-\Phi(x,2)\big)+\big(\Phi(y+1,2)-\Phi(x,2)\big)+\psi_6(z,x)\\
=&\psi_6(z,x)>0.
\end{aligned}
$$

Subcase 2.3. $d(s_1)=1$. Then $d(s_2)=d(s_3)=\cdots=d(s_{x-1})=1$ by (5.3). By Lemma 2.1,

$$
\begin{aligned}
&AZI(T_0^*)-AZI(T_0)\\
\geq&\sum_{i=3}^{z}\psi(z+1,1)+\sum_{i=1}^{y-1}\psi(y+1,1)-\sum_{i=3}^{x-1}\big(\psi(x,1)+\psi(x-1,1)\big)\\
&+\big(\Phi(z+1,1)-\Phi(x,1)\big)+\big(\Phi(y+1,1)-\Phi(x,1)\big)+\psi_6(z,x)\\
=&(z-2)\psi(z+1,1)+(y-1)\psi(y+1,1)-(x-3)\big(\psi(x,1)+\psi(x-1,1)\big)\\
&+\big(\Phi(z+1,1)-\Phi(x,1)\big)+\big(\Phi(y+1,1)-\Phi(x,1)\big)+\psi_6(z,x)\\
=&(z-1)\psi(z+1,1)+\Phi(z,1)+(y-1)\psi(y+1,1)+\Phi(y+1,1)\\
&-(x-1)\psi(x,1)-(x-3)\psi(x-1,1)-2\Phi(x-1,1)+\psi_6(z,x)\\
=&\big((z-1)\psi(z+1,1)+\Phi(z+1,1)\big)-\big((x-2)\psi(x,1)+\Phi(x,1)\big)+(y-1)\psi(y+1,1)\\
&+\Phi(y+1,1)-\big((x-3)\psi(x-1,1)+\Phi(x-1,1)\big)-\psi(z+1,1)+\psi_6(z,x)\\
>&-\psi(z+1,1)+\psi_6(z,x)\qquad\text{(by Lemma 5.2, as } x\geq 4)\\
>&\psi_6(z,x)>0\qquad\text{(by Lemma 2.1(i)).}
\end{aligned}
$$

Case 3. $\Delta \geq 7, t \geq 2$ **and** $d_2 = 3$**.** Then $y \geq z-1$ and $t = 2$ by Lemma 5.6, as $d_2 = 3$. Let $T_0^* = T_0 - v_2s_1 + v_0s_1$. Then, $T_0^* \in \mathbb{T}_n^k$. Since $x = d_2 = 3$, by Lemma 5.9, it follows that

$$\begin{aligned} AZI(T_0^*) - AZI(T_0) =& \psi(z+1, y) + \Phi(z+1, x-1) - \Phi(z, x) + \sum_{i=3}^{z} \psi(z+1, d(w_i)) \\ & - \sum_{i=2}^{x-1} \psi(x, d(s_i)) + \Phi(z+1, d(s_1)) - \Phi(x, d(s_1)) \\ \geq & \psi(z+1, y) + \Phi(z+1, 2) - \Phi(z, 3). \end{aligned} \tag{5.5}$$

Subcase 3.1. $\Delta = 7$**.** Then $6 \leq y \leq 7$, and $t = 2$ by Lemma 5.6, as $d_2 = 3$ and $v_2 = w_2$. If $y = 7$, then $AZI(T_0^*) - AZI(T_0) \geq \psi(8, 7) + \Phi(8, 2) - \Phi(7, 3) > 1.76 > 0$, a contradiction. Thus, $y = 6$, and so $12 \leq k \leq 7 + (6-2) + (3-2) = 12$ by Lemma 5.8. This implies that $k = 12$ and $\pi = \left(7, 6, 3, 2^{(n-15)}, 1^{(12)}\right)$.

If $n \geq 26$, then $AZI(T_0) \leq \Phi(7, 6) + \Phi(7, 3) + 8(n-3) < \Phi(7, 7) + 8(n-2) = AZI(W_0)$ by Lemma 2.2 and (5.2), as T_0 is a greedy tree of $\mathscr{T}(\pi)$.

If $20 \leq n \leq 25$, then $AZI(T_0) = \Phi(7, 6) + \Phi(7, 3) + 16(n-15) + 2\Phi(3, 1) + (25-n)\Phi(6, 1) < \Phi(7, 7) + 16(n-14) + (26-n)\Phi(7, 1) = AZI(W_0)$ by Lemma 2.3 and (5.2), as $\big(\Phi(7, 7) + 16(n-14) + (26-n)\Phi(7, 1)\big) - \big(\Phi(7, 6) + \Phi(7, 3) + 16(n-15) + 2\Phi(3, 1) + (25-n)\Phi(6, 1)\big) > 3.5 + (26-n)\Phi(7, 1) - (25-n)\Phi(6, 1) = (3781n + 42850)/27000 > 0$.

If $15 \leq n \leq 19$, then $AZI(T_0) = \Phi(7, 6) + \Phi(7, 3) + 16(n-15) + 2\Phi(3, 1) + 5\Phi(6, 1) + (20-n)\Phi(7, 1) < \Phi(7, 7) + 16(n-14) + (26-n)\Phi(7, 1) = AZI(W_0)$ by Lemma 2.3 and (5.2), as $\big(\Phi(7, 7) + 16(n-14) + (26-n)\Phi(7, 1)\big) - \big(\Phi(7, 6) + \Phi(7, 3) + 16(n-15) + 2\Phi(3, 1) + 5\Phi(6, 1) + (20-n)\Phi(7, 1)\big) > 6\Phi(7, 1) - 5.1 > 0$.

Subcase 3.2. $\Delta \geq 8$**.** Then, $y \geq z - 1 \geq 7$. By Lemma 5.1,

$$\begin{aligned} AZI(T_0^*) - AZI(T_0) \geq & \psi(z+1, z-1) + \Phi(z+1, 2) - \Phi(z, 3) \\ = & \frac{3\psi_7(z)}{8(2z-3)^3(z+1)^3} > 0, \qquad (\text{as } z \geq 8) \end{aligned}$$

where $\psi_7(z) = 4z^8 - 6z^7 - 433z^6 + 2344z^5 - 4467z^4 + 2714z^3 + 921z^2 - 612z - 585$.

Case 4. $\Delta = 6$**.** Then $t \geq 2$. Otherwise, $k \leq 10$ by Lemma 5.8, a contradiction. Two subcases occur as follows.

Subcase 4.1. $t \geq 3$**.** Then, $6 = z \geq y \geq x \geq z - 1 = 5$ by Lemma 5.6. Let $T_0^* = T_0 - v_3h_1 + v_0h_1$. Then, $T_0^* \in \mathbb{T}_n^k$.

$$\begin{aligned} & AZI(T_0^*) - AZI(T_0) \\ = & \psi(z+1, y) + \psi(z+1, x) + \Phi(z+1, b-1) - \Phi(z, b) \\ & + \sum_{i=4}^{z} \psi(z+1, d(w_i)) - \sum_{i=2}^{b-1} \psi(b, d(h_i)) + \Phi(z+1, d(h_1)) - \Phi(b, d(h_1)) \\ \geq & \psi(z+1, y) + \psi(z+1, x) + \Phi(z+1, b-1) - \Phi(z, b) \qquad (\text{by Lemma 5.9}) \\ \geq & 2\psi(7, 5) + \Phi(7, b-1) - \Phi(6, b) \qquad (\text{by Lemma 5.1}) \\ = & \frac{14977b^3 - 96000b^2 + 171660b + 43660}{108(b+4)^3} > 0, \qquad (\text{as } b \geq 3) \end{aligned} \tag{5.6}$$

a contradiction.

Subcase 4.2. $t = 2$**.** Then, $5 \leq y \leq 6$ by Lemma 5.6.

We first suppose that $y = 6$. Let $T_0^* = T_0 - v_2s_1 + v_0s_1$. Then, $T_0^* \in \mathbb{T}_n^k$. By Lemma 5.9 and (5.5), we have

$$\begin{aligned} AZI(T_0^*) - AZI(T_0) \geq & \psi(z+1, y) + \Phi(z+1, x-1) - \Phi(z, x) \\ \geq & \psi(7, 6) + \Phi(7, x-1) - \Phi(6, x) \\ > & 9.005 + \Phi(7, x-1) - \Phi(6, x) \\ = & \frac{27201x^3 - 184188x^2 + 292248x + 46664}{200(x+4)^3} \\ > & 0 \qquad (\text{as } x \geq 3 \text{ and } x \text{ is an integer}). \end{aligned}$$

We now suppose that $y = 5$. Then, $x = y = 5$ by Lemma 5.8, as $k \geq 12$ and $t = 2$. In this case, $k = 12$ and $\pi = \left(6, 5^{(2)}, 2^{(n-15)}, 1^{(12)}\right)$, where $n \geq 15$.

If $n \geq 26$, then $AZI(T_0) \leq 2\Phi(6, 5) + 8(n-3) < \Phi(7, 7) + 8(n-2) = AZI(W_0)$ by Lemma 2.2 and (5.2), as T_0 is a greedy tree of $\mathscr{T}(\pi)$.

If $19 \le n \le 25$, then $AZI(T_0) = 2\Phi(6,5)+16(n-15)+(27-n)\Phi(5,1) < \Phi(7,7)+16(n-14)+(26-n)\Phi(7,1) = AZI(W_0)$ by Lemma 2.2 and (5.2), as $\big(\Phi(7,7)+16(n-14)+(26-n)\Phi(7,1)\big) - \big(2\Phi(6,5)+16(n-15)+(27-n)\Phi(5,1)\big) > 10+(26-n)\Phi(7,1)-(27-n)\Phi(5,1) = (631n-2501)/1728 > 0$.

If $15 \le n \le 18$, then $AZI(T_0) = 2\Phi(6,5)+8\Phi(5,1)+16(n-15)+(19-n)\Phi(6,1) < \Phi(7,7)+16(n-14)+(26-n)\Phi(7,1) = AZI(W_0)$ by Lemma 2.2 and (5.2), as $\big(\Phi(7,7)+16(n-14)+(26-n)\Phi(7,1)\big) - \big(2\Phi(6,5)+8\Phi(5,1)+16(n-15)+(19-n)\Phi(6,1)\big) > (26-n)\Phi(7,1)-(19-n)\Phi(6,1)-5.7 = (3781n+74386)/27000 > 0$.

Case 5. $\Delta = 5$. Then $t \ge 3$ and thus $d_3 \ge 3$ by Lemma 5.8, as $k \ge 12$.

Subcase 5.1. $d_3 \ge 4$. Then, $y \ge x \ge b \ge 4$. Let $T_0^* = T_0 - v_3h_1 + v_0h_1$. Then, $T_0^* \in \mathbb{T}_n^k$. By Lemma 5.9 and (5.6), we have

$$\begin{aligned} AZI(T_0^*) - AZI(T_0) &\ge \psi(z+1,y)+\psi(z+1,x)+\Phi(z+1,b-1)-\Phi(z,b)\\ &= \psi(6,y)+\psi(6,x)+\Phi(6,b-1)-\Phi(5,b)\\ &\ge 2\psi(6,4)+\Phi(6,b-1)-\Phi(5,b) \text{ (by Lemma 5.1)}\\ &= \frac{3(11245b^3-66522b^2+96786b-1998)}{343(x+3)^3} > 0, \qquad (\text{as } x \ge 4) \end{aligned}$$

a contradiction.

Subcase 5.2. $d_3 = 3$. Then, $t = 3$ by Lemma 5.6, as $d_3 = 3$. Combining with $t = 3$ and $k \ge 12$, we have $x = y = 5$ and $b = 3$ by Lemma 5.8. This implies that $k = 12$ and $\pi = \big(5^{(3)}, 3, 2^{(n-16)}, 1^{(12)}\big)$, where $n \ge 16$.

If $n \ge 26$, then $AZI(T_0) \le 2\Phi(5,5)+\Phi(5,3)+8(n-4) < \Phi(7,7)+8(n-2) = AZI(W_0)$ by Lemma 2.2 and (5.2), as T_0 is a greedy tree of $\mathscr{T}(\pi)$.

If $16 \le n \le 25$, then $AZI(T_0) = 2\Phi(5,5)+\Phi(5,3)+2\Phi(3,1)+16(n-16)+(26-n)\Phi(5,1) < \Phi(7,7)+16(n-14)+(26-n)\Phi(7,1) = AZI(W_0)$ by Lemma 2.2 and (5.2), as $\big(\Phi(7,7)+16(n-14)+(26-n)\Phi(7,1)\big) - \big(2\Phi(5,5)+\Phi(5,3)+2\Phi(3,1)+16(n-16)+(26-n)\Phi(5,1)\big) > 16.5+(26-n)\Phi(7,1)-(26-n)\Phi(5,1) = (631n+12106)/1728 > 0$.

Case 6. $\Delta \le 4$. Then $12 \le k \le 4+4\times(4-2) = 12$ by Lemmas 5.7 and 5.8. This implies that $k = 12$ and $t = \Delta = 4$, and so $\pi = \big(4^{(5)}, 2^{(n-17)}, 1^{(12)}\big)$.

If $n \ge 26$, then $AZI(T_0) \le 4\Phi(4,4)+8(n-5) < \Phi(7,7)+8(n-2) = AZI(W_0)$ by Lemma 2.2 and (5.2), as T_0 is a greedy tree of $\mathscr{T}(\pi)$.

If $17 \le n \le 25$, then $AZI(T_0) = 4\Phi(4,4)+16(n-17)+(29-n)\Phi(4,1) < \Phi(7,7)+16(n-14)+(26-n)\Phi(7,1) = AZI(W_0)$ by Lemma 2.2 and (5.2), as $\big(\Phi(7,7)+16(n-14)+(26-n)\Phi(7,1)\big) - \big(4\Phi(4,4)+16(n-17)+(29-n)\Phi(4,1)\big) > 40+(26-n)\Phi(7,1)-(29-n)\Phi(4,1) = (169n+2710)/216 > 0$. □

Proof of Theorem 1.4. Let T_0 be an AZI-maximum tree of $\mathbb{T}_k^n$ and let W_0 be the unique greedy tree of $\mathscr{T}(\pi_0)$, where $\pi_0 = \Big(\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, 2^{(n-k-2)}, 1^{(k)}\Big)$. By Lemma 5.12 and Theorem 1.3, we have $T_0 \in \mathscr{T}(\pi_0)$ and $AZI(T_0) = AZI(W_0)$. Next, we show that $AZI(W_0) = f(n,k)$, where $f(n,k)$ is defined in Theorem 1.4. Actually, this depends on the structure of W_0.

Since $\Phi(2,y) = 8$ holds for any real number y, we only need to consider the edge v_0v_1 of W_0 and those pendent edges adjacent to either v_0 or v_1 in W_0.

If $0 \le n-k-2 \le \lceil \frac{k}{2} \rceil$, then there are exactly $\lfloor \frac{k}{2} \rfloor$ pendent edges adjacent to v_1 and exactly $\lceil \frac{k}{2} \rceil + k + 2 - n$ pendent edges adjacent to v_0.

If $\lceil \frac{k}{2} \rceil \le n-k-2 < k$, then there are exactly $2k+2-n$ pendent edges adjacent to v_1, and v_0 is not adjacent to any pendent edge.

If $n-k-2 \ge k$, then neither v_0 nor v_1 is adjacent to any pendent edge.

Since the structure of W_0 is unique, from the above arguments, we have $AZI(W_0) = f(n,k)$. Recall that $AZI(W_0) = AZI(T_0)$ and $T_0 \in \mathscr{T}(\pi_0)$. We have $T_0 \in \mathbb{T}_0$, as $d(v_0) > d(v_1)$ if k is odd and $d(v_0) = d(v_1)$ if k is even. Conversely, if $T_0 \in \mathbb{T}_0$, then it is easily checked that $AZI(T_0) = AZI(W_0)$. This completes the proof. □

6. Further discussion

Let H_0 be an extremal graph with maximum AZI of $\mathbb{G}_k^n$, where $n-1 \ge k \ge 1$. By Lemma 2.3, we have $\mathcal{R}(H_0) = K_{n-k}$. This implies that H_0 is obtained from K_{n-k} by attaching k pendent vertices to some vertices of K_{n-k}. However, the exact graphs that attain the maximum AZI of $\mathbb{G}_k^n$ are still unknown in general.

The bound $k \ge 12$ of Theorem 1.4 is optimal. To see this, we consider the class of trees with 11 pendent vertices and 25 vertices. Let $\pi = \big(7, 6, 2^{(12)}, 1^{(11)}\big)$, and let W_1 and W_2 be the two trees as shown in Fig. 1.1. From Theorem 1.3, W_1 is an AZI-maximum tree of $\mathscr{T}(\pi)$. However, $AZI(W_1) = \Phi(7,6)+23\times 8 < 239.7 < 240 < \Phi(6,5)+\Phi(6,4)+22\times 8 = AZI(W_2)$. Thus, Theorem 1.4 does not hold for $k = 11$.

As a supplement of Theorem 1.4, we list the maximum AZI of $\mathbb{T}_k^n$ for other k values in Table 6.1. Since the optimal (greedy) trees for $k = 2, 3$ are unique, we only consider the case of $4 \le k \le 11$. To show Table 6.1, we need the following (6.1), which can be proved similarly to the proof of Case 1 of Lemma 5.12.

Table 6.1
The maximum AZI of $\mathbb{T}_k^n$ for $4 \le k \le n-2$.

	The optimal degree sequence	The range of n	The maximum AZI of $\mathbb{T}_k^n$
$k \ge 12$	$\left(\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, 2^{(n-k-2)}, 1^{(k)}\right)$	$n \ge k+2$	$f(n,k)$
$k=11$	$(7,6,2^{(n-13)},1^{(11)})$	$13 \le n \le 24$	$f(n,11)$
	$(6,5,4,2^{(n-14)},1^{(11)})$	$n \ge 25$	$\Phi(6,5)+\Phi(6,4)+8(n-3)$
$k=10$	$(6^{(2)},2^{(n-12)},1^{(10)})$	$n \ge 12$	$f(n,10)$
$k=9$	$(6,5,2^{(n-11)},1^{(9)})$	$11 \le n \le 20$	$f(n,9)$
	$(5,4^{(2)},2^{(n-12)},1^{(9)})$	$n \ge 21$	$2\Phi(5,4)+8(n-3)$
$k=8$	$(5^{(2)},2^{(n-10)},1^{(8)})$	$10 \le n \le 18$	$f(n,8)$
	$(5,4,3,2^{(n-11)},1^{(8)})$	$n = 19, 20$	$\Phi(5,4)+\Phi(5,3)+8(n-3)$
	$(4,3^{(4)},2^{(n-13)},1^{(8)})$	$n \ge 21$	$4\Phi(4,3)+8(n-5)$
$k=7$	$(5,4,2^{(n-9)},1^{(7)})$	$9 \le n \le 16$	$f(n,7)$
	$(4^{(2)},3,2^{(n-10)},1^{(7)})$	$n = 17$	$\Phi(4,4)+\Phi(4,3)+112$
	$(4,3^{(3)},2^{(n-11)},1^{(7)})$	$n \ge 18$	$3\Phi(4,3)+8(n-4)$
$k=6$	$(4^{(2)},2^{(n-8)},1^{(6)})$	$8 \le n \le 14$	$f(n,6)$
	$(4,3^{(2)},2^{(n-9)},1^{(6)})$	$n \ge 15$	$2\Phi(4,3)+8(n-3)$
$k=5$	$(4,3,2^{(n-7)},1^{(5)})$	$7 \le n \le 12$	$f(n,5)$
	$(3^{(3)},2^{(n-8)},1^{(5)})$	$n \ge 13$	$2\Phi(3,3)+8(n-3)$
$k=4$	$(3^{(2)},2^{(n-6)},1^{(4)})$	$n \ge 6$	$f(n,4)$

$$d_0 - d_1 \le 1 \text{ if } t = 1 \text{ for } d_0 \ge 4. \tag{6.1}$$

When $k \le 11$, if $t \ge 5$, then $\Delta \ge 5$ by Lemma 5.7, and thus $11 \ge k \ge \Delta + (t-1)(\Delta - 3) + 1 \ge 14$ by Lemmas 5.6 and 5.8, a contradiction. Thus,

$$t \le 4 \text{ for } k \le 11.$$

We only give a proof for $k = 11$ in the following, and the case of $4 \le k \le 10$ can be proved similarly.

If $t = 1$, then

$$11 = k = d_0 + d_1 - 2 \ge 2d_0 - 3$$

by (6.1) and Lemma 5.8. This implies that $d_0 \le 7$. Combining this with $d_0 + d_1 - 2 = 11$, we can conclude that the degree sequence of the optimal (greedy) tree is equal to $(7,6,2^{(n-13)},1^{(11)})$.

If $t = 2$, then $d_1 \ge d_0 - 1$ by Lemma 5.6 and thus $11 = k = d_0 + d_1 + d_2 - 4 \ge 2d_0 - 2$ by Lemma 5.8. This implies that $d_0 \le 6$. Combining this with $11 = d_0 + d_1 + d_2 - 4$ and $d_1 \ge d_0 - 1$, we can deduce that the degree sequences of the optimal (greedy) trees is equal to $(6,5,4,2^{(n-14)},1^{(11)})$, $(6^{(2)},3,2^{(n-14)},1^{(11)})$ or $(5^{(3)},2^{(n-14)},1^{(11)})$.

If $t = 3$, then $d_1 \ge d_2 \ge d_0 - 1$ by Lemma 5.6 and thus $11 = k = d_0 + d_1 + d_2 + d_3 - 6 \ge 3d_0 - 5$ by Lemma 5.8. This implies that $d_0 \le 5$. Combining this with $11 = d_0 + d_1 + d_2 + d_3 - 6$ and $d_1 \ge d_2 \ge d_0 - 1$, we can deduce that the degree sequences of the optimal (greedy) trees is equal to $(5^{(2)},4,3,2^{(n-15)},1^{(11)})$ or $(5,4^{(3)},2^{(n-15)},1^{(11)})$. Similarly, we can show that the degree sequence of the optimal (greedy) tree is equal to $(4^{(4)},3,2^{(n-16)},1^{(11)})$ for $t = 4$.

If $n \ge 27$, then every pendent vertex is adjacent to a 2-vertex in the greedy tree, and thus the AZI of greedy trees of these seven degree sequences are $\Phi(7,6)+8(n-2)$, $\Phi(6,6)+\Phi(6,3)+8(n-3)$, $\Phi(6,5)+\Phi(6,4)+8(n-3)$, $2\Phi(5,5)+8(n-3)$, $\Phi(5,5)+\Phi(5,4)+\Phi(5,3)+8(n-4)$, $3\Phi(5,4)+8(n-4)$ and $3\Phi(4,4)+\Phi(4,3)+8(n-5)$, respectively. It is straightly check that $\Phi(6,5)+\Phi(6,4)+8(n-3)$ is the maximum AZI of $\mathbb{T}_{11}^n$.

Otherwise, $13 \le n \le 26$. In this case, we can calculate the AZI of optimal greedy trees of these seven degree sequences for each n with $13 \le n \le 26$. With the help of Matlab, we can check straightly that the greedy tree with degree sequence $(6,5,4,2^{(n-14)},1^{(11)})$ has the maximum AZI of $\mathbb{T}_{11}^n$ for $25 \le n \le 26$, and the greedy tree with degree sequence $(7,6,2^{(n-13)},1^{(11)})$ obtains the maximum AZI of $\mathbb{T}_{11}^n$ for $13 \le n \le 24$.

Declaration of competing interest

There is no competing interest.

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On general *ABC*-type index of connected graphs☆

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ABSTRACT

For a simple connected graph $G = (V, E)$, define

$$ABC_\alpha(G;\beta) = \sum_{uv\in E}\left[\frac{d_G(u)+d_G(v)-\beta}{d_G(u)d_G(v)}\right]^\alpha,$$

for any $\alpha \in \mathbb{R}\setminus\{0\}$ and $\beta \in \mathbb{R}$. This topological index generalizes the famous *ABC* index, augmented Zagreb index, and inverse sum indeg index. Let $\Gamma(\pi)$ be the class of connected graphs with given degree sequence π. In this paper, under different conditions of α and β, we show that (*i*) For any connected graph G with $uv \notin E(G)$, $ABC_\alpha(G+uv;\beta) > ABC_\alpha(G;\beta)$ holds; (*ii*) For any given degree sequence π with minimum degree 1, there exists a **special extremal** *BFS*-**graph** (see Definition 1.2) for $ABC_\alpha(G;\beta)$ in the class of $\Gamma(\pi)$; (*iii*) For any given c-cyclic degree sequence π with minimum degree 1 and $c \in \{0, 1, 2\}$, there exists a **precise maximum extremal** *BFS*-**graph** (see Definition 1.3) for $ABC_\alpha(G;\beta)$ in the class of $\Gamma(\pi)$. These extend the main results of (Chen et al., 2021; Lin et al., 2013; Lin et al., 2018; Chen and Hao, 2018).

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1. Introduction

Throughout this paper, we only consider undirected simple connected graphs, and $G = (V, E)$ is a simple graph. As usual, let $d_G(u)$ and $N_G(u)$ denote the degree and neighbor set of vertex u in G. When there are no ambiguities, we simplify $d_G(u)$ and $N_G(u)$ as $d(u)$ and $N(u)$, respectively. If $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d(v_i)$, $1 \le i \le n$, then $\pi = (d_1, d_2, \ldots, d_n)$ is called the **degree sequence** of G. In what follows, we always suppose that $d_1 \ge d_2 \ge \cdots \ge d_n$ and denote by $\Gamma(\pi)$ the class of connected graphs with degree sequence π. A connected graph with n vertices and $n + c - 1$ edges will be referred as a c-**cyclic graph**. Particularly, when $c = 0$, 1, and 2, a c-cyclic graph is also called a tree, unicyclic graph, and bicyclic graph, respectively.

To study the strain energy of cycloalkanes and the stability of alkanes, E. Estrada et al. [1] put forward the notation of **atom-bond connectivity index**, $ABC(G)$ for a graph G, where

$$ABC(G) = \sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}.$$

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Later, to better understand the correlation properties of the atom-bond connectivity index for the heat of formation of alkanes, B. Furtula et al. [2] generalized the atom-bond connectivity index to the **general atom-bond connectivity index** $ABC_\alpha(G)$, where

$$ABC_\alpha(G) = \sum_{uv\in E(G)} \left[\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}\right]^\alpha \text{ for any } \alpha \in \mathbb{R}\setminus\{0\}. \tag{1.1}$$

We would like to point out that $ABC_{-3}(G)$ is also known as the **augmented Zagreb index** $AZI(G)$ of graph G, which received much attention recently (see [3–5]).

Another famous topological index similar with $ABC(G)$, is the **inverse sum indeg index** $ISI(G)$ of graph G [6], where

$$ISI(G) = \sum_{uv\in E(G)} \left[\frac{d_G(u)+d_G(v)}{d_G(u)d_G(v)}\right]^{-1}.$$

The inverse sum indeg index is shown to have a nice predicting ability for the total surface area of octane isomers [7]. Motivated from (1.1), we may establish the general case for $ISI(G)$, that is,

$$ISI_\alpha(G) = \sum_{uv\in E(G)} \left[\frac{d(u)+d(v)}{d(u)d(v)}\right]^\alpha. \tag{1.2}$$

Actually, we can unify $ABC_\alpha(G)$ and $ISI_\alpha(G)$ to a **general** ABC**-type index** $ABC_\alpha(G;\beta)$ for a graph G, where

$$ABC_\alpha(G;\beta) = \sum_{uv\in E(G)} \left[\frac{d_G(u)+d_G(v)-\beta}{d_G(u)d_G(v)}\right]^\alpha \text{ for any } \alpha \in \mathbb{R}\setminus\{0\} \text{ and } \beta\in\mathbb{R}. \tag{1.3}$$

It is easily checked that $ABC(G) = ABC_{\frac{1}{2}}(G;2)$, $AZI(G) = ABC_{-3}(G;2)$ and $ISI(G) = ABC_{-1}(G;0)$.

Recently, the research on extremal problem of (general) atom-bond connectivity index has received much attention [8–17]. In this line, Chen et al. [9] showed the following useful property of ABC_α for connected graphs.

Theorem 1.1 ([9]). *Let G be a connected graph with two non-adjacent vertices u and v. If $\alpha \le 1/2$ and $\alpha \ne 0$, then $ABC_\alpha(G+uv;2) > ABC_\alpha(G;2)$.*

In this paper, we will extent Theorem 1.1 to general ABC-type index for special α and β, that is,

Theorem 1.2. *Let G be a connected graph with at least three vertices and non-adjacent vertices u and v. If either $0<\alpha\le 1/2$, $-1\le\beta\le 2$ or $\alpha<0$, $\beta\le 2$ holds, then $ABC_\alpha(G+uv;\beta) > ABC_\alpha(G;\beta)$.*

We cannot replace the condition "$-1\le\beta\le 2$" of Theorem 1.2 by "$\beta\le 2$", since we have $ABC_\alpha(G+uv;\beta) < ABC_\alpha(G;\beta)$ in the case $\alpha = 1/2$ and $\beta = -10$ if $d(u) = d(v) = 5$ and each neighbor of either u or v is a vertex with degree two in G.

It is interesting to determine the extremal graphs for different topological indices in the class of connected graphs with given degree sequences. In this line, Lin et al. showed that there exists a BFS-graph with maximal ISI index [18] (resp. minimal ABC index [19], and maximum AZI index [20]) in the class of $\Gamma(\pi)$, where a BFS-graph is defined as follows:

Definition 1.1. Let G be a connected graph. We say that G is a BFS-**graph** if there exists a vertex ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ satisfying:
(*i*) $d(v_1)\ge d(v_2)\ge\cdots\ge d(v_n)$ and $h(v_1)\le h(v_2)\le\cdots\le h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1;
(*ii*) let $v\in N(u)\backslash N(w)$ and $z\in N(w)\backslash N(u)$ such that $h(v) = h(u)+1$ and $h(z) = h(w)+1$. If $u\prec w$, then $v\prec z$.

Definition 1.2. For a c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$ and $n\ge 3$, if G is a BFS-graph such that $\{v_1, v_2, v_3\}$ forms a triangle of G when $c\ge 1$, then G is called a **special extremal** BFS-**graph**.

The following results extend the main results of [18–20].

Theorem 1.3. *For any given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$,*
(*i*) *if either $\alpha<0$, $\beta\le 2$ or $\alpha\ge 1$, $\beta\le 0$, $(\alpha-1)^2+\beta^2\ne 0$ holds, then there exists a special extremal BFS-graph with maximum $ABC_\alpha(G;\beta)$ in the class of $\Gamma(\pi)$;*
(*ii*) *if $0<\alpha\le 1$, $0\le\beta\le 2$ and $(\alpha-1)^2+\beta^2\ne 0$, then there exists a special extremal BFS-graph with minimum $ABC_\alpha(G;\beta)$ in the class of $\Gamma(\pi)$.*

Hereafter, we use the symbol $p^{(q)}$ to define q copies of the real number p. In [21] the authors show that for any tree degree sequence π there exists a unique BFS-tree, here denoted by $T_M(\pi)$. The BFS-trees are also called greedy trees in the literature, e.g. [19,20]. In fact, we can also construct a unique unicyclic BFS-graph $U_M(\pi)$ by the following breadth-first-search method for any unicyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$ (see [22]): The unique cycle of $U_M(\pi)$ is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Select the vertex v_1 as the root vertex and begin with v_1 of the

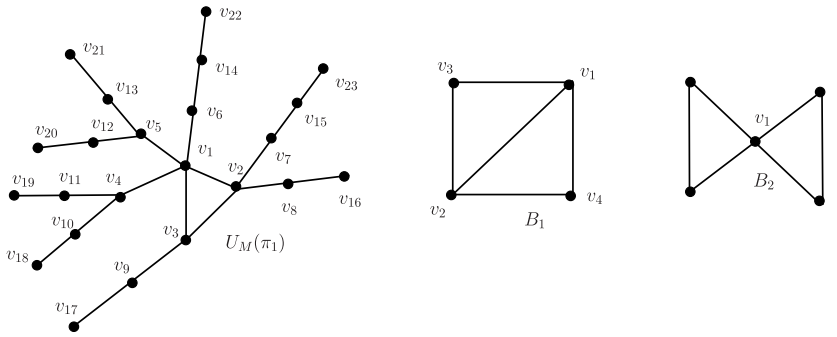


Fig. 1. The graphs $U_M(\pi_1)$, B_1 and B_2.

zeroth layer. Select the vertices v_2, v_3, v_4, v_5,..., v_{d_1+1} as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$. Let $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$ and $N(v_3) = \{v_1, v_2, v_{d_1+d_2}, \ldots, v_{d_1+d_2+d_3-3}\}$. Then, append $d_4 - 1$ vertices to v_4 such that $N(v_4) = \{v_1, v_{d_1+d_2+d_3-2}, \ldots, v_{d_1+d_2+d_3+d_4-4}\}$, and so on. Informally, the *BFS*-unicyclic graph is constructed from a *BFS*-tree by adding an edge between v_2 and v_3. As an example, consider the unicyclic degree sequence $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, $U_M(\pi_1)$ is depicted in Fig. 1.

Denote by $\mathcal{R}(G)$ the **reduced graph** obtained from G by recursively deleting pendant vertices to the resultant graph until no pendant vertices remain. If $c \geq 1$ and G is a c-cyclic graph, then $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a c-cyclic graph.

Some paths P_{l_1}, P_{l_2}, ..., P_{l_k} are said to have almost equal lengths if their lengths pairwise differ at most by 1, that is, $|l_i - l_j| \leq 1$ for $1 \leq i < j \leq k$. Let B_1 and B_2 be the two bicyclic graphs depicted in Fig. 1. If $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence with $d_n = 1$, then $\sum_{i=1}^{n} d_i = 2n + 2$, which implies that π should be one of the following two cases. When $d_n = 1$, we construct a unique bicyclic graph $B_M(\pi)$ of $\Gamma(\pi)$ as follows:
(*i*) If $d_n = 1$ and $d_1 \geq d_2 \geq 3$, then let $B_M(\pi)$ be a *BFS*-graph such that $\mathcal{R}(B_M(\pi)) = B_1$ and the remaining vertices appear in a *BFS*-ordering.
(*ii*) If $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$, then let $B_M(\pi)$ be the bicyclic graph with n vertices obtained from B_2 by attaching $d_1 - 4$ paths of almost equal lengths to the v_1 of B_2 (see Fig. 1).

Definition 1.3. For a given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, we say that G is a **precise maximum extremal graph** of $\Gamma(\pi)$, if G has maximum $ABC_\alpha(G; \beta)$ among all graphs of $\Gamma(\pi)$ for $\alpha < 0$ and $\beta \leq 2$.

Theorem 1.4. *For any c-cyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, then*
(*i*) *$T_M(\pi)$ is a precise maximum extremal graph for $c = 0$;*
(*ii*) *$U_M(\pi)$ is a precise maximum extremal graph for $c = 1$;*
(*iii*) *$B_M(\pi)$ is a precise maximum extremal graph for $c = 2$.*

Remark 1.1. *Recall that $ABC(G) = ABC_{\frac{1}{2}}(G; 2)$, $AZI(G) = ABC_{-3}(G; 2)$ and $ISI(G) = ABC_{-1}(G; 0)$. Thus, Theorem 1.3 also holds for $ABC(G)$, $AZI(G)$ and $ISI(G)$, that is the main results of [18–20]. Moreover, Theorem 1.4 also holds for $AZI(G)$ and $ISI(G)$.*

Here, we have to point out that extremal graphs of $ABC_\alpha(G; \beta)$ in the class of $\Gamma(\pi)$ maybe be not *BFS*-graphs. For instance, some examples can be found in [19,20,22].

2. The proof of Theorem 1.2

In this section, we define $\Phi_\alpha(x, y; \beta)$ and $\psi_\alpha(x, y; \beta)$ as follows:

$$\Phi_\alpha(x, y; \beta) = \left(\frac{x + y - \beta}{xy}\right)^\alpha, \text{ and } \psi_\alpha(x, y; \beta) = \left(\frac{x + y - \beta}{xy}\right)^\alpha - \left(\frac{x + y - \beta - 1}{(x - 1)y}\right)^\alpha,$$

where $\min\{x, y\} \geq 1$, $\max\{x, y\} \geq 2$ and $\beta \leq 2$. Since $x + y - \beta - 1 \geq 0$ and 0^α is meaningless for $\alpha < 0$, in the rest discussion we always suppose that $x + y - \beta - 1 > 0$ for $\alpha < 0$.

Lemma 2.1. *Let x, y, α and β be four real numbers with $y \geq 1$. If $x \geq 2 \geq \beta$, then*

$$\psi_\alpha(x, y; \beta) \begin{cases} \geq 0, & \text{if } \alpha(y - \beta) \leq 0, \\ < 0, & \text{if } \alpha(y - \beta) > 0. \end{cases} \tag{2.1}$$

Proof. If $y = \beta$, then $\psi_\alpha(x, y; \beta) = 0$, and so (2.1) holds. Next, we suppose that $y \neq \beta$. To show (2.1), we define $g(z) = z^\alpha$, let $z_1 = \frac{x+y-\beta}{xy}$ and $z_2 = \frac{x+y-\beta-1}{(x-1)y}$.

By the Lagrange Mean Value Theorem and since

$$z_1 - z_2 = \frac{x+y-\beta}{xy} - \frac{x+y-\beta-1}{(x-1)y} = -\frac{y-\beta}{(x-1)xy},$$

we have

$$\begin{aligned}\psi_\alpha(x,y;\beta) &= g(z_1) - g(z_2)\\ &= \alpha(z_1-z_2)\xi^{\alpha-1}\\ &= -\frac{\alpha(y-\beta)}{(x-1)xy}\xi^{\alpha-1}\begin{cases} > 0, & \text{if } \alpha(y-\beta) < 0,\\ < 0, & \text{if } \alpha(y-\beta) > 0,\end{cases}\end{aligned} \tag{2.2}$$

where $\xi \in (z_2, z_1)$ if $y < \beta$, and $\xi \in (z_1, z_2)$ if $y > \beta$, and thus the result holds. □

Lemma 2.2. *Let x be an integer with $x \geq 1$, α and β be two real numbers. If $1 < \beta \leq 2$ and $\alpha < 0$, then*

$$\left[\left(\frac{x+2-\beta}{x+1}\right)^\alpha - \left(\frac{x+1-\beta}{x}\right)^\alpha\right](x-1) \geq \left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha. \tag{2.3}$$

Proof. It is easily checked that (2.3) holds for $x = 1$ or $x = 2$. Thus, we suppose that $x \geq 3$ in the following. By the Lagrange Mean Value Theorem, there exist $\xi_1 \in \left(\frac{x+1-\beta}{x}, \frac{x+2-\beta}{x+1}\right)$ and $\xi_2 \in \left(\frac{3-\beta}{2}, \frac{4-\beta}{3}\right)$ such that

$$\left(\frac{x+2-\beta}{x+1}\right)^\alpha - \left(\frac{x+1-\beta}{x}\right)^\alpha = \frac{\alpha(\beta-1)}{x(x+1)}\xi_1^{\alpha-1}, \text{ and } \left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha = \frac{\alpha(\beta-1)}{6}\xi_2^{\alpha-1}. \tag{2.4}$$

To show (2.3), it suffices to show that

$$6\xi_2^{1-\alpha} \leq \frac{x(x+1)}{x-1}\xi_1^{1-\alpha}. \tag{2.5}$$

Since $\xi_1 \in \left(\frac{x+1-\beta}{x}, \frac{x+2-\beta}{x+1}\right)$ and $\xi_2 \in \left(\frac{3-\beta}{2}, \frac{4-\beta}{3}\right)$, to show (2.5), we only need to show that

$$g(3) = 6\left(\frac{4-\beta}{3}\right)^{1-\alpha} \leq \frac{x(x+1)}{x-1}\left(\frac{x+1-\beta}{x}\right)^{1-\alpha} = g(x). \tag{2.6}$$

Since $(x+2)(x-1) \geq x^2$ and $x(x+2-\beta) > (x+1)(x+1-\beta)$, we have

$$\frac{g(x+1)}{g(x)} = \frac{(x+2)(x-1)}{x^2}\left[\frac{x(x+2-\beta)}{(x+1)(x+1-\beta)}\right]^{1-\alpha} > 1,$$

and thus $g(x) \geq g(3)$. This completes the proof. □

Lemma 2.3. *For any real numbers $\alpha < 0$ and $1 < \beta \leq 2$, the function*

$$f(\beta) = \left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha$$

is strictly decreasing with respect to β.

Proof. We just need to prove

$$f'(\beta) = -\alpha\left[\frac{(4-\beta)^{\alpha-1}}{3^\alpha} - \frac{(3-\beta)^{\alpha-1}}{2^\alpha}\right] < 0,$$

which is equivalent to

$$\left(\frac{2}{3}\right)^\alpha < \left(\frac{3-\beta}{4-\beta}\right)^{\alpha-1}. \tag{2.7}$$

Since $\beta > 1$ and $0 < 3-\beta < 4-\beta$, we have

$$\left(\frac{2}{3}\right)^\alpha < \left(\frac{3-\beta}{4-\beta}\right)^\alpha < \left(\frac{3-\beta}{4-\beta}\right)^{\alpha-1}.$$

This implies that (2.7) holds, and thus $f(\beta)$ is strictly decreasing for $1 < \beta \leq 2$. □

Lemma 2.4. *Let x and y be two integers with $x \geq y \geq 2$, α and β be two real numbers. If $1 < \beta \leq 2$ and $\alpha < 0$, then*

$$\Phi_\alpha(x+1, y+1; \beta) + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha > 0. \tag{2.8}$$

Proof. First we show that

$$\Phi_\alpha(x+1, y+1; \beta) \geq \left(\frac{6-\beta}{9}\right)^\alpha. \tag{2.9}$$

Since $\alpha < 0$, it suffices to show that $9(x+y+2-\beta) \leq (6-\beta)(x+1)(y+1)$. Denote by $g(x, y; \beta) = 9(x+y+2-\beta) - (6-\beta)(x+1)(y+1)$. Since $\frac{\partial g(x,y;\beta)}{\partial \beta} = x+y+xy-8 \geq 0$, $g(x, y; \beta) \leq g(x, y; 2) = 5x+5y-4xy-4 = f(x, y)$. Now, since $\frac{\partial f(x,y)}{\partial x} = 5-4y < 0$, we have $g(x, y; \beta) \leq f(x, y) \leq f(2, y) = 3(2-y) \leq 0$. Therefore, (2.9) holds.

Next we show that

$$\left(\frac{6-\beta}{9}\right)^\alpha + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha > 0. \tag{2.10}$$

Notice that $\left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha$ is strictly decreasing with respect to β and $\left(\frac{6-\beta}{9}\right)^\alpha$ is strictly increasing with respect to β.

Case 1. $1 < \beta \leq 1.8$. We have

$$\begin{aligned}
&\left(\frac{6-\beta}{9}\right)^\alpha + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha \\
>&\left(\frac{5}{9}\right)^\alpha + 2\left(\frac{2.2}{3}\right)^\alpha - 2\left(\frac{1.2}{2}\right)^\alpha \\
=&0.6^\alpha\left[\left(\frac{25}{27}\right)^\alpha + 2\left(\frac{11}{9}\right)^\alpha - 2\right] = 0.6^\alpha h_1(\alpha).
\end{aligned}$$

By a routine calculation, we have

$$h_1'(\alpha) = \left(\frac{25}{27}\right)^\alpha \ln\frac{25}{27} + 2\left(\frac{11}{9}\right)^\alpha \ln\frac{11}{9} = \left(\frac{11}{9}\right)^\alpha\left[\left(\frac{25}{33}\right)^\alpha \ln\frac{25}{27} + 2\ln\frac{11}{9}\right],$$

and $h_1''(\alpha) = \left(\frac{25}{27}\right)^\alpha \left(\ln\frac{25}{27}\right)^2 + 2\left(\frac{11}{9}\right)^\alpha \left(\ln\frac{11}{9}\right)^2 > 0$.

Since $h_1'(\alpha) = 0$ has a unique root

$$\alpha_1 = \frac{\ln\left[-2\ln(11/9)/\ln(25/27)\right]}{\ln(25/33)} < -5.945 < 0$$

and $h_1''(\alpha) > 0$, we have

$$h_1(\alpha) \geq h_1(\alpha_1) > 0.185 > 0,$$

and thus (2.10) holds.

Case 2. $1.8 < \beta \leq 1.9$. We have

$$\begin{aligned}
&\left(\frac{6-\beta}{9}\right)^\alpha + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha \\
>&\left(\frac{4.2}{9}\right)^\alpha + 2\left(\frac{2.1}{3}\right)^\alpha - 2\left(\frac{1.1}{2}\right)^\alpha \\
=&\left(\frac{1.1}{2}\right)^\alpha\left[\left(\frac{28}{33}\right)^\alpha + 2\left(\frac{14}{11}\right)^\alpha - 2\right] = \left(\frac{1.1}{2}\right)^\alpha h_2(\alpha).
\end{aligned}$$

It is easily checked that $h_2'(\alpha) = 0$ has a unique root

$$\alpha_2 = \frac{\ln\left[-2\ln(14/11)/\ln(28/33)\right]}{\ln(2/3)} < -2.65 < 0$$

and $h_2''(\alpha) > 0$, we have

$$h_2(\alpha) \geq h_2(\alpha_2) > 0.6 > 0,$$

and thus (2.10) holds.

Case 3. $1.9 < \beta \leq 2$. We have

$$\left(\frac{6-\beta}{9}\right)^\alpha + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha$$

$$> \left(\frac{4.1}{9}\right)^{\alpha} + 2\left(\frac{2}{3}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}$$
$$= \left(\frac{1}{2}\right)^{\alpha}\left[\left(\frac{41}{45}\right)^{\alpha} + 2\left(\frac{4}{3}\right)^{\alpha} - 2\right] = \left(\frac{1}{2}\right)^{\alpha} h_3(\alpha).$$

It is easily checked that $h_3'(\alpha) = 0$ has a unique root

$$\alpha_3 = \frac{\ln\left[-2\ln(4/3)/\ln(41/45)\right]}{\ln(41/60)} < -4.78 < 0$$

and $h_3''(\alpha) > 0$, we have

$$h_3(\alpha) \geq h_3(\alpha_3) > 0.066 > 0,$$

and thus (2.10) holds. □

Lemma 2.5. *Let x and y be two real numbers with $\min\{x, y\} \geq 1$ and $x + y > 2$. If $0 < \alpha \leq 1/2$ and $-1 \leq \beta \leq 2$, then*

$$f(x, y; \beta) = \frac{x-\beta}{x} \cdot \left(\frac{x+y+1-\beta}{x}\right)^{\alpha-1} < 1. \tag{2.11}$$

Proof. If $0 < \beta \leq 2$, then it is easily to see that (2.11) holds. Next, we suppose that $-1 \leq \beta \leq 0$. Note that

$$f(x, y; \beta) = \frac{x-\beta}{x} \cdot \left(\frac{x}{x+y+1-\beta}\right)^{1-\alpha}$$
$$\leq \frac{x-\beta}{x} \cdot \sqrt{\frac{x}{x+y+1-\beta}} = \frac{x-\beta}{\sqrt{x(x+y+1-\beta)}}.$$

Thus, to show (2.11), it suffices to show that $(x-\beta)^2 < x(x+y+1-\beta)$. Let $g(\beta) = x(x+y+1-\beta) - (x-\beta)^2 = x\beta + x + xy - \beta^2$. Since $g'(\beta) = x - 2\beta > 0$, we have $g(\beta) \geq g(-1) = xy - 1 > 0$, and hence $(x-\beta)^2 < x(x+y+1-\beta)$, as desired. □

Proof of Theorem 1.2. Suppose that $d(u) \geq d(v) \geq 1$. By (1.3), we have

$$ABC_\alpha(G + uv; \beta) - ABC_\alpha(G; \beta)$$
$$= \sum_{y \in N_G(u)} \psi_\alpha\big(d(u)+1, d(y); \beta\big) + \sum_{y \in N_G(v)} \psi_\alpha\big(d(v)+1, d(y); \beta\big) + \Phi_\alpha\big(d(u)+1, d(v)+1; \beta\big).$$

Case 1. $0 < \alpha \leq 1/2$ and $-1 \leq \beta \leq 2$. For any vertex w of G, denote by $N_G^*(w) = \{y : d_G(w) > \beta\}$. By (2.2) with $x = d(u) + 1$, for any vertex $y \in N_G^*(u)$, which satisfies $d(y) > \beta$, we have

$$\psi_\alpha\big(d(u)+1, d(y); \beta\big) = -\frac{\alpha\big(d(y)-\beta\big)}{d(u)\big(d(u)+1\big)d(y)}\xi^{\alpha-1}$$
$$\geq -\frac{\alpha\big(d(y)-\beta\big)}{d(u)\big(d(u)+1\big)d(y)}\left[\frac{d(u)+d(y)+1-\beta}{\big(d(u)+1\big)d(y)}\right]^{\alpha-1}$$
$$= -\frac{\alpha}{d(u)\big(d(u)+1\big)^{\alpha}}\frac{d(y)-\beta}{d(y)}\left[\frac{d(u)+d(y)+1-\beta}{d(y)}\right]^{\alpha-1}$$
$$> -\frac{\alpha}{d(u)\big(d(u)+1\big)^{\alpha}}. \text{ (by Lemma 2.5)}$$

By Lemma 2.1, for any vertex $y \in N_G(u) \setminus N_G^*(u)$, we have $\psi_\alpha\big(d(u)+1, d(y); \beta\big) \geq 0$, as $\alpha > 0$. Thus,

$$ABC_\alpha(G + uv; \beta) - ABC_\alpha(G; \beta)$$
$$\geq \sum_{y \in N_G^*(u)} \psi_\alpha\big(d(u)+1, d(y); \beta\big) + \sum_{y \in N_G^*(v)} \psi_\alpha\big(d(v)+1, d(y); \beta\big) + \Phi_\alpha\big(d(u)+1, d(v)+1; \beta\big)$$
$$> -\frac{\alpha}{\big(d(u)+1\big)^{\alpha}} - \frac{\alpha}{\big(d(v)+1\big)^{\alpha}} + \left[\frac{d(u)+d(v)+2-\beta}{\big(d(u)+1\big)\big(d(v)+1\big)}\right]^{\alpha}$$
$$\geq -\frac{2\alpha}{\big(d(v)+1\big)^{\alpha}} + \frac{1}{\big(d(v)+1\big)^{\alpha}} \geq 0. \text{ (since } d(u) \geq d(v) \geq 1)$$

Case 2. $\alpha < 0$ and $\beta \le 1$. By Lemma 2.1, for any vertex y of $N_G^*(u)$, we have $\psi_\alpha\big(d(u)+1, d(y); \beta\big) > 0$. Combining this with $\beta \le 1 \le d(v) \le d(u)$ and Lemma 2.1,

$$\begin{aligned}
&ABC_\alpha(G+uv;\beta) - ABC_\alpha(G;\beta)\\
\ge &\sum_{y\in N_G(u)\setminus N_G^*(u)} \psi_\alpha\big(d(u)+1, d(y);\beta\big) + \sum_{y\in N_G(v)\setminus N_G^*(v)} \psi_\alpha\big(d(v)+1, d(y);\beta\big) + \Phi_\alpha\big(d(u)+1, d(v)+1;\beta\big)\\
= &\Phi_\alpha\big(d(u)+1, d(v)+1;\beta\big) > 0.
\end{aligned}$$

Case 3. $\alpha < 0$ and $1 < \beta \le 2$. Since G is connected, then $|\{y \mid y \in N_G(u), d(y) = 1\}| \le d(u) - 1$. First we suppose $d(v) \ge 2$. Combining this with $1 < \beta \le 2 \le d(v) \le d(u)$, Lemmas 2.1, 2.2 and 2.4,

$$\begin{aligned}
&ABC_\alpha(G+uv;\beta) - ABC_\alpha(G;\beta)\\
\ge &\sum_{y\in N_G(u)\setminus N_G^*(u)} \psi_\alpha\big(d(u)+1, d(y);\beta\big) + \sum_{y\in N_G(v)\setminus N_G^*(v)} \psi_\alpha\big(d(v)+1, d(y);\beta\big) + \Phi_\alpha\big(d(u)+1, d(v)+1;\beta\big)\\
\ge &\big(d(u)-1\big)\psi_\alpha\big(d(u)+1, 1;\beta\big) + \big(d(v)-1\big)\psi_\alpha\big(d(v)+1, 1;\beta\big) + \Phi_\alpha\big(d(u)+1, d(v)+1;\beta\big)\\
\ge &\Phi_\alpha\big(d(u)+1, d(v)+1;\beta\big) + 2\left(\frac{4-\beta}{3}\right)^\alpha - 2\left(\frac{3-\beta}{2}\right)^\alpha \quad \text{(by Lemma 2.2)}\\
> &0. \quad \text{(by Lemma 2.4)}
\end{aligned}$$

Next we suppose $d(v) = 1$. Then $d(u) \ge 1$. For any vertex y of $N_G(v)$, since $d(y) \ge 2 \ge \beta$, $\psi_\alpha\big(d(v)+1, d(y);\beta\big) \ge 0$. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
&ABC_\alpha(G+uv;\beta) - ABC_\alpha(G;\beta)\\
\ge &\sum_{y\in N_G(u)\setminus N_G^*(u)} \psi_\alpha\big(d(u)+1, d(y);\beta\big) + \Phi_\alpha\big(d(u)+1, 2;\beta\big)\\
\ge &\big(d(u)-1\big)\psi_\alpha\big(d(u)+1, 1;\beta\big) + \Phi_\alpha\big(d(u)+1, 2;\beta\big)\\
\ge &\left(\frac{d(u)+3-\beta}{2\big(d(u)+1\big)}\right)^\alpha + \left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha \quad \text{(by Lemma 2.2)}\\
\ge &\left(\frac{4-\beta}{4}\right)^\alpha + \left(\frac{4-\beta}{3}\right)^\alpha - \left(\frac{3-\beta}{2}\right)^\alpha\\
\ge &\left(\frac{4-\beta}{3}\right)^\alpha > 0.
\end{aligned}$$

This completes the proof of Theorem 1.2. □

3. The proofs of Theorems 1.3–1.4

This section is dedicated to the proofs of Theorems 1.3–1.4. We need to introduce more notations. A symmetric bivariate function $f(x, y)$ defined on positive real numbers is called **escalating** (resp. **de-escalating**) if

$$f(x_1, x_2) + f(y_1, y_2) \ge \ (\text{resp., } \le\ ) f(x_2, y_1) + f(x_1, y_2) \tag{3.1}$$

holds for any $x_1 \ge y_1 > 0$ and $x_2 \ge y_2 > 0$, and the inequality in (3.1) is strict if $x_1 > y_1$ and $x_2 > y_2$.

In [23], Wang defined the **connectivity function** of a connected graph G associated with a symmetric bivariate function $f(x, y)$ to be

$$M_f(G) = \sum_{uv\in E(G)} f(d(u), d(v)).$$

It is easily to see that $ABC_\alpha(G;\beta)$ is just a special case of $M_f(G)$.

The proofs of Theorems 1.3–1.4 rely on the following two lemmas:

Lemma 3.1 ([22]). *For any given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, there exists a BFS-graph G such that $M_f(G)$ is maximized in $\Gamma(\pi)$ when $f(x, y)$ is escalating and $M_f(G)$ is minimized in $\Gamma(\pi)$ when $f(x, y)$ is de-escalating.*

Lemma 3.2 ([22]). *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a given c-cyclic degree sequence with $d_n = 1$. In the class of $\Gamma(\pi)$,*
(i) if $c = 0$, then $T_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $T_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;

(ii) if $c = 1$, then $U_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $U_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;
(iii) if $c = 2$, then $B_M(\pi)$ has maximum $M_f(G)$ when $f(x, y)$ is escalating, and $B_M(\pi)$ has minimum $M_f(G)$ when $f(x, y)$ is de-escalating;

From Lemmas 3.1–3.2, to show Theorems 1.3–1.4, it suffices to show that the following proposition.

Proposition 3.1. *(i) If either $\alpha < 0$, $\beta \le 2$ or $\alpha \ge 1$, $\beta \le 0$, $(\alpha-1)^2+\beta^2 \ne 0$ holds, then $ABC_\alpha(G;\beta)$ is escalating;*
(ii) if $0 < \alpha \le 1$, $0 \le \beta \le 2$ and $(\alpha-1)^2+\beta^2 \ne 0$ holds, then $ABC_\alpha(G;\beta)$ is de-escalating.

Lemma 3.3. *For $x \ge 2$ and $y \ge 1$,*
(i) if either $\alpha < 0$, $\beta \le 2$ or $\alpha \ge 1$, $\beta \le 0$, $(\alpha-1)^2+\beta^2 \ne 0$ holds, then $\psi_\alpha(x, y+1;\beta) > \psi_\alpha(x, y;\beta)$;
(ii) if $0 < \alpha \le 1$, $0 \le \beta \le 2$ and $(\alpha-1)^2+\beta^2 \ne 0$ holds, then $\psi_\alpha(x, y+1;\beta) < \psi_\alpha(x, y;\beta)$.

Proof. Let $\lambda = -\alpha$. Then,

$$\begin{aligned}\frac{\partial \psi_\alpha(x,y;\beta)}{\partial y} &= \frac{\lambda x^\lambda y^{\lambda-1}(x-\beta)}{(x+y-\beta)^{\lambda+1}} - \frac{\lambda(x-1)^\lambda y^{\lambda-1}(x-\beta-1)}{(x+y-\beta-1)^{\lambda+1}}\\ &= \lambda y^{\lambda-1}\left[\frac{x^\lambda(x-\beta)}{(x+y-\beta)^{\lambda+1}} - \frac{(x-1)^\lambda(x-\beta-1)}{(x+y-\beta-1)^{\lambda+1}}\right]\\ &= \lambda y^{\lambda-1}\left[h(x,y) - h(x-1,y)\right],\end{aligned}$$

where $h(x,y) = \frac{(x-\beta)x^\lambda}{(x+y-\beta)^{\lambda+1}}$. By a routine calculation, we have

$$\begin{aligned}\frac{\partial h(x,y)}{\partial x} &= \frac{\left(\lambda(x-\beta)x^{\lambda-1}+x^\lambda\right)(x+y-\beta)^{\lambda+1} - (\lambda+1)(x+y-\beta)^\lambda(x-\beta)x^\lambda}{(x+y-\beta)^{2\lambda+2}}\\ &= \frac{x^{\lambda-1}}{(x+y-\beta)^{\lambda+2}}\left[\lambda(x-\beta)(x+y-\beta) - \lambda(x-\beta)x + x(x+y-\beta) - x(x-\beta)\right]\\ &= \frac{x^{\lambda-1}}{(x+y-\beta)^{\lambda+2}}\left[(\lambda+1)xy - (x-\beta)\lambda\beta - \lambda\beta y\right].\end{aligned}$$

Case 1. $\alpha < 0$ and $\beta \le 2$. Then $\lambda > 0$.
Subcase 1.1. $1 < \beta \le 2$. If $y = 1$, then the result holds by Lemma 2.1, as $\psi_\alpha(x, 1;\beta) < 0 \le \psi_\alpha(x, 2;\beta)$. Otherwise, $y \ge 2$. Since $x \ge 2$ and $y \ge 2$, we have

$$\lambda(x-\beta)(y-\beta) + xy \ge xy > 0.$$

Subcase 1.2. $\beta \le 1$. Since $x \ge 2$ and $y \ge 1$, we have

$$\lambda(x-\beta)(y-\beta) + xy \ge xy > 0.$$

Thus, we can conclude that $\frac{\partial h(x,y)}{\partial x} > 0$ holds in both cases, which means that $\frac{\partial \psi_\alpha(x,y;\beta)}{\partial y} > 0$ and thus $\psi_\alpha(x, y+1;\beta) > \psi_\alpha(x, y;\beta)$ for $x \ge 2$ and $y \ge 1$.
Case 2. $\alpha \ge 1$, $\beta \le 0$, and $(\alpha-1)^2+\beta^2 \ne 0$. Then, $\lambda \le -1$. Since $x \ge 2$ and $y \ge 1$, we have

$$(\lambda+1)xy - (x-\beta)\lambda\beta - \lambda y\beta < 0,$$

where the inequality is strict as $(\lambda+1)^2+\beta^2 \ne 0$. Therefore, we have $\frac{\partial h(x,y)}{\partial x} < 0$, which means that $\frac{\partial \psi_\alpha(x,y;\beta)}{\partial y} > 0$ and thus $\psi_\alpha(x, y+1;\beta) > \psi_\alpha(x, y;\beta)$ for $x \ge 2$ and $y \ge 1$.
Case 3. $0 < \alpha \le 1$, $0 \le \beta \le 2$, and $(\alpha-1)^2+\beta^2 \ne 0$. Then $-1 \le \lambda < 0$. Since $x \ge 2 \ge \beta$ and $y \ge 1$, we have

$$(\lambda+1)xy - (x-\beta)\lambda\beta - \lambda\beta y > 0,$$

where the inequality is strict as $(\lambda+1)^2+\beta^2 \ne 0$. Thus, we have $\frac{\partial h(x,y)}{\partial x} > 0$, which means that $\frac{\partial \psi_\alpha(x,y;\beta)}{\partial y} < 0$ and thus $\psi_\alpha(x, y+1;\beta) < \psi_\alpha(x, y;\beta)$ for $x \ge 2$ and $y \ge 1$. □

Proof of Proposition 3.1. If either $\alpha < 0$, $\beta \le 2$ or $\alpha \ge 1$, $\beta \le 0$, $(\alpha-1)^2+\beta^2 \ne 0$ holds, we just need to prove that

$$\Phi_\alpha(x_1, x_2;\beta) + \Phi_\alpha(y_1, y_2;\beta) - \Phi_\alpha(x_1, y_2;\beta) - \Phi_\alpha(y_1, x_2;\beta) \ge 0 \tag{3.2}$$

holds for any $x_1 \ge y_1 > 0$ and $x_2 \ge y_2 > 0$, and that the inequality in (3.2) is strict if $x_1 > y_1$ and $x_2 > y_2$.

Let $t = x_1 - y_1 \geq 0$. If $t = 0$, then $x_1 = y_1$ and thus the equality in (3.2) holds. Next, we suppose that $t \geq 1$. Since x_1 and y_1 are both positive integers, we have

$$\begin{aligned}
&\Phi_\alpha(x_1, x_2; \beta) + \Phi_\alpha(y_1, y_2; \beta) - \Phi_\alpha(x_1, y_2; \beta) - \Phi_\alpha(y_1, x_2; \beta)\\
=&\big[\Phi_\alpha(x_1, x_2; \beta) - \Phi_\alpha(y_1, x_2; \beta)\big] - \big[\Phi_\alpha(x_1, y_2; \beta) - \Phi_\alpha(y_1, y_2; \beta)\big]\\
=&\sum_{i=1}^{t}\big[\Phi_\alpha(y_1 + i, x_2; \beta) - \Phi_\alpha(y_1 + i - 1, x_2; \beta)\big] - \sum_{i=1}^{t}\big[\Phi_\alpha(y_1 + i, y_2; \beta) - \Phi_\alpha(y_1 + i - 1, y_2; \beta)\big]\\
=&\sum_{i=1}^{t}\big[\psi_\alpha(y_1 + i, x_2; \beta) - \psi_\alpha(y_1 + i, y_2; \beta)\big] \geq 0. \qquad \text{(From } x_2 \geq y_2 \text{ and Lemma 3.3)}
\end{aligned} \tag{3.3}$$

Thus, (3.2) holds and the inequality in (3.2) is strict if $x_1 > y_1$ and $x_2 > y_2$ by (3.3) and Lemma 3.3, which means that $ABC_\alpha(G; \beta)$ is escalating if either $\alpha < 0$, $\beta \leq 2$ or $\alpha \geq 1$, $\beta \leq 0$, $(\alpha - 1)^2 + \beta^2 \neq 0$ holds.

If $0 < \alpha \leq 1$, $0 \leq \beta \leq 2$ and $(\alpha - 1)^2 + \beta^2 \neq 0$ holds, similarly we have

$$\big[\Phi_\alpha(x_1, x_2; \beta) + \Phi_\alpha(y_1, y_2; \beta)\big] - \big[\Phi_\alpha(x_1, y_2; \beta) + \Phi_\alpha(y_1, x_2; \beta)\big] \leq 0, \tag{3.4}$$

and the inequality in (3.4) is strict if $x_1 > y_1$ and $x_2 > y_2$, which means that $ABC_\alpha(G; \beta)$ is de-escalating. □

4. Concluding remarks

In the former sections, we show that $ABC_\alpha(G; \beta)$ is escalating if either $\alpha < 0$, $\beta \leq 2$ or $\alpha \geq 1$, $\beta \leq 0$, $(\alpha - 1)^2 + \beta^2 \neq 0$ holds, and $ABC_\alpha(G; \beta)$ is de-escalating if $0 < \alpha \leq 1$, $0 \leq \beta \leq 2$ and $(\alpha - 1)^2 + \beta^2 \neq 0$ holds. Let H be a connected c-cyclic graph on $n - p$ vertices, then $K_p \vee H$ is called a p-**cone** c-**cyclic graph**, where K_p is a complete graph with p vertices. It is worth to observe that for $p = 0$, $K_0 \vee H = H$, therefore any connected graph can be seen as a 0-cone graph. Recently, in the class of p-cone c-cyclic graphs, the extremal graphs for $M_f(G)$ when $f(x, y)$ is escalating or de-escalating function have been discussed in [24]. Thus, we can apply Proposition 3.1 to extend Theorems 1.3–1.4 to the p-cone c-cyclic graphs.

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The minimal augmented Zagreb index of k-apex trees for $k \in \{1, 2, 3\}$

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ABSTRACT

For a graph G containing no component isomorphic to the 2-vertex path graph, the augmented Zagreb index (AZI) of G is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3.$$

This topological index has been proved to be closely correlated with the formation heat of heptanes and octanes. A k-apex tree is a connected graph G admitting a k-subset of vertices X such that $G - X$ is a tree, but for any subset of vertices X' of order less than k, $G - X'$ is not a tree. In this paper, we determine the minimum AZI among all k-apex trees for $k \in \{1, 2, 3\}$.

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1. Introduction

Throughout this paper, we restrict to simple and connected graphs. For a graph $G = (V(G), E(G))$ and $v \in V(G)$, we denote by $N(v)$ the neighbor set of v, and by $|N(v)| = d(v)$ the degree (or valency) of v. As usual, let $\Delta(G) = \max\{d(v) : v \in V(G)\}$ be the maximum degree of G. If $d(v) = r$, then v is said to be an r-vertex. A 1-vertex is also called a pendant vertex, while a vertex with degree at least two is called a non-pendant vertex. Similarly, an edge uv of G is called a pendant (resp., non-pendant) if one (resp., none) of its end-vertices is a pendant vertex. We will omit the graph in the argument whenever it is clear from the context.

In Chemical Graph Theory, various topological indices, determined by the combinatorial structure of the graph, are correlated to the chemical and physical property of the corresponding molecule. Among such topological indices we have the atom-bond connectivity (ABC) index of G defined in [6] as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}.$$

The above index is closely correlated with the alkanes heat of formation, and a quantum-chemical explanation for this correlation is provided in [5]. Further studies by Furtula et al. [7] extended the ABC index to the generalized ABC index of

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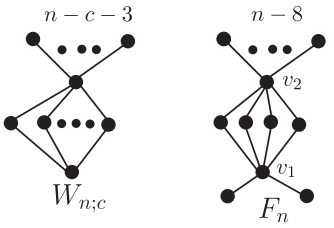


Fig. 1.1. The graphs $W_{n;c}$ and F_n.

G, that is,

$$ABC_\alpha(G) = \sum_{uv\in E(G)} \left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^\alpha.$$

In particular, $ABC_{-3}(G)$ is called the augmented Zagreb index (AZI) of G, where G does not admit components isomorphic to the 2-vertex path graph. Hence,

$$AZI(G) = \sum_{uv\in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3.$$

The authors of [7] also showed that the AZI performs better compared to the ABC index in predicting the heat of formation of heptanes and octanes. We refer the reader to [8–11,17,19] for further chemical applications of the AZI, ABC index, and other topological indices.

We introduce here the additional notations used in the paper. Let X be a subset of $V(G)$, and by $G-X$ we denote the graph obtained from G by deleting the vertices of X and the edges incident to any of them. In particular, $G-\{v\}$ is shortened to $G-v$. As usual, by P_n, C_n, and K_n, we denote the path, the cycle, and the complete graph on n vertices, respectively. Let G and H be two disjoint graphs, the join $G\vee H$ is the graph whose vertex set is $V(G\vee H)=V(G)\cup V(H)$ and the edge set is $E(G\vee H)=E(G)\cup E(H)\cup\{uv: u\in V(G) \text{ and } v\in V(H)\}$. The join of two co-cliques of orders s and $n-s$ is $K_{s,n-s}$, also called the complete bipartite graph. Particularly, $K_{1,n-1}$ is the star on n vertices. If G is a (connected) graph on n vertices and $n+c-1$ edges, then G is said to be a c-cyclic graph. Clearly, G is a tree (resp., unicyclic graph, bicyclic graph) when $c=0$ (resp., $c=1$, $c=2$). Hereafter, by $\mathbb{U}(n)$ (resp., $\mathbb{B}(n)$), we denote the class of unicyclic (resp., bicyclic) graphs on n vertices. As shown in Figure 1.1, let $W_{n;c}$ be the c-cyclic graph on n vertices obtained from $K_{2,c+1}$ by attaching $n-c-3$ pendant vertices to a $(c+1)$-vertex of $K_{2,c+1}$, and let F_n be the tricyclic graph obtained from $K_{2,4}$ by attaching two pendant vertices to v_1 and $n-8$ pendant vertices to v_2, where $\{v_1,v_2\}$ are the two 4-vertices of $K_{2,4}$.

A quasi-tree is a graph G having a vertex $v\in V(G)$ such that $G-v$ is a tree [21]. The latter concept has been generalized to k-apex trees by Xu et al. in [20] as in the following definition.

Definition 1.1. *[20, 22]* For $k\geq 1$, a k-apex tree is a (connected) graph G admitting a k-subset of vertices $V_k\subseteq V(G)$, such that $G-V_k$ is a tree, but $G-X$ is not a tree for any $X\subseteq V(G)$ and $|X|<k$. The subset V_k is called a **k**-quasi vertex set of G.

Recently, extremal results of AZI have received the attention of several scholars. The first result was given in [7] by Furtula et al., who showed that the star $K_{1,n-1}$ is the unique graph minimizing the AZI among all trees on $n\geq 2$ vertices. Afterwards, Huang et al. [12] and Zhan et al. [23] independently proved that the graphs obtained from $K_{1,n-1}$ by adding either one edge, or two non-adjacent edges minimize the AZI in the class of unicyclic and bicyclic graphs on $n\geq 5$ vertices, respectively. Ali [1] showed that $W_{n;3}$ is the unique minimizer for the AZI among all tricyclic graphs on n vertices ($n\geq 6$). Lin et al. [14] identified that the doubly balanced stars uniquely maximize the AZI among all trees with n vertices for $n\geq 19$, and they also posed the problem to characterize the extremal graphs for the AZI among all connected graphs on n vertices and m edges, with $m\geq n$. The latter problem was attacked by Liu et al. [15], who showed that $W_{n;c}$ uniquely minimizes the AZI of c-cyclic graphs on n vertices for $n\geq 2c+1$ and $c\geq 3$.

On the other hand, many extremal results on the topological indices of k-apex trees are also reported, for example, the extremal (weighted) Harary index of k-apex trees has been determined in [20,21], the extremal matching energy of k-apex trees has been studied in [22], and the unified extremal results for general sum-connectivity, Zeroth-order general Randić index, second Zagreb index and general spectral radius of k-apex trees have been determined in [16].

In this paper, we shall consider the extremal AZI of k-apex trees, and our main results are described in the subsequent theorems. Let $\mathbb{T}_n^k$ denote the class of k-apex trees on n vertices.

Theorem 1.1. *Let $G\in\mathbb{T}_n^1$. If $n\geq 6$, then*

$$AZI(G)\geq AZI\big(K_1\vee(K_2\cup(n-3)K_1)\big),$$

with equality if and only if $G=K_1\vee(K_2\cup(n-3)K_1)$.

Theorem 1.2. *Let $G \in \mathbb{T}_n^2$. If $n \geq 9$, then*

$$AZI(G) \geq AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big),$$

with equality if and only if $G = K_1 \vee (2K_2 \cup (n-5)K_1)$.

Theorem 1.3. *Let $G \in \mathbb{T}_n^3$. If $n \geq 14$, then*

$$AZI(G) \geq AZI\big(F_n\big),$$

with equality if and only if $G = F_n$.

We only determine the minimal AZI of k-apex trees for $k \in \{1, 2, 3\}$. As for the case of c-cyclic graphs, we believe that identifying the minimal AZI of k-apex trees for $k \geq 4$ is a difficult task. The remainder of this paper is organized as follows. In Section 2, we recall some preliminary results to be used later. In Section 3 we prove Theorem 1.1, and in Section 4 we prove Theorem 1.2. Finally, the more challenging proof of Theorem 1.3 is given in Section 5.

2. Preliminaries

Let the vertices of C_3 be labeled v_1, v_2 and v_3. By $Q_n(q_1, q_2, q_3)$ we denote the unicyclic graph obtained by attaching q_i pendant vertices to v_i, where $q_i \geq 0$ for $i \in \{1, 2, 3\}$ and $q_1 + q_2 + q_3 = n - 3$.

Lemma 2.1. *[23] If $q_1 \geq q_2 \geq q_3$ and $q_2 \geq 1$, then $AZI\big(Q_n(q_1+1, q_2-1, q_3)\big) < AZI\big(Q_n(q_1, q_2, q_3)\big)$.*

Lemma 2.2. *[3] Let G be a connected graph with two non-adjacent vertices u and v. If $\alpha \leq 1/2$ and $\alpha \neq 0$, then $ABC_\alpha(G+uv) > ABC_\alpha(G)$.*

Hereafter, let $\Psi(x, y)$ denote the function below defined:

$$\Psi(x, y) = \left(\frac{xy}{x+y-2}\right)^3.$$

Lemma 2.3. *[13] Let x and y be two real numbers, where $\min\{x, y\} \geq 1$.*
(i) $\Psi(1, y)$ is decreasing for $y \geq 2$.
(ii) $\Psi(2, y) = 8$ for any real number y.
(iii) If $y \geq 3$ is fixed, then $\Psi(x, y) > 8$ is increasing for $x \geq 3$.

Lemma 2.4. *[2] For a real number p, let*

$$f(x, y) = \left(\frac{xy}{x+y-2}\right)^3 - \left(\frac{(x-p)y}{x+y-p-2}\right)^3,$$

where $\min\{x, y\} \geq 2$. If $x > p \geq 1$, then the function $f(x, y)$ is increasing on y for $y \geq 2$.

Lemma 2.5. *[18] Let G be a connected graph on n vertices, e edges, p pendant vertices, maximum degree Δ, and minimum non-pendant vertex degree δ_1. Then,*

$$AZI(G) \geq p\left(\frac{\Delta}{\Delta-1}\right)^3 + (e-p)\left(\frac{\delta_1^2}{2\delta_1-2}\right)^3.$$

3. The proof of Theorem 1.1

Let $C_{n,p}$ be the unicyclic graph obtained from C_{n-p} by attaching p pendant vertices to a vertex of the cycle C_{n-p}, where $0 \leq p \leq n-3$. In this section, we shall prove a stronger result than Theorem 1.1, that is,

Theorem 3.1. *Let $G \in \mathbb{T}_n^1 \setminus \{K_1 \vee (K_2 \cup (n-3)K_1)\}$. If $n \geq 6$, then*

$$AZI(G) \geq AZI(C_{n,n-4}) > AZI\big(K_1 \vee (K_2 \cup (n-3)K_1)\big),$$

where the equality holds if and only if $G = C_{n,n-4}$.

Lemma 3.1. *[12, 23] If $n \geq 5$ and $G \in \mathbb{B}(n)$, then*

$$AZI(G) \geq 48 + (n-5)\Psi(n-1, 1) = (n-5)\left(\frac{n-1}{n-2}\right)^3 + 48,$$

where the equality holds if and only if $G = K_1 \vee \big(2K_2 \cup (n-5)K_1\big)$.

Lemma 3.2. *[12, 23] If $n \geq 6$ and $G \in \mathbb{U}(n) \setminus \{K_1 \vee \big(K_2 \cup (n-3)K_1\big)\}$, then*

$$AZI(G) \geq AZI(C_{n,n-4}) = (n-4)\left(\frac{n-2}{n-3}\right)^3 + 32 > AZI\big(K_1 \vee (K_2 \cup (n-3)K_1)\big),$$

where the equality holds if and only if $G = C_{n,n-4}$.

Lemma 3.3. *If* $n \geq 6$, *then*

$$AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big) > AZI\big(C_{n,n-4}\big).$$

Proof. By Lemmas 3.1 and 3.2, we have

$$\begin{aligned} &AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big) - AZI\big(C_{n,n-4}\big) \\ &\quad = 16 + (n-5)\Psi(1,n-1) - (n-4)\Psi(1,n-2) \\ &\quad = \frac{15n^6 - 231n^5 + 1467n^4 - 4909n^3 + 9117n^2 - 8905n + 3577}{(n-2)^3(n-3)^3} > 0, \end{aligned}$$

as claimed. □

Proof of Theorem 3.1. Let $G \in \mathbb{T}_n^1 \setminus \big\{K_1 \vee (K_2 \cup (n-3)K_1)\big\}$ such that $AZI(G)$ is minimal. By Definition 1.1, G is not a tree. If G is a bicyclic graph, then Lemmas 3.1 and 3.3 imply that $AZI(G) \geq AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big) > AZI\big(C_{n,n-4}\big)$. Since $C_{n,n-4} \in \mathbb{T}_n^1 \setminus \big\{K_1 \vee (K_2 \cup (n-3)K_1)\big\}$, G can not be a bicyclic graph. Since $AZI(G) > AZI\big(C_{n,n-4}\big)$ for any bicyclic graph G, in view of Lemma 2.2, we conclude that $AZI(G) > AZI\big(C_{n,n-4}\big)$ for any c-cyclic graph G with $c \geq 2$. Hence, G is a unicyclic graph. Now, the result follows from Lemma 3.2. □

4. The proof of Theorem 1.2

This section is devoted to the proof of Theorem 1.2. Let G be a c-cyclic graph with $c > 0$ (trees are not considered). The **base graph** of G, denoted by $\mathcal{R}(G)$, is the subgraph of G obtained by stepwise deleting the pendant vertices, until the obtained graph has no more pendant vertices. Clearly, $\mathcal{R}(G)$ is uniquely determined, and it keeps the same cyclomatic number of G. On the other hand, G is obtained from $\mathcal{R}(G)$ by attaching some hanging trees to the vertices of $\mathcal{R}(G)$. In the forthcoming discussion, by T_v we denote a rooted tree whose root is v (the root is a vertex of T_v).

Lemma 4.1. *Let* $G \in \mathbb{T}_n^k$. *If* $k \geq 2$ *and* G *is a unicyclic graph whose unique cycle is* C_g, *then* $|V(T_u)| \geq k$ *holds for each vertex* u *of* C_g. *Moreover,* $G[V_k]$ *is a rooted tree for each* k*-quasi vertex set* V_k *of* G.

Proof. If $|V(T_u)| \leq k-1$ holds for some vertex u of C_g, then $G - V(T_u)$ is a tree, contrary to Definition 1.1. Thus, $|V(T_u)| \geq k$ holds for each vertex u of C_g, as claimed. Now, we prove the additional statement.

If $V_k \cap V(C_g) = \emptyset$, then C_g is also a cycle of $G - V_k$, and thus $G - V_k$ is not a tree. This implies that $V_k \cap V(C_g) \neq \emptyset$. Suppose that $V_k \cap V(C_g) = \{u_1, u_2, \ldots, u_s\}$. If $s \geq 2$, then $|V(T_{u_1})| \leq k-1$, contrary to $|V(T_{u_1})| \geq k$. Thus, $s = 1$ and so $V(T_{u_1}) = V_k$. □

Lemma 4.2. *If* $n \geq 8$, *then* $AZI\big(Q_n(n-5,1,1)\big) > AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big)$.

Proof. By Lemmas 2.3 and 3.1, we have

$$\begin{aligned} &AZI\big(Q_n(n-5,1,1)\big) - AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big) \\ &\quad = 2\Psi(1,3) + \Psi(3,3) + 2\Psi(3,n-3) + (n-5)\Psi(1,n-3) - (n-5)\Psi(1,n-1) - 48 \\ &\quad > 18 + 2\Psi(3,n-3) - 48 + (n-5)\big(\Psi(1,n-3) - \Psi(1,n-1)\big) \\ &\quad > 18 + 2\Psi(3,5) - 48 > 0, \end{aligned}$$

as desired. □

A **special cycle** C is a cycle whose vertices have degree at least three. In the remainder of this section, let G be a graph of $\mathbb{T}_n^2$ such that $AZI(G)$ is minimum. Note that $K_1 \vee (2K_2 \cup (n-5)K_1) \in \mathbb{T}_n^2$. Thus, if $AZI(G) > AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big)$, then we get a contradiction to the choice of G.

Lemma 4.3. *If* $n \geq 9$, *then* G *is not a unicyclic graph with girth* $g \geq 4$.

Proof. Assume, by way of contradiction, that G is a unicyclic graph with girth $g \geq 4$. By Lemma 4.1 C_g is a special cycle of G. Hence, by Lemma 2.3, each edge of C_g contributes to $AZI(G)$ at least $\Psi(3,3)$, and, for each 2-quasi vertex set V_2 of G, the edge belonging to $G[V_2]$ of G contributes to $AZI(G)$ exactly $\Psi(3,1)$. Furthermore, by Lemma 2.3, the other $n-g-1$ edges of G contribute to $AZI(G)$ at least $(n-g-1)\Psi(1,\Delta)$. Since $\Delta \leq n-5$ by Lemma 4.1, it is

$$\begin{aligned} AZI(G) &\geq g\Psi(3,3) + \Psi(3,1) + (n-g-1)\Psi(n-5,1) \\ &\geq 4\Psi(3,3) + \Psi(3,1) + (n-5)\Psi(n-5,1) \\ &> 48 + (n-5)\Psi(n-5,1) > AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big), \end{aligned}$$

by Lemmas 2.3 and 3.1. The latter is a contradiction to the choice of G. □

Lemma 4.4. *If $n \geq 9$, then G is not a unicyclic graph with girth $g = 3$.*

Proof. Assume, by way of contradiction, that G is a unicyclic graph with girth $g = 3$. By Lemma 4.1, C_3 is a special triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Let G contain exactly p pendant vertices. Then, $p \leq n-3$. We consider the following three cases:

Case 1. $p = n-3$. By Lemmas 2.1 and 4.1 we have $G = Q_n(n-5, 1, 1)$, and thus Lemma 4.2 implies that $AZI(G) > AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big)$, a contradiction.

Case 2. $p = n-4$. By Lemma 4.1, G is the unicyclic graph obtained from C_3 by attaching a pendant vertex to v_3 and two rooted trees T_{v_1} and T_{v_2} to v_1 and v_2, respectively, where $\min\big\{|V(T_{v_1})|, |V(T_{v_2})|\big\} \geq 2$. Since $p = n-4$, there exists exactly one non-pendant vertex $u \in V(T_{v_1}) \cup V(T_{v_2})$. Without loss of generality, we assume that $u \in V(T_{v_1})$ and $\{u_1, u_2, \ldots, u_s\}$ are all pendant neighbor of u. Then, $s \geq 1$.

Recall that $p = n-4$. Thus, $\{v_1, v_2, v_3, u\}$ are all non-pendant vertices of G, and $uv_1 \in E(G)$, as $u \in V(T_{v_1})$. Moreover, $\Delta \leq n-4$ by Lemma 4.1.

If $\Delta = 3$, then $d(v_1) = d(v_2) = d(v_3) = 3$. Hence, G is obtained from $Q_6(1,1,1)$ by attaching one or two pendant vertices to the pendant vertex of $Q_6(1,1,1)$. The latter implies that $n \leq 8$, a contradiction. Thus, $\Delta = \max\{d(u), d(v_1), d(v_2)\} \geq 4$.

If $d(u) \geq 3$, by Lemmas 2.3 and 4.1, the four edges $\{uv_1, v_1v_2, v_1v_3, v_2v_3\}$ contribute to $AZI(G)$ at least $3\Psi(3,3) + \Psi(4,3) > 47$. If $d(u) = 2$, by Lemmas 2.3 and 4.1, the edges $\{uv_1, v_1v_2, v_1v_3, v_2v_3\}$ contribute to $AZI(G)$ at least $\Psi(3,3) + 2\Psi(4,3) + 8 > 47$. In both cases, by Lemma 2.3 the remaining $n-4$ pendant edges of G contribute to $AZI(G)$ at least $(n-4)\Psi(1,\Delta)$. Combining the latter with Lemma 2.3 and $\Delta \leq n-4$, we have

$$\begin{aligned} AZI(G) &> 47 + (n-4)\Psi(1,\Delta) \\ &> 48 + (n-5)\Psi(1,\Delta) \\ &> 48 + (n-5)\Psi(1,n-1) = AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big), \end{aligned}$$

by Lemma 3.1. This is a contradiction to the choice of G.

Case 3. $p \leq n-5$. In this case, G contains at least $n-p \geq 5$ non-pendant edges. By Lemma 4.1, there exist five non-pendant edges of G contributing to $AZI(G)$ at least $16 + 3\Psi(3,3) > 50$, and all other $n-5$ edges contribute to $AZI(G)$ as least $(n-5)\Psi(1,\Delta)$ by Lemma 2.3. Thus,

$$AZI(G) > 50 + (n-5)\Psi(1,\Delta) > 48 + (n-5)\Psi(1,n-1) = AZI\big(K_1 \vee (2K_2 \cup (n-5)K_1)\big)$$

by Lemmas 2.3 and 3.1. This is a contradiction to the choice of G. □

Proof of Theorem 1.2.. Assume that G is a graph of $\mathbb{T}_n^2$ such that $AZI(G)$ is minimum. By Definition 1.1, G is not a tree. By Lemmas 4.3 and 4.4, G is not a unicyclic graph. Now, by Lemmas 2.2 and 3.1, we can conclude that $G = K_1 \vee \big(2K_2 \cup (n-5)K_1\big)$. □

5. The proof of Theorem 1.3

Let u_0 be a vertex in the base graph of G. If $|V(T_{u_0})| = q \geq 3$, then denote by $G^*(u_0)$ the graph obtained from G by deleting all vertices of $V(T_{u_0}) \setminus \{u_0\}$ and then adding one new edge between u_0 and a pendant vertex of $K_{1,q-2}$. From the definition, it is easily checked that

For $k \geq 2$, if G is a k-apex tree, then $G^*(u_0)$ is also a k-apex tree. (5.1)

Proposition 5.1. *Let $G \neq G^*(u_0)$, $u_0 \in \mathcal{R}(G)$ with $N(u_0) \cap V(\mathcal{R}(G)) = \{v_0, w_0\}$, and $d(v_0) \geq d(w_0) \geq 3$. Suppose that $|V(T_{u_0})| = q \geq 3$ and $V(T_{u_0}) \setminus \{u_0\}$ contains exactly t non-pendant vertices. If one of the following conditions holds: (i) $t = 0$, $d(v_0) = 3$ and $q \geq 7$; (ii) $t = 0$, $d(v_0) \geq 4$ and $q \geq 5$. (iii) $t = 1$, $d(u_0) = 3$ and $q \geq 6$; (iv) $t = 1$, $d(u_0) \geq 4$ and $q \geq 5$; (v) $t \geq 2$; then $AZI(G) > AZI\big(G^*(u_0)\big)$.*

Proof. We first prove (*i*) and (*ii*). Assume $t = 0$, then $G[V(T_{u_0})] = K_{1,q-1}$, so $d(u_0) = q+1$. From the definition of AZI, we have

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) = {} & \Psi(q+1, d(v_0)) + \Psi(q+1, d(w_0)) + (q-1)\Psi(q+1,1) \\ & - \Psi(3, d(v_0)) - \Psi(3, d(w_0)) - 16 - (q-3)\Psi(q-2,1). \end{aligned}$$

If $d(v_0) = 3$, then $d(w_0) = 3$. Hence,

$$\begin{aligned} & AZI(G) - AZI\big(G^*(u_0)\big) \\ &= 2\big(\Psi(q+1,3) - \Psi(3,3)\big) + (q-1)\Psi(q+1,1) - 16 - (q-3)\Psi(q-2,1) \\ &= 2\left(\left(\frac{3q+3}{q+2}\right)^3 - \left(\frac{9}{4}\right)^3\right) + (q-1)\left(\frac{q+1}{q}\right)^3 - 16 - (q-3)\left(\frac{q-2}{q-3}\right)^3 \\ &= \frac{551q^8 - 5280q^7 + 6903q^6 + 29402q^5 - 31068q^4 - 66024q^3 - 3520q^2 - 6528q - 2304}{32q^3(q-3)^2(q+2)^3} > 0 \end{aligned}$$

for $q \geq 7$. This implies that (i) holds.

If $d(v_0) \geq 4$ and $q \geq 5$, then Lemmas 2.3 and 2.4 imply that

$$\begin{aligned} AZI(G) - AZI(G^*(u_0)) &\geq \Psi(q+1,4) - \Psi(3,4) + \Psi(q+1,3) - \Psi(3,3) + (q-1)\Psi(q+1,1) - 16 - (q-3)\Psi(q-2,1) \\ &> \Psi(q+1,4) + \Psi(q+1,3) + (q-1)\Psi(q+1,1) - (q-3)\Psi(q-2,1) - 41.5 \\ &= f(q)/\big(2q^3(q-3)^2(q+3)^3(q+2)^3\big), \end{aligned}$$

where $f(q) = 103q^{11} - 9q^{10} - 2886q^9 - 3238q^8 + 24909q^7 + 49977q^6 - 51198q^5 - 194022q^4 - 135648q^3 - 18252q^2 - 14904q - 3888$. Since $f(q) > 0$ for $q \geq 5$, (ii) holds.

Next we prove (iii) and (iv). Assume now $t = 1$, then $q \geq 5$ and $V(T_{u_0}) \setminus \{u_0\}$ contains exactly one non-pendant vertex, say x_0. In this case, $d(u) \leq q$ for each $u \in V(T_{u_0})$, and $u_0x_0 \in E(G)$. If $d(x_0) = 2$, then the two edges adjacent to x_0 contribute 16 to $AZI(G)$. Combining the latter with Lemmas 2.3 and 2.4, we get

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &\geq \Psi(d(u_0),d(v_0)) + \Psi(d(u_0),d(w_0)) + \Psi(3,3) + (q-2)\Psi(q,1) \\ &\quad - \Psi(3,d(v_0)) - \Psi(3,d(w_0)) - 16 - (q-3)\Psi(q-2,1) \\ &> 2\big(\Psi(d(u_0),3) - \Psi(3,3)\big) + \Psi(3,3) + (q-2)\Psi(q,1) - 16 \\ &\quad - (q-3)\Psi(q-2,1). \end{aligned}$$

If $d(u_0) \geq 5$, then $q \geq d(u_0) \geq 5$. By Lemma 2.3(iii),

$$\begin{aligned} &2\big(\Psi(d(u_0),3) - \Psi(3,3)\big) + \Psi(3,3) + (q-2)\Psi(q,1) - 16 - (q-3)\Psi(q-2,1) \\ &\geq 2\big(\Psi(5,3) - \Psi(3,3)\big) + \Psi(3,3) + (q-2)\Psi(q,1) - 16 - (q-3)\Psi(q-2,1) \\ &= \frac{311q^5 - 2991q^4 + 10290q^3 - 15586q^2 + 10455q - 2735}{64(q-3)^2(q-1)^3} > 0, \end{aligned}$$

and, consequently, $AZI(G) > AZI\big(G^*(u_0)\big)$.

Thus, it remains to consider the case $3 \leq d(u_0) \leq 4$. Recall that x_0 is the unique non-pendant vertex of $V(T_{u_0}) \setminus \{u_0\}$. Thus, $d(x_0) = q + 2 - d(u_0) \geq q - 2 \geq 3$, as $q \geq 5$. From the definition of AZI and Lemma 2.4, we have

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &= \Psi(d(u_0),d(v_0)) + \Psi(d(u_0),d(w_0)) + \Psi(d(u_0),d(x_0)) \\ &\quad + (d(u_0)-3)\Psi(d(u_0),1) + (d(x_0)-1)\Psi(d(x_0),1) - \Psi(3,d(v_0)) \\ &\quad - \Psi(3,d(w_0)) - 16 - (q-3)\Psi(q-2,1). \end{aligned}$$

If $d(u_0) = 3$ and $q \geq 6$, then

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &= \Psi(3,q-1) + (q-2)\Psi(q-1,1) - 16 - (q-3)\Psi(q-2,1) \\ &= \frac{12q^7 - 201q^6 + 1332q^5 - 4541q^4 + 8546q^3 - 8775q^2 + 4536q - 972}{q^3(q-2)^2(q-3)^2} \\ &> 0, \end{aligned}$$

and so (iii) holds.

If $d(u_0) = 4$ and $q \geq 5$, then Lemma 2.4 implies that

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &\geq 2\big(\Psi(4,3) - \Psi(3,3)\big) + \Psi(4,q-2) + \Psi(4,1) \\ &\quad + (q-3)\Psi(q-2,1) - 16 - (q-3)\Psi(q-2,1) \\ &> \Psi(4,q-2) - 9 = \frac{64(q-2)^3}{q^3} - 9 \\ &= \frac{55q^3 - 384q^2 + 768q - 512}{q^3} > 0 \end{aligned}$$

and thus (iv) holds.

Finally, we show (v). In this case, since $G \neq G^*(u_0)$, we have $q \geq 5$, $d(u) \leq q - 1$ for each vertex $u \in V(T_{u_0})$ and T_{u_0} contains at least two non-pendant edges, which contribute at least 16 to $AZI(G)$.

If $d(u) \leq q - 2$ for each vertex $u \in V(T_{u_0})$, then Lemma 2.3 implies that

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &\geq \Psi(d(u_0),d(v_0)) + \Psi(d(u_0),d(w_0)) + 16 + (q-3)\Psi(q-2,1) \\ &\quad - \big(\Psi(3,d(v_0)) + \Psi(3,d(w_0)) + 16 + (q-3)\Psi(q-2,1)\big) \geq 0, \end{aligned}$$

where $AZI(G) = AZI\big(G^*(u_0)\big)$ holds if and only if $q - 3$ pendant vertices are adjacent to a vertex x_0 with degree $q - 2$, $d(u_0) = 3$ and T_{u_0} contains a 2-vertex which is adjacent to both x_0 and u_0, that is, $G = G^*(u_0)$, a contradiction.

If $d(u) = q-1$ for some vertex $u \in V(T_{u_0})$, then $u = u_0$ and the other two non-pendant vertices of $V(T_{u_0}) \setminus \{u_0\}$ are both 2-vertices, as $t \geq 2$. Thus,

$$\begin{aligned} AZI(G) - AZI\big(G^*(u_0)\big) &= \Psi(q-1, d(v_0)) + \Psi(q-1, d(w_0)) + 24 + (q-4)\Psi(q-1,1) \\ &\quad -\Psi(3, d(v_0)) - \Psi(3, d(w_0)) - 16 - (q-3)\Psi(q-2,1) \\ &> 8 + (q-4)\Psi(q-1,1) - (q-3)\Psi(q-2,1), \end{aligned}$$

as $d(u_0) = q-1 \geq 4$. Since $q \geq 5$,

$$8 + (q-4)\Psi(q-1,1) - (q-3)\Psi(q-2,1) = \frac{(q-4)(7q^4 - 62q^3 + 202q^2 - 287q + 151)}{(q-3)^2(q-2)^3} > 0.$$

Thus, (v) also holds. □

Recall that $W_{n;c}$ and F_n are the graphs as shown in Figure 1.1. By an elementary computation, we have

$$AZI(W_{n;4}) = (n-7)\left(\frac{n-2}{n-3}\right)^3 + 80, \tag{5.2}$$

and

$$AZI(F_n) = \frac{8432}{125} + (n-8)\left(\frac{n-4}{n-5}\right)^3 < 67.5 + (n-8)\Psi(n-4,1). \tag{5.3}$$

Lemma 5.1. *[15] Let G be a c-cyclic graph with n vertices. If $n \geq 2c+1$ and $c \geq 3$, then $AZI(G) \geq AZI(W_{n;c})$ with equality if and only if $G = W_{n;c}$.*

Corollary 5.1. *If G is a c-cyclic graph with $n \geq 9$ vertices and $c \geq 4$, then $AZI(G) > AZI(F_n)$.*

Proof. Since $n \geq 9$, from Lemmas 2.2 and 5.1, we have $AZI(G) \geq AZI(W_{n;4})$. Note that

$$\begin{aligned} &AZI(W_{n;4}) - AZI(F_n) \\ &= (n-7)\left(\frac{n-2}{n-3}\right)^3 + 80 - \frac{8432}{125} - (n-8)\left(\frac{n-4}{n-5}\right)^3 \big(by(5.2)and(5.3)\big) \\ &= \frac{1693n^6 - 41007n^5 + 410241n^4 - 2164401n^3 + 6336990n^2 - 9744700n + 6145000}{125(n-3)^3(n-5)^3} > 0 \end{aligned}$$

as $n \geq 9$. Thus, $AZI(G) > AZI(F_n)$. □

In the remainder of this section, let G be a graph of $\mathbb{T}_n^3$ such that $AZI(G)$ is minimum. Since $F_n \in \mathbb{T}_n^3$, if $AZI(G) > AZI(F_n)$, then we get a contradiction to the choice of G.

Lemma 5.2. *If $n \geq 9$, then G is not a unicyclic graph with girth $g \geq 5$.*

Proof. Assume, by way of contradiction, that G is a unicyclic graph with girth $g \geq 5$. Since $g \geq 5$ and C_g is a special cycle by Lemma 4.1, we have $\Delta \leq n-6$. Once again, Lemma 4.1 confirms the existence of a rooted tree T_{u_0} with $|V(T_{u_0})| = 3$ such that either $d(u_0) = 4$, or $d(u_0) = 3$. By Lemma 2.3, the two edges of T_{u_0} contribute at least $2\Psi(4,1)$ to $AZI(G)$.

Case 1. $g \geq 6$. Then, each of the g edges of C_g contributes at least $\Psi(3,3)$ to $AZI(G)$, and each of the other $n-g-2$ edges of G contributes at least $\Psi(1,\Delta)$ to $AZI(G)$. By Lemma 2.3 and (5.3), it follows that

$$\begin{aligned} AZI(G) &\geq g\Psi(3,3) + 2\Psi(4,1) + (n-g-2)\Psi(1,\Delta) \\ &\geq 6\Psi(3,3) + 2\Psi(4,1) + (n-8)\Psi(1,n-4) \\ &> 73 + (n-8)\Psi(1,n-4) > AZI(F_n), \end{aligned}$$

a contradiction.

Case 2. $g = 5$. If $d(u) \geq 4$ for some vertex $u \in V(C_5)$, then the five edges of C_5 contribute at least $3\Psi(3,3) + 2\Psi(4,3)$ to $AZI(G)$, and each of the other $n-7$ edges of G contributes at least $\Psi(1,\Delta)$ to $AZI(G)$ by Lemma 2.3. Combining this with Lemma 2.3,

$$\begin{aligned} AZI(G) &\geq 3\Psi(3,3) + 2\Psi(1,4) + 2\Psi(4,3) + (n-7)\Psi(1,\Delta) \\ &\geq 3\Psi(3,3) + 2\Psi(1,4) + 2\Psi(4,3) + (n-7)\Psi(1,n-6) \\ &> 67.5 + (n-8)\Psi(1,n-6) > AZI(F_n), \end{aligned}$$

a contradiction.

If $d(u) = 3$ for each vertex $u \in V(C_5)$, then Lemma 4.1 implies the existence of a rooted tree T_{u_0} with $V(T_{u_0}) = \{u_0, w_1, w_2\}$ such that $d(u_0) = 3$ and $d(w_1) = 2 > 1 = d(w_2)$. This implies that the five edges of C_5 and two edges of T_{u_0} contribute at least $5\Psi(3,3) + 2 \times 8 > 72.5$ to $AZI(G)$. Since each of the other $n-7$ edges of G contributes at least $\Psi(1,\Delta)$ to $AZI(G)$,

from Lemma 2.3 and (5.3) it follows that

$$\begin{aligned} AZI(G) &\geq 5\Psi(3,3) + 2\times 8 + (n-7)\Psi(1,\Delta) \\ &> 72.5 + (n-7)\Psi(1,n-6) \\ &> 67.5 + (n-8)\Psi(1,n-6) > AZI(F_n), \end{aligned}$$

a contradiction. □

Lemma 5.3. *If $n \geq 9$, then G is not a unicyclic graph with girth $g = 4$.*

Proof. Assume, by way of contradiction, that G is a unicyclic graph with girth $g = 4$. By Lemma 4.1, $\Delta < n-4$.

We first suppose that C_4 contains at least three 3-vertices. By Lemma 4.1, if $d(u) = 3$ for $u \in V(C_4)$, then T_u contains at least one non-pendant edge of G. Combining this with Lemmas 2.3 and 4.1,

$$\begin{aligned} AZI(G) &\geq 4\Psi(3,3) + 24 + (n-7)\Psi(1,\Delta) \\ &> 4\Psi(3,3) + 24 + (n-7)\Psi(1,n-4) \\ &> 69.5 + (n-7)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

We next suppose that C_4 contains at least three vertices with degree at least four. By Lemmas 2.3 and 4.1,

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,4) + 2\Psi(4,3) + (n-4)\Psi(1,\Delta) \\ &> 69.5 + (n-8)\Psi(1,\Delta) \\ &> 67.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

The last possibility is that C_4 contains exactly two 3-vertices and two vertices with degree at least four. In this case, since T_u contains at least one non-pendant edge of G in the case of $d(u) = 3$, Lemmas 2.3 and 4.1 imply that

$$\begin{aligned} AZI(G) &\geq 4\Psi(4,3) + 16 + (n-6)\Psi(1,\Delta) \\ &> 73 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction. □

Lemma 5.4. *If $n \geq 14$, then G is not a unicyclic graph with girth $g = 3$.*

Proof. Assume, by way of contradiction, that G is a unicyclic graph with girth $g = 3$. By Lemma 4.1, $\Delta < n-4$ and there exists $u_0 \in C_3$ such that $|V(T_{u_0})| = 3$. Thus, either $d(u_0) = 4$ or $d(u_0) = 3$. We suppose that $V(C_3) = \{u_0, v_0, w_0\}$, where $d(v_0) \geq d(w_0) \geq 3$ by Lemma 4.1. Suppose that $|V(T_{v_0})| = q_1$ and $|V(T_{w_0})| = q_2$.

Case 1. $d(u_0) = 4$**.** Then, except for $\{v_0, w_0\}$, u_0 is adjacent with exactly two pendant vertices.

If $q_1 \geq 6$, then $G = G^*(v_0)$ by Proposition 5.1 and (5.1), as $d(u_0) = 4$. This implies that $d(v_0) = d(w_0) = 3$, v_0 is adjacent to a 2-vertex and w_0 contains three non-pendant neighbors, as $q_2 = |V(T_{w_0})| \geq 3$ by Lemma 4.1. By the definition of AZI, (5.3) and Lemma 2.3,

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + \Psi(3,3) + 24 + 2\Psi(4,1) + (n-8)\Psi(\Delta,1) \\ &> 67.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned} \tag{5.4}$$

a contradiction.

Thus, $q_1 \leq 5$ and hence $q_2 \geq 6$, as $n = q_1 + q_2 + 3 \geq 14$. By Proposition 5.1 and (5.1), $G = G^*(w_0)$, and thus w_0 is adjacent to a 2-vertex and $d(w_0) = 3$.

In this case, either $d(v_0) \geq 4$ or $d(v_0) = 3$ with three non-pendant neighbors. From (5.4), we may suppose that $d(v_0) \geq 4$, and thus Lemma 2.3 implies that

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + \Psi(4,4) + 16 + 2\Psi(4,1) + (n-7)\Psi(\Delta,1) \\ &> 68 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

Case 2. $d(u_0) = 3$**.** Then, exactly for $\{v_0, w_0\}$, u_0 is adjacent to one 2-vertex, which is adjacent to a pendant vertex, as $|V(T_{u_0})| = 3$.

Subcase 2.1. $d(w_0) \geq 4$**.** If G contains at least five non-pendant vertices, then $d(v_0) \geq d(w_0) \geq 4$ implies that

$$AZI(G) \geq 2\Psi(4,3) + \Psi(4,4) + 24 + (n-6)\Psi(\Delta,1)$$

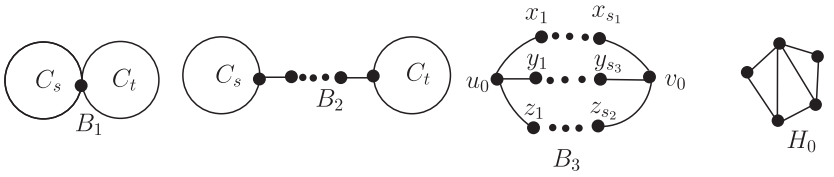


Fig. 5.1. The graphs B_1, B_2, B_3 and H_0.

$$> 72.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n),$$

a contradiction.

Otherwise, G contains exactly four non-pendant vertices. By Proposition 5.1 and (5.1), we have $\max\{q_1, q_2\} \le 5$, as $d(v_0) \ge d(w_0) \ge 4$. This implies that $n = 3 + q_1 + q_2 \le 13$, a contradiction.

Subcase 2.2. $d(w_0) = 3$ and $d(v_0) \ge 4$. Then, $V(T_{w_0}) \setminus \{w_0\}$ contains at least one non-pendant vertex, as $|V(T_{w_0})| \ge 3$ by Lemma 4.1. If either $q_2 = 3$ or $V(T_{w_0}) \setminus \{w_0\}$ contains at least two non-pendant vertices, then from $d(v_0) \ge 4$ it follows that

$$\begin{aligned} AZI(G) &\ge 2\Psi(4,3) + \Psi(3,3) + 32 + (n-7)\Psi(\Delta,1) \\ &> 72 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

Thus, $V(T_{w_0}) \setminus \{w_0\}$ contains exactly one non-pendant vertex, say x_0, and $d(x_0) = q_2 - 1 \ge 3$. By Lemma 2.3 and $d(v_0) \ge 4$,

$$\begin{aligned} AZI(G) &\ge 2\Psi(4,3) + 2\Psi(3,3) + 16 + (n-6)\Psi(\Delta,1) \\ &> 68 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \text{ a contradiction.} \end{aligned}$$

Subcase 2.3. $d(w_0) = d(v_0) = 3$. If G contains at least seven non-pendant vertices, then

$$\begin{aligned} AZI(G) &\ge 3\Psi(3,3) + 40 + (n-8)\Psi(\Delta,1) \\ &> 74 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \text{ a contradiction.} \end{aligned}$$

Thus, G contains exactly six non-pendant vertices, as C_3 is a special triangle. Suppose that x_0 is a neighbor of v_0 and y_0 is a neighbor of w_0, where $\{x_0, y_0\} \cap V(C_3) = \emptyset$. Then, $d(x_0) = q_1 - 1$ and $d(y_0) = q_2 - 1$. Since $n = 3 + q_1 + q_2 \ge 14$, we have $\max\{q_1, q_2\} \ge 5$. Thus,

$$\begin{aligned} AZI(G) &\ge 3\Psi(3,3) + 24 + \Psi(4,3) + (n-7)\Psi(\Delta,1) \\ &> 72.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

This completes the proof. □

Lemma 5.5. *If G is a bicyclic graph, then G contains at least one special cycle.*

Proof. Assume, to the contrary, that G contains no special cycle. Then, every cycle of G contains a 2-vertex. Denote by G_1 the unicyclic graph with $n-1$ vertices obtained from G by deleting one 2-vertex from one cycle of G. Then, the unique cycle of G_1 also contains a 2-vertex u and thus $G_1 - u$ is a tree, contrary with Definition 1.1. □

Hereafter, let B_1, B_2, and B_3 be the three bicyclic graphs and H_0 be the tricyclic graph as shown in Figure 5.1.

Lemma 5.6. *If $n \ge 9$, then G is not a bicyclic graph with $\mathcal{R}(G) \in \{B_1, B_2\}$.*

Proof. Assume, to the contrary, that G is a bicyclic graph with $\mathcal{R}(G) = B_j$ for $j \in \{1, 2\}$. Suppose that G contains q non-pendant vertices and C_t is the special cycle of G by Lemma 5.5.

We first suppose that $j = 2$. Then, $\Delta < n - 4$ and $t \ge 3$. By Lemma 2.3 and (5.3),

$$\begin{aligned} AZI(G) &\ge 3\Psi(3,3) + 32 + (n-6)\Psi(\Delta,1) \\ &> 68 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction. Thus, $j = 1$ and so $q \ge 5$.

If either $q \geq 7$ or $t \geq 4$, then Lemma 5.5 implies that $\Delta \leq n-4$ and

$$\begin{aligned} AZI(G) &\geq \Psi(3,3) + 2\Psi(4,3) + 32 + (n-6)\Psi(\Delta,1) \\ &> 73 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction. Thus, $5 \leq q \leq 6$ and $t = 3$.

Denote by $\{u_0, v_0, w_0\}$ the three vertices of the special triangle such that u_0 is the common vertex of two cycle and $d(v_0) \geq d(w_0) \geq 3$. Then, $\Delta \leq n-3$.

Case 1. $\Delta \leq n-4$. If $d(v_0) \geq 4$, then

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + \Psi(4,4) + 24 + (n-5)\Psi(\Delta,1) \\ &> 73.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

If $d(v_0) = 3$, then $d(w_0) = 3$ and thus

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + 2\Psi(3,1) + \Psi(3,3) + 24 + (n-7)\Psi(\Delta,1) \\ &> 70.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

Case 2. $\Delta = n-3$. This implies there are exactly $n-7$ pendant vertices adjacent to u_0, as G contains a special triangle. Combining this with $n \geq 9$, we have

$$\begin{aligned} &AZI(G) - AZI(F_n) \\ &> 2\Psi(n-3,3) + 2\Psi(3,1) + \Psi(3,3) + 24 + (n-7)\Psi(n-3,1) - 67.5 - (n-8)\left(\frac{n-4}{n-5}\right)^3 \\ &> 2\Psi(n-3,3) + (n-7)\Psi(n-3,1) - 25.5 - (n-8)\left(\frac{n-4}{n-5}\right)^3 \\ &= \frac{f(n)}{2(n-5)^3(n-2)^3(n-4)^3} > 0, \end{aligned}$$

where $f(n) = 59n^9 - 2271n^8 + 38523n^7 - 377801n^6 + 2359860n^5 - 9733082n^4 + 26499486n^3 - 45914412n^2 + 45931000n - 20210288$. □

Lemma 5.7. *If $n \geq 9$, then G is not a bicyclic graph with $\mathcal{R}(G) = B_3$.*

Proof. Assume, to the contrary, that G is a bicyclic graph with $\mathcal{R}(G) = B_3$. Without loss of generality, we suppose that $s_1 \geq s_2 \geq s_3$ (see Figure 5.1). Since $G \in \mathbb{T}_n^3$, we have $\min\left\{|V(T_{u_0})|, |V(T_{v_0})|\right\} \geq 3$, where u_0 and v_0 are the two 3-vertices of B_3 (see Figure 5.1). Thus, $d(u_0) \geq d(v_0) \geq 4$ and $\Delta \leq n-4$. By Lemma 5.5, let C_t be a special cycle of G.

If $s_3 \geq 1$, then $t \geq 4$ and

$$\begin{aligned} AZI(G) &\geq 4\Psi(4,3) + 16 + (n-5)\Psi(\Delta,1) \\ &> 74 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction. Thus, $s_3 = 0$ and so $u_0v_0 \in E(G)$.

We first suppose that G contains at least five non-pendant vertices. Then,

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + \Psi(4,4) + 24 + (n-5)\Psi(\Delta,1) \\ &> 73.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

We next suppose that G contains exactly four non-pendant vertices, and thus $\mathcal{R}(G) = K_4 - e$. If $d(u_0) \geq 5$, then

$$\begin{aligned} AZI(G) &\geq 2\Psi(4,3) + \Psi(5,4) + 16 + (n-4)\Psi(\Delta,1) \\ &> 70.5 + (n-8)\left(\frac{n-4}{n-5}\right)^3 > AZI(F_n), \end{aligned}$$

a contradiction.

Thus, $d(u_0) = 4$ and so $d(v_0) = 4$. This implies that u_0 and v_0 are adjacent to precisely a pendant vertex, respectively. Let x_0 be the pendant neighbor of u_0. Then, $G - \{u_0, x_0\}$ is a tree, contrary with $G \in \mathbb{T}_n^3$. □

An $(s^{\geq}, t^{\geq})$ edge uv is an edge with $d(u) \geq s$ and $d(v) \geq t$. By Lemma 2.3(iii),

if $\min\{s,t\} \geq 3$, then $\Psi(s^{\geq}, t^{\geq}) \geq \Psi(s,t)$.

Proof of Theorem 1:3... From Corollary 5.1 and Lemmas 5.2–5.7, we can conclude that G is a tricyclic graph. Suppose that G contains p pendant vertices. Denote by G_1 the resultant graph obtained from G by deleting all these pendant vertices. Then, each edge of G_1 is a non-pendant edge of G.

Case 1. $p \leq n-7$. By (5.3) and Lemmas 2.3 and 2.5,

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq 8(n+2) - p\big(8 - \Psi(\Delta,1)\big) - 67.5 - (n-8)\Psi(n-4,1) \\ &\geq 8(n+2) - (n-7)\big(8 - \Psi(\Delta,1)\big) - 67.5 - (n-8)\Psi(n-4,1) \\ &\geq 72 + (n-7)\Psi(n-1,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &= \frac{11n^6 - 243n^5 + 2199n^4 - 10269n^3 + 25620n^2 - 31806n + 15442}{2(n-2)^3(n-5)^3} > 0, \end{aligned}$$

as $n \geq 14$.

Case 2. $p = n-6$. This implies that G_1 contains six vertices and eight edges, and thus G contains exactly eight non-pendant edges.

If G contains one $(4^{\geq}, 3^{\geq})$ edge, then

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq \Psi(4,3) + 56 + (n-6)\Psi(\Delta,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &> 2 + (n-6)\Psi(n-1,1) - (n-8)\Psi(n-4,1) \qquad (5.5) \\ &= \frac{4n^6 - 87n^5 + 780n^4 - 3623n^3 + 9000n^2 - 11103n + 5346}{(n-2)^3(n-5)^3} > 0, \end{aligned}$$

a contradiction.

If G contains two $(3^{\geq}, 3^{\geq})$ edges, then (5.5) implies that

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq 2\Psi(3,3) + 48 + (n-6)\Psi(\Delta,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &> 3 + (n-6)\Psi(n-1,1) - (n-8)\Psi(n-4,1) > 0, \end{aligned}$$

a contradiction.

Thus, G and, therefore, G_1 contain at most one $(3^{\geq}, 3^{\geq})$ edge and no $(4^{\geq}, 3^{\geq})$ edge. Since G_1 is a tricyclic graph with six vertices and eight edges, we have $G_1 = K_{2,4}$ (see the table of connected graphs with six vertices [4]). Combining this with $G \in \mathbb{T}_n^3$, we have $G = F_n$ by Definition 1.1.

Case 3. $n-5 \leq p \leq n-4$. If G contains at least five $(3^{\geq}, 3^{\geq})$ edges, then

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq 5\Psi(3,3) + 8 + (n-4)\Psi(\Delta,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &\geq 5\Psi(3,3) + 8 + (n-4)\Psi(n-1,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &= \frac{93n^6 - 1761n^5 + 14157n^4 - 60527n^3 + 139650n^2 - 157092n + 67144}{64(n-2)^3(n-5)^3} \\ &> 0, \end{aligned}$$

as G contains at least six non-pendant edges. Thus, G contains at most four $(3^{\geq}, 3^{\geq})$ edges and so $p = n-5$. This implies that G_1 is a tricyclic graph with five vertices and thus G contains exactly seven non-pendant edges.

Recall that G contains exactly seven non-pendant edges. Thus, if G contains at least one $(4^{\geq}, 4^{\geq})$ edges, then

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq \Psi(4,4) + 48 + (n-5)\Psi(\Delta,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &\geq \Psi(4,4) + 48 + (n-5)\Psi(n-1,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &= \frac{133n^6 - 2793n^5 + 24513n^4 - 112495n^3 + 276720n^2 - 336162n + 158434}{54(n-2)^3(n-5)^3} \\ &> 0, \end{aligned}$$

and so G contains no $(4^{\geq}, 4^{\geq})$ edge.

Now, since G contains at most four $(3^{\geq}, 3^{\geq})$ edges and no $(4^{\geq}, 4^{\geq})$ edge, we can conclude that $G_1 = H_0$ (see Figure 5.1) by the table of connected graphs with five vertices [4]. In this case, G contains two $(4^{\geq}, 3^{\geq})$ edges and one $(3^{\geq}, 3^{\geq})$ edge, we have

$$\begin{aligned} AZI(G) - AZI(F_n) &\geq 2\Psi(4,3) + \Psi(3,3) + 32 + (n-5)\Psi(\Delta,1) - 67.5 - (n-8)\Psi(n-4,1) \\ &> 3 + (n-5)\Psi(n-1,1) - (n-8)\Psi(n-4,1) \\ &> 0, \end{aligned}$$

by (5.5). □

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Extremal polygonal cacti for bond incident degree indices☆

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ABSTRACT

For a connected graph G, the general sum-connectivity index $\chi_\alpha(G)$, general Platt index $Pl_\alpha(G)$ and second Zagreb index $M_2(G)$ are defined as $\chi_\alpha(G) = \sum_{uv\in E(G)}\big(d(u)+d(v)\big)^\alpha$, $Pl_\alpha(G) = \sum_{uv\in E(G)}\big(d(u)+d(v)-2\big)^\alpha$ and $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$, where $d(u)$ is the degree of vertex u. A k-polygonal cactus is a connected graph in which every edge lies on exactly one cycle of length k. In this paper, we shall determine the minimum value and maximum value for $\chi_\alpha(G)$, $Pl_\alpha(G)$ and $M_2(G)$, respectively, among the class of k-polygonal cacti with n cycles for $k \geq 3$, $n \geq 3$ and $\alpha > 1$. Furthermore, when $\alpha > 1$, we determine the unique extremal maximum k-polygonal cactus with n cycles for $k \geq 3$ and $n \geq 3$, and we also identify the unique extremal minimum k-polygonal cactus with n cycles for $3 \leq k \leq 5$ and $n \geq 3$.

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1. Introduction

Throughout this paper, G denotes a simple connected undirected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u)$ and $N_G(u)$ be the degree and neighbor set of vertex u in G, respectively. If $u \in V(G)$ and $G-u$ is not connected, then u is said to be a *cut-vertex* of G.

A *cactus graph*, or cactus for short, is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus is either an edge or a cycle. A cycle of length k is denoted by C_k, and C_k is always called a *k-polygon* in the sequel. If each block of a cactus G is a k-polygon, then G is called a *k-polygonal cactus*. Hereafter, if there is no risk of confusion, we always call a k-polygon as a polygon, and we always simplify $d_G(u)$ and $N_G(u)$ as $d(u)$ and $N(u)$, respectively.

Let $\mathcal{G}_{n,k}$ be the class of k-polygonal cacti with $n \geq 3$ blocks. Suppose that $G \in \mathcal{G}_{n,k}$ and C_k is a polygon of G. If C_k contains exactly one cut-vertex, then C_k is called a *pendent polygon*. While C_k is called a *non-pendent polygon* if C_k contains at least two cut-vertices. A *star-like cactus* $W_{n,k}$ is a special k-polygonal cactus with n polygons such that all polygons have a common vertex. From the definition, $W_{n,k}$ is unique, all polygons of $W_{n,k}$ are pendent polygons and $W_{n,k}$ contains exactly one vertex with degree being equal to $2n$, while the degree of all the other vertices of $W_{n,k}$ is equal to two.

A *cactus chain* is a special k-polygonal cactus such that each polygon has at most two cut-vertices, and each cut-vertex is shared by exactly two polygons. When G is a cactus chain, then the number of polygons is called the *length* of G. For

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convenience, we use the notation $\mathcal{T}_{n,k}$ to denote the class of cactus chains of length n such that each polygon is a k-polygon. From the definition, each cactus chain of $\mathcal{T}_{n,k}$ has exactly $n-2$ non-pendent polygons and two pendent polygons. When $k=3$ and $n\geq 3$, it is easy to see that the cactus chain of $\mathcal{T}_{n,k}$ is unique. However, when $k\geq 4$ and $n\geq 3$, $\mathcal{T}_{n,k}$ is not unique. Hereafter, we define two special classes of cactus chains of $\mathcal{T}_{n,k}$ for $n\geq 3$ and $k\geq 3$ as follows:

Let $\mathcal{H}_{n,k}=\{G\colon G \text{ is a cactus chain of } \mathcal{T}_{n,k} \text{ such that each pair of cut-vertices, which lies in the same non-pendent polygon of } G \text{ is adjacent}\}$, and let $\mathcal{R}_{n,k}=\{G\colon G \text{ is a cactus chain of } \mathcal{T}_{n,k} \text{ such that each pair of cut-vertices, which lies in the same non-pendent polygon of } G \text{ is not adjacent}\}$.

From the above definitions, $\mathcal{H}_{n,k}$ is unique for $k\geq 3$, $\mathcal{R}_{n,3}$ is an empty set, both $\mathcal{R}_{n,4}$ and $\mathcal{R}_{n,5}$ are unique, and $\mathcal{R}_{n,k}$ is not unique for $k\geq 6$.

Since the bond incident degree indices have important applications on Biology and Biochemistry [5,7,8], more and more bond incident degree indices have been constructed. Among the bond incident degree indices, the *Randić index* $R(G)$ [14] and *second Zagreb index* $M_2(G)$ [9] are two famous topological indices, where

$$R(G)=\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{-\frac{1}{2}},\quad \text{and}\quad M_2(G)=\sum_{uv\in E(G)}d(u)d(v).$$

Bollobás and Erdős [4] generalized the concepts of Randić index and second Zagreb index to the *general Randić index* $R_\alpha(G)$, where

$$R_\alpha(G)=\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{\alpha}.$$

Similarly with the general Randić index of G, the *general sum-connectivity index* [21] $\chi_\alpha(G)$ of G is constructed as:

$$\chi_\alpha(G)=\sum_{uv\in E(G)}\big(d(u)+d(v)\big)^{\alpha}.$$

Particularly, $\chi_{-\frac{1}{2}}(G)$ is known as the *sum-connectivity index* of G [20], $\chi_2(G)$ is also called the *hyper-Zagreb index* of G [15], while $2\chi_{-1}(G)$ is equal to the *harmonic index* of G [6].

The *"reformulated first Zagreb index"* $EM_1(G)$ of G [13] is a slight modification to $\chi_2(G)$, where

$$EM_1(G)=\sum_{uv\in E(G)}\big(d(u)+d(v)-2\big)^{2}.$$

As an extension of the reformulated first Zagreb index, Ali and Dimitrov [1] constructed the *general Platt index* $Pl_\alpha(G)$ as

$$Pl_\alpha(G)=\sum_{uv\in E(G)}\big(d(u)+d(v)-2\big)^{\alpha}.$$

For more mathematical results on bond incident degree indices, one can refer to [2,3,17,18].

In this paper, we shall determine the minimum value and maximum value of general sum-connectivity index, general Platt index and second Zagreb index, respectively, among the class of k-polygonal cacti with n polygons for $k\geq 3$ and $n\geq 3$, that is,

Theorem 1.1. *Let $\alpha>1$ be a real number and let G be a cactus of $\mathcal{G}_{n,k}$, where $n\geq 3$ and $k\geq 3$. (i) If $k=3$, then $\chi_\alpha(G)\geq 2^{2\alpha+1}+2n\times 6^\alpha+(n-2)\times 8^\alpha$, $Pl_\alpha(G)\geq 2^{\alpha+1}+n\times 2^{2\alpha+1}+(n-2)\times 6^\alpha$ and $M_2(G)\geq 32n-24$, where the equality holds if and only if $G\in\mathcal{T}_{n,3}$.*

(ii) If $k\geq 4$, then $\chi_\alpha(G)\geq (kn-4n+4)\times 4^\alpha+(4n-4)\times 6^\alpha$, $Pl_\alpha(G)\geq (kn-4n+4)\times 2^\alpha+(n-1)\times 4^{\alpha+1}$ and $M_2(G)\geq 4(kn+4n-4)$, where the equality holds if $G\in\mathcal{R}_{n,k}$. Furthermore, if $k\in\{4,5\}$, then the equality holds if and only if $G\in\mathcal{R}_{n,k}$.

Theorem 1.2. *Let G be a cactus of $\mathcal{G}_{n,k}$, where $k\geq 3$ and $n\geq 3$. If $\alpha>1$ is a real number, then $\chi_\alpha(G)\leq\chi_\alpha(W_{n,k})$, $Pl_\alpha(G)\leq Pl_\alpha(W_{n,k})$ and $M_2(G)\leq M_2(W_{n,k})$, where each equality holds if and only if $G\cong W_{n,k}$.*

At the end of this section, we shall point out that $\mathcal{R}_{n,k}$ is not unique for $k\geq 6$, but $\chi_\alpha(G)$, $Pl_\alpha(G)$ and $M_2(G)$ are equal to the same value for each $G\in\mathcal{R}_{n,k}$, respectively. Furthermore, when $k\geq 6$, the cacti of $\mathcal{R}_{n,k}$ are not all the extremal minimum cacti of $\mathcal{G}_{n,k}$ in Theorem 1.1 (see Remark 2.1 of Section 2).

2. The proof of Theorem 1.1

In order to study on the graph invariants based on adjacency vertex degree, Wang [17] recently proposed the concept of escalating function as follows:

A symmetric bivariate function $f(x,y)$ defined on positive real numbers is called *escalating* if

$$f(x_1,x_2)+f(y_1,y_2)\geq f(x_2,y_1)+f(x_1,y_2) \tag{2.1}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (2.1) is strict if $x_1 > y_1 > 0$ and $x_2 > y_2 > 0$. Furthermore, an escalating function $f(x, y)$ is called *special escalating* if $f(x, y)$ satisfies

$$4f(2r, 2) \geq f(2r-2, 4) + f(2r-2, 2) + f(4, 2) + f(4, 4) \text{ holds for } r \geq 3$$

and $f(x_1, x_2) \geq f(y_1, y_2)$ holds for any $x_1 \geq y_1 \geq 2$ and $x_2 \geq y_2 \geq 2$.

It is interesting to unify these former topological indices by a definition. To do this, Hollas [11] constructed a new invariant $BID(G)$ of graph G as

$$BID(G) = \sum_{uv \in E(G)} f\big(d(u), d(v)\big). \tag{2.2}$$

In some literatures, $BID(G)$ was called the *bond incident degree index* [1,16] of G, and it was also called the *connectivity function* of G by Wang [17].

Hereafter, let $n_{s,t}$ be the number of edges connecting the vertices of degrees s and t, and let $G\big[X\big]$ be the subgraph of G induced by X, where X is a subset of $V(G)$.

Lemma 2.1. *Let G be a cactus of $\mathcal{T}_{n,k}$, where $k \geq 4$ and $n \geq 3$. If $f(x, y)$ is an escalating function and $G \notin \mathcal{R}_{n,k} \cup \mathcal{H}_{n,k}$, then $BID(G_1) < BID(G) < BID(G_2)$, where $G_1 \in \mathcal{R}_{n,k}$ with $BID(G_1) = \big(kn - 4n + 4\big)f(2, 2) + \big(4n - 4\big)f(4, 2)$ and $G_2 \in \mathcal{H}_{n,k}$ with $BID(G_2) = \big(n(k-3) + 2\big)f(2, 2) + 2nf(4, 2) + \big(n - 2\big)f(4, 4)$.*

Proof. Since $G \in \mathcal{T}_{n,k}$, G contains exactly $n-2$ non-pendent polygons and two pendent polygons. We suppose that G contains exactly p non-pendent polygons, whose two cut-vertices in the same polygon are adjacent. This means that G contains exactly $n-2-p$ non-pendent polygons, whose two cut-vertices in the same polygon are not adjacent. From the structure of G, there are three types of edges, that is, $n_{2,2} = 2(k-2) + p(k-3) + (n-2-p)(k-4) = p + (k-4)n + 4$, $n_{2,4} = 4(n-2-p) + 2p + 4 = 2\big(2n - p - 2\big)$ and $n_{4,4} = p$. Thus, we have

$$BID(G) = \Big(p + (k-4)n + 4\Big)f(2, 2) + 2\big(2n - p - 2\big)f(4, 2) + pf(4, 4).$$

We consider the function

$$\Psi(z) = \Big(z + (k-4)n + 4\Big)f(2, 2) + 2\big(2n - z - 2\big)f(4, 2) + zf(4, 4).$$

Since $f(x, y)$ is escalating, we have $\Psi'(z) = f(2, 2) - 2f(4, 2) + f(4, 4) > 0$. Thus, $\Psi(z)$ is a strictly increasing function on z. Consequently, $\Psi(0) \leq \Psi(z) \leq \Psi(n-2)$, where the left equality holds if and only if $p = 0$ (that is, $G \in \mathcal{R}_{n,k}$), and the right equality holds if and only if $p = n-2$ (that is, $G \in \mathcal{H}_{n,k}$).

Since $G_1 \in \mathcal{R}_{n,k}$ and $G_2 \in \mathcal{H}_{n,k}$, we have $BID\big(G_1\big) = \Psi(0) = \big(kn - 4n + 4\big)f(2, 2) + \big(4n - 4\big)f(4, 2)$ and $BID\big(G_2\big) = \Psi(n-2) = \big(n(k-3) + 2\big)f(2, 2) + 2nf(4, 2) + (n-2)f(4, 4)$. Recall that $G \notin \mathcal{R}_{n,k} \cup \mathcal{H}_{n,k}$. Thus, $BID\big(G_1\big) = \Psi(0) < BID(G) < \Psi(n-2) = BID\big(G_2\big)$. ■

Suppose that $G \in \mathcal{G}_{n,k}$ and $C_k^{(1)}, C_k^{(2)}, \ldots, C_k^{(s)}$ are s cycles of length k in G, where $k \geq 3$, $s \geq 1$ and $n \geq 3$. Let $V_1 = V\left(C_k^{(1)}\right) \cup V\left(C_k^{(2)}\right) \cup \cdots \cup V\left(C_k^{(s)}\right)$ and let u_1 be a cut-vertex of $C_k^{(1)}$ in G such that u_1 is not a cut-vertex of $G\big[V_1\big]$. If $G\big[V_1\big]$ is a cactus chain and each k-polygon of $\left\{C_k^{(1)}, C_k^{(2)}, \ldots, C_k^{(s)}\right\}$ has at most two cut-vertices in G, $C_k^{(s)}$ is a pendent polygon of G, the degree of each vertex of $V_1 \setminus \{u_1\}$ is at most four in G, then $G\big[V_1\big]$ is called a *pendent cactus chain* of length s of G. Furthermore, if $G\big[V_1\big]$ is a pendent cactus chain of length $s \geq 2$, then $C_k^{(s-1)}$ is called a *neighbor polygon* of the pendent cactus chain. Hereafter, we denote $L_{s,k}$ as a pendent cactus chain of length s in a k-polygonal cactus.

From the definition, if $G\big[V_1\big]$ is a pendent cactus chain of length $s \geq 2$, then for $1 \leq i \leq s-1$ and $2 \leq j \leq s-1$, each $C_k^{(i)}$ contains exactly two cut-vertices in G and the degree of every cut-vertex of $C_k^{(j)}$ is equal to four in G.

Definition 2.1. Let G be a cactus of $\mathcal{G}_{n,k}$ and let $C_k^{(1)}, C_k^{(2)}, \ldots, C_k^{(s+t)}$ be $s+t$ cycles of length k of G such that $G\left[V\left(C_k^{(1)}\right) \cup V\left(C_k^{(2)}\right) \cup \cdots \cup V\left(C_k^{(s)}\right)\right]$ and $G\left[V\left(C_k^{(s+1)}\right) \cup V\left(C_k^{(s+2)}\right) \cup \cdots \cup V\left(C_k^{(s+t)}\right)\right]$ are two pendent cactus chains of length $s \geq 1$ and $t \geq 1$, respectively.

(*i*) If $u_0 \in V\left(C_k^{(1)}\right) \cap V\left(C_k^{(s+1)}\right)$ and $d_G(u_0) \geq 6$, then u_0 is called a *singular vertex* of G.

(*ii*) If $C_k^{(0)}$ is a k-polygon of G with at least three cut-vertices in G such that $V\left(C_k^{(1)}\right) \cap V\left(C_k^{(0)}\right) = \{v_0\}$ and $V\left(C_k^{(s+1)}\right) \cap V\left(C_k^{(0)}\right) = \{w_0\}$ with $d_G(w_0) = d_G(v_0) = 4$, then $C_k^{(0)}$ is called a *special polygon* of G.

Lemma 2.2. *Let G be a cactus of $\mathcal{G}_{n,k}$, where $k \geq 4$ and $n \geq 4$. Let $L_{s,k}$ be a pendent cactus chain of length $s \geq 2$ such that $C_k^{(s-1)}$ is the neighbor polygon and $C_k^{(s)}$ is the pendent polygon of $L_{s,k}$. Let w_1 and w_2 be two cut-vertices of $C_k^{(s-1)}$: $w_1w_2 \cdots w_kw_1$, and $N_G(w_2) \cap V\left(C_k^{(s)}\right) = \{u, v\}$. Let $G' = G - w_2u - w_2v + w_3u + w_3v$. If $f(x, y)$ is an escalating function, then $BID(G) > BID(G')$.*

Proof. If $s \geq 3$, then we have

$$BID(G) - BID(G') = f(4,4) + f(2,2) - 2f(4,2) > 0,$$

as $f(x,y)$ is escalating. Otherwise, $s = 2$. In this case, we suppose that $d_G(w_1) = 2r$, where $r \geq 2$. Since $f(x,y)$ is escalating, we have

$$BID(G) - BID(G') = f(2r,4) + f(2,2) - f(2r,2) - f(4,2) > 0.$$

This completes the proof of this result. ■

Lemma 2.3. *Let G be a cactus of $\mathcal{G}_{n,k}$, where $k \geq 3$ and $n \geq 3$. If $f(x,y)$ is a special escalating function and G contains a singular vertex, then $BID(G)$ is not minimum in $\mathcal{G}_{n,k}$.*

Proof. By contradiction, we assume that $BID(G)$ is minimum in $\mathcal{G}_{n,k}$. Let u_0 be a singular vertex of G with $d_G(u_0) = 2r$, where $r \geq 3$. For convenience, we suppose that u_0 is a common vertex of two pendent cactus chains $L_{t,k}$ and $L_{s,k}$ in G, where $s \geq t \geq 1$. Suppose that $C_k^{(t)} : u_1u_2 \cdots u_ku_1$ and $C_k^{(s)} : w_1w_2 \cdots w_kw_1$ are the pendent polygons of $L_{t,k}$ and $L_{s,k}$, respectively, where u_1 and w_1 are the two cut-vertices of G. Let $G' = G - u_1u_2 - u_1u_k + w_3u_2 + w_3u_k$. By the definition of G', it is easy to see that

Observation 1. If $t \geq 2$, then u_0 is also a singular vertex of G' such that u_0 is a common vertex of two pendent cactus chains $L_{t-1,k}$ and $L_{s+1,k}$ in G'.

Now, we suppose that $u_0v_0 \in E(G)$ with $d_G(v_0) = 2q$, where $u_0v_0 \notin E(L_{t,k}) \cup E(L_{s,k})$. Let $E_1 = E(L_{t,k}) \cup E(L_{s,k}) \cup \{u_0v_0\}$ and also let $E_2 = E(G) \setminus E_1$. For any edge $uv \in E_2$, since $d_G(u) \geq d_{G'}(u)$ and $d_G(v) \geq d_{G'}(v)$, we have $f\big(d_G(u), d_G(v)\big) \geq f\big(d_{G'}(u), d_{G'}(v)\big)$. Thus,

$$BID(G) - BID(G') \geq \sum_{uv \in E(G)\setminus E_2} f\big(d_G(u), d_G(v)\big) - \sum_{uv \in E(G')\setminus E_2} f\big(d_{G'}(u), d_{G'}(v)\big). \tag{2.3}$$

Case 1. $k = 3$. We consider the following two subcases:

Subcase 1.1. $t = 1$. If $s > t = 1$, since $f(x,y)$ is special escalating and $2r \geq 6$, (2.3) implies that

$$\begin{aligned} BID(G) - BID(G') &\geq f(2r,2q) + 3f(2r,2) + f(2r,4) + f(4,2) + f(2,2) - f(2r-2,4) \\ &\quad - f(2r-2,2) - 3f(4,2) - f(4,4) - f(2r-2,2q) \\ &\geq f(2r,2q) + f(2r,4) + f(2,2) - f(2r-2,2q) - f(2r,2) - f(4,2) \\ &\geq f(2r,4) + f(2,2) - f(2r,2) - f(4,2) > 0, \end{aligned}$$

which is contrary with the choice of G.

Otherwise, $s = t = 1$. Since $f(x,y)$ is special escalating and $2r \geq 6$, by (2.3) we have

$$\begin{aligned} &BID(G) - BID(G') \\ &\geq f(2r,2q) + 4f(2r,2) + f(2,2) - f(2r-2,2) - f(2r-2,4) - 3f(4,2) - f(2r-2,2q) \\ &\geq f(2r,2q) + f(4,4) + f(2,2) - 2f(4,2) - f(2r-2,2q) \\ &\geq f(4,4) + f(2,2) - 2f(4,2) > 0, \end{aligned}$$

which is contrary with the choice of G.

Subcase 1.2. $t \geq 2$. If $t \geq 3$, then it is easy to see that $BID(G) = BID(G')$. Now, by Observation 1, there exists a cactus G_1 of $\mathcal{G}_{n,k}$ such that $BID(G) = BID(G_1)$, u_0 is also a singular vertex of G_1 and u_0 is a common vertex of two pendent cactus chains $L_{t-1,k}$ and $L_{s+1,k}$ in G_1. By repeating the above process, we can conclude that there exists a cactus G_2 of $\mathcal{G}_{n,k}$ such that $BID(G) = BID(G_2)$, u_0 is also a singular vertex of G_2 and u_0 is a common vertex of two pendent cactus chains $L_{2,k}$ and $L_{s+t-2,k}$ in G_2.

Otherwise, $t = 2$. Since $f(x,y)$ is special escalating, we have

$$BID(G) - BID(G') = f(2r,4) + f(4,2) - f(2r,2) - f(4,4) > 0.$$

Now, from the above arguments and Observation 1, we can conclude that there exists a cactus G_3 of $\mathcal{G}_{n,k}$ such that $BID(G) > BID(G_3)$, a contradiction.

Case 2. $k \geq 4$. We also divide the proof into two subcases as follows:

Subcase 2.1. $t \geq 2$. Let u and v be the two cut-vertices in the neighbor polygon of $L_{t,k}$. If $uv \in E(G)$, then by Lemma 2.2 we have another $G_4 \in \mathcal{G}_{n,k}$ such that $BID(G) > BID(G_4)$, a contradiction. Otherwise, $uv \notin E(G)$. It is easy to see that $BID(G) = BID(G')$. Now, by Observation 1, there exists a cactus G_5 of $\mathcal{G}_{n,k}$ such that $BID(G) = BID(G_5)$, u_0 is also a singular vertex of G_5 and u_0 is a common vertex of two pendent cactus chains $L_{t-1,k}$ and $L_{s+1,k}$ in G_5. By repeating the above process,

we can conclude that there exists a cactus G_6 of $\mathcal{G}_{n,k}$ such that $BID(G) = BID(G_6)$, u_0 is also a singular vertex of G_6 and u_0 is a common vertex of two pendent cactus chains $L_{1,k}$ and $L_{s+t-1,k}$ in G_6.

Subcase 2.2. $t = 1$. In this subcase, let $N(u_0) \cap V(L_{s,k}) = \{u, v\}$ with $d_G(u) \geq d_G(v)$. We suppose that $d_G(u) = 2p$. Then, $2p \geq 2 = d_G(v)$. Since

$$4f(2r, 2) \geq f(2r-2, 4) + f(2r-2, 2) + f(4, 2) + f(4, 4) \text{ and } f(2r, 2q) \geq f(2r-2, 2q),$$

from (2.3) it follows that

$$\begin{aligned} &BID(G) - BID(G') \\ &\geq f(2r, 2q) + 3f(2r, 2) + f(2r, 2p) + 2f(2, 2) - f(2r-2, 2p) - f(2r-2, 2) \\ &\quad - 4f(4, 2) - f(2r-2, 2q) \\ &\geq f(2r-2, 4) + f(4, 4) + 2f(2, 2) + f(2r, 2p) - f(2r-2, 2p) - f(2r, 2) - 3f(4, 2). \end{aligned} \tag{2.4}$$

If $p \geq 2$, then (2.4) implies that

$$\begin{aligned} BID(G) - BID(G') &\geq f(2r, 4) + f(4, 4) + 2f(2, 2) - f(2r, 2) - 3f(4, 2) \\ &> f(2r, 2) + f(4, 2) + 2f(4, 2) - f(2r, 2) - 3f(4, 2) = 0, \end{aligned}$$

a contradiction.

Otherwise, $p = 1$. Since $f(2r-2, 4) + f(2, 2) > f(2r-2, 2) + f(4, 2)$, from (2.4), we have

$$BID(G) - BID(G') > f(4, 4) + f(2, 2) - 2f(4, 2) > 0,$$

a contradiction. ■

Lemma 2.4. *Let $f(x, y)$ be an escalating function, and let G be a cactus of $\mathcal{G}_{n,k}$, where $n \geq 4$. If G contains a special polygon, then $BID(G)$ is not minimum in $\mathcal{G}_{n,k}$ for $3 \leq k \leq 5$, and there exists $G_0 \in \mathcal{G}_{n,k}$ such that $BID(G) \geq BID(G_0)$ and G_0 contains no special polygon for $k \geq 6$.*

Proof. We assume that $BID(G)$ is minimum in $\mathcal{G}_{n,k}$ and G contains a special polygon $C_k^{(0)}$. Let $L_{t,k}$ and $L_{s,k}$ be two pendent cactus chains of G such that $V(L_{t,k}) \cap V\left(C_k^{(0)}\right) = \{u_0\}$ and $V(L_{s,k}) \cap V\left(C_k^{(0)}\right) = \{w_0\}$, where $s \geq t \geq 1$. Suppose that $C_k^{(t)}: u_1u_2 \cdots u_ku_1$ and $C_k^{(s)}: w_1w_2 \cdots w_kw_1$ are the pendent polygons of $L_{t,k}$ and $L_{s,k}$, respectively, such that u_1 and w_1 are two cut-vertices of G. Let $G' = G - u_1u_2 - u_1u_k + w_3u_2 + w_3u_k$. By the definition of G', it is easy to see that

Observation 1. If $t \geq 2$, then $C_k^{(0)}$ is also a special polygon of G' and that $L_{t-1,k}$ and $L_{s+1,k}$ are two pendent cactus chains of G' such that $V(L_{t-1,k}) \cap V\left(C_k^{(0)}\right) = \{u_0\}$ and $V(L_{s+1,k}) \cap V\left(C_k^{(0)}\right) = \{w_0\}$.

We now consider the following two cases:

Case 1. $k = 3$. In this case, we suppose that $V\left(C_k^{(0)}\right) \setminus \{u_0, w_0\} = \{v_0\}$ and we suppose that $d_G(v_0) = 2r_1$. Since $C_k^{(0)}$ is a special polygon of G, we have $r_1 \geq 2$. If $t \geq 2$, then it is easy to see that $BID(G) = BID(G')$. By Observation 1, there exists $G_1 \in \mathcal{G}_{n,k}$ such that $BID(G) = BID(G_1)$, where $C_k^{(0)}$ is also a special polygon of G_1 such that $L_{1,k}$ and $L_{s+t-1,k}$ are two pendent cactus chains of G_1, $V(L_{1,k}) \cap V\left(C_k^{(0)}\right) = \{u_0\}$ and $V(L_{s+t-1,k}) \cap V\left(C_k^{(0)}\right) = \{w_0\}$. Otherwise, $t = 1$. Since $f(x, y)$ is escalating, we have

$$BID(G) - BID(G') = f(2r_1, 4) + f(2, 2) - f(2r_1, 2) - f(4, 2) > 0,$$

which is contrary with the choice of G. In this case, the result follows.

Case 2. $k \geq 4$. In this case, we suppose that $N_G(u_0) \cap V\left(C_k^{(0)}\right) = \{x_0, y_0\}$, and we suppose that $d_G(x_0) = 2r_2$ and $d_G(y_0) = 2r_3$, where $r_2 \geq r_3 \geq 1$. We consider the following two subcases:

Subcase 2.1. $t \geq 2$. Let u and v be the two cut-vertices of the neighbor polygon of $L_{t,k}$. If $uv \in E(G)$, since $f(x, y)$ is escalating, we have

$$BID(G) - BID(G') = f(4, 4) + f(2, 2) - 2f(4, 2) > 0,$$

a contradiction. Otherwise, $uv \notin E(G)$. In this case, it is easy to see that $BID(G) = BID(G')$. By Observation 1, there exists $G_2 \in \mathcal{G}_{n,k}$ such that $BID(G) \geq BID(G_2)$, where $C_k^{(0)}$ is also a special polygon of G_2 such that $L_{1,k}$ and $L_{s+t-1,k}$ are two pendent cactus chains of G_2, $V(L_{1,k}) \cap V\left(C_k^{(0)}\right) = \{u_0\}$ and $V(L_{s+t-1,k}) \cap V\left(C_k^{(0)}\right) = \{w_0\}$.

Subcase 2.2. $t = 1$. By the definition of G and G', we have

$$BID(G) - BID(G') = f(2r_2, 4) + f(2r_3, 4) + 2f(2, 2) - f(2r_2, 2) - f(2r_3, 2) - 2f(4, 2). \tag{2.5}$$

Subcase 2.2.1. $k = 4$. In this case, we have $r_2 \geq 2$. If $r_2 \geq r_3 \geq 2$, since $f(x, y)$ is escalating, we have $BID(G) > BID(G')$ by (2.5), a contradiction. If $r_2 \geq 2$ and $r_3 = 1$, since $f(x, y)$ is escalating, (2.5) implies that

$$BID(G) - BID(G') = f(2r_2, 4) + f(2, 2) - f(2r_2, 2) - f(4, 2) > 0,$$

a contradiction.

Subcase 2.2.2. $k \geq 6$. If $r_2 \geq 2$, by the proof of $k = 4$, from (2.5), we have $BID(G) > BID(G')$, a contradiction. Thus, $r_2 = r_3 = 1$. In this case, $BID(G) = BID(G')$ by (2.5). By repeating this process, we can conclude that there exists $G_0 \in \mathcal{G}_{n,k}$ such that $BID(G) = BID(G_0)$ and G_0 contains no special polygon.

Subcase 2.2.3. $k = 5$. If $r_2 \geq 2$, by the proof of $k = 4$, from (2.5), we have $BID(G) > BID(G')$, a contradiction. Thus $r_2 = r_3 = 1$. In this case, we may suppose that $V\left(C_k^{(0)}\right) \setminus \{u_0, w_0, x_0, y_0\} = \{v_0\}$ and $d_G(v_0) = 2r_4$. Then $r_4 \geq 2$. Let $G'' = G - w_1w_2 - w_1w_k + u_3w_2 + u_3w_k$.

If $s = 1$, then $s = t = 1$ and hence

$$BID(G) - BID(G'') = f(2r_4, 4) + f(2, 2) - f(2r_4, 2) - f(4, 2) > 0,$$

a contradiction. Otherwise, $s \geq 2$. By Lemma 2.2 and the choice of G, we may suppose that the two cut-vertices of the non-pendent polygon of $L_{s,k}$ are not adjacent. It is easy to see that $BID(G) = BID(G'')$. By repeating this process, we can conclude that there exists $G_3 \in \mathcal{G}_{n,k}$ such that $BID(G) = BID(G_3)$, $C_k^{(0)}$ is also a special polygon of G_3 and that $L_{t+s-1,k}$ and $L_{1,k}$ are two pendent cactus chains of G_3, where $V\left(L_{t+s-1,k}\right) \cap V\left(C_k^{(0)}\right) = \{u_0\}$ and $V\left(L_{1,k}\right) \cap V\left(C_k^{(0)}\right) = \{w_0\}$.

Let G_3'' be the graph obtained from G_3 by a similar method as G'' constructing from G. By an elementary computation and $r_4 \geq 2$, we have

$$BID(G_3) - BID(G_3'') = f(2r_4, 4) + f(2, 2) - f(2r_4, 2) - f(4, 2) > 0,$$

a contradiction. ■

The distance $dist(u, v)$ between the vertices u and v of a connected graph G is equal to the length of (number of edges in) a shortest path that connects u and v in G. Let C_k and C_k' be two k-polygons of a connected graph G and let u_0 be a vertex of G. Then, we denote by $dist\ (u_0, C_k) = \min\left\{dist(u_0, v)\colon v \in V(C_k)\right\}$ and $dist\left(C_k, C_k'\right) = \min\left\{dist(u, v)\colon u \in V(C_k) \text{ and } v \in V(C_k')\right\}$. Sometimes, we write $dist_G(u, v)$, $dist_G\ (u_0, C_k)$ and $dist_G\left(C_k, C_k'\right)$ in place of $dist(u, v)$, $dist\ (u_0, C_k)$ and $dist\left(C_k, C_k'\right)$ in order to indicate the dependence on G, respectively.

In what follows, we always suppose that G contains exactly $p(G)$ polygons, say $C_k^{(1)}, C_k^{(2)}, \ldots, C_k^{(p(G))}$, such that each polygon of $\left\{C_k^{(1)}, C_k^{(2)}, \ldots, C_k^{(p(G))}\right\}$ contains at least three cut-vertices and G contains exactly $q(G)$ cut-vertices, say $u_1, u_2, \ldots, u_{q(G)}$, such that each vertex of $\{u_1, u_2, \ldots, u_{q(G)}\}$ is the common vertex of at least three polygons, namely, $\{u_1, u_2, \ldots, u_{q(G)}\}$ is the class of vertices with degrees at least six.

Lemma 2.5. *Let G be a cactus of $\mathcal{G}_{n,k}$, where $k \geq 3$ and $n \geq 3$. If G contains neither singular vertex nor special polygon, then G must be a cactus chain.*

Proof. We firstly prove the following claim:

Claim 1. *If $p(G) + q(G) = 0$, then G is a cactus chain.*

Proof of Claim 1. Let u be a cut-vertex of G and let C_k be a non-pendent polygon of G. Since $p(G) = q(G) = 0$, C_k contains exactly two cut-vertices and $d_G(u) = 4$, equivalently, u is the common vertex of two polygons. Now, we prove Claim 1 by induction on n. When $n = 3$, it is easy to see that G is a cactus chain, as $p(G) = q(G) = 0$. Next we suppose that Claim 1 already holds for $n = m - 1 \geq 3$, and suppose that G is a cactus of $\mathcal{G}_{m,k}$ with $p(G) + q(G) = 0$. Let C_k' be a pendent polygon of G, and let G' be the cactus obtained from G by deleting the vertices in $V(C_k') \setminus \{u'\}$, where u' is the cut vertex of C_k'. It is easy to see that $p(G') + q(G') = 0$ and $G' \in \mathcal{G}_{m-1,k}$. By the induction hypothesis, G' is already a cactus chain.

Since $p(G) = q(G) = 0$, u' is in a pendent polygon of G' (otherwise, $p(G) \geq 1$ or $q(G) \geq 1$) and u' is not a cut-vertex of G' (otherwise, $q(G) \geq 1$), that is, G is also a cactus chain. This completes the proof of Claim 1. ■

We secondly prove this result by contradiction, and we assume that G is not a cactus chain. By Claim 1, we have $p(G) + q(G) \geq 1$. We now consider the following two cases:

Case 1. $p(G) + q(G) \geq 2$. Let

$$h_1 = \min\left\{dist_G\left(u_i, u_j\right) :\ 1 \leq i \leq j \leq q(G)\right\},$$

$$h_2 = \min\left\{dist_G\left(u_i, C_k^{(j)}\right) :\ 1 \leq i \leq q(G) \text{ and } 1 \leq j \leq p(G)\right\},$$

$$\text{and } h_3 = \min\left\{dist_G\left(C_k^{(i)}, C_k^{(j)}\right) :\ 1 \leq i \leq j \leq p(G)\right\}.$$

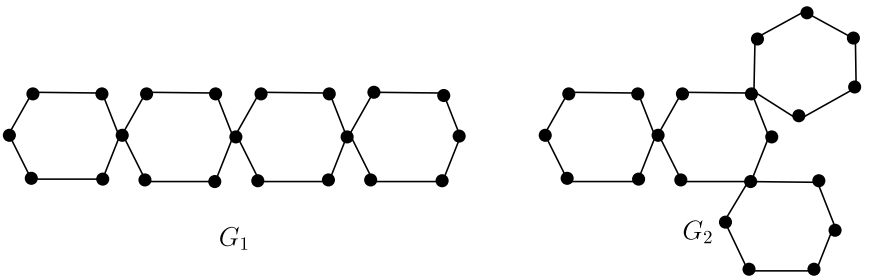


Fig. 2.1. The graphs G_1 and G_2.

Denote by

$$h_0 = \max\{h_1, h_2, h_3\}.$$

Subcase 1.1. $h_0 = h_1$. Without loss of generality, we suppose that $h_0 = h_1 = dist_G(u_1, u_2)$. By the definition of h_0 and Claim 1, both u_1 and u_2 are singular vertices, a contradiction.

Subcase 1.2. $h_0 = h_2$. Without loss of generality, we suppose that $h_0 = h_2 = dist_G\left(u_1, C_k^{(1)}\right)$. By the definition of h_0 and Claim 1, u_1 is a singular vertex and $C_k^{(1)}$ is a special polygon, a contradiction.

Subcase 1.3. $h_0 = h_3$. Without loss of generality, we suppose that $h_0 = h_3 = dist_G\left(C_k^{(1)}, C_k^{(2)}\right)$. By the definition of h_0 and Claim 1, $C_k^{(1)}$ and $C_k^{(2)}$ are both special polygons, a contradiction.

Case 2. $p(G) + q(G) = 1$. If $p(G) = 1$ and $q(G) = 0$, then $C_k^{(1)}$ is a special polygon of G, a contradiction. Otherwise, $p(G) = 0$ and $q(G) = 1$, then u_1 is a singular vertex of G, a contradiction. ■

In the following, when $f(x, y)$ is a special escalating function, we shall determine the minimum value of connectivity function among the class of k-polygonal cacti with n polygons for $k \geq 3$ and $n \geq 3$, that is,

Theorem 2.1. *Let $f(x, y)$ be a special escalating function and also let G be a cactus of $\mathcal{G}_{n,k}$, where $n \geq 3$ and $k \geq 3$.*
(i) If $k = 3$, then

$$BID(G) \geq 2f(2, 2) + 2nf(4, 2) + (n - 2)f(4, 4)$$

with equality holding if and only if $G \in \mathcal{T}_{n,3}$.
(ii) If $k \geq 4$, then

$$BID(G) \geq (kn - 4n + 4)f(2, 2) + (4n - 4)f(4, 2),$$

where the equality holds if $G \in \mathcal{R}_{n,k}$. Furthermore, if $k \in \{4, 5\}$, then the equality holds if and only if $G \in \mathcal{R}_{n,k}$.

Proof. We consider the following three cases:

Case 1. $k = 3$. Since $\mathcal{T}_{n,3}$ is unique, according to Lemmas 2.3–2.5, $BID(G)$ is minimum if and only if $G \in \mathcal{T}_{n,3}$. By an elementary computation, we have

$$BID(G) = 2f(2, 2) + 2nf(4, 2) + (n - 2)f(4, 4)$$

for $G \in \mathcal{T}_{n,3}$, and hence (i) holds.

Case 2. $4 \leq k \leq 5$. According to Lemmas 2.3–2.5, $BID(G)$ is minimum for $G \in \mathcal{T}_{n,k}$. Note that $\mathcal{R}_{n,k}$ is unique for $4 \leq k \leq 5$. By Lemma 2.1, we can conclude that $BID(G)$ is minimum if and only if $G \in \mathcal{R}_{n,k}$.

Case 3. $k \geq 6$. Then, Lemmas 2.1, 2.3–2.5 imply that $BID(G)$ is minimum for $G \in \mathcal{R}_{n,k}$.
When $k \geq 4$, by an elementary computation, we have

$$BID(G) = (kn - 4n + 4)f(2, 2) + (4n - 4)f(4, 2)$$

for $G \in \mathcal{R}_{n,k}$. Thus, (ii) also holds. ■

Remark 2.1. When $k \geq 6$, $\mathcal{R}_{n,k}$ is not unique but $BID(G) = (kn - 4n + 4)f(2, 2) + (4n - 4)f(4, 2)$ holds for each $G \in \mathcal{R}_{n,k}$. Furthermore, it is easy to see that $BID(G_1) = BID(G_2) = 12(f(2, 2)+f(4, 2))$, where G_1 and G_2 are shown in Fig. 2.1. However, $G_2 \notin \mathcal{R}_{4,6}$.

The proof of Theorem 1.1. In [12,19], it has been shown that both $Pl_\alpha(G)$ and $\chi_\alpha(G)$ are escalating for $\alpha > 1$ and $M_2(G)$ is also escalating. Combining with this, it is easy to see that $f(x,y) = (x+y)^\alpha$, $f(x,y) = (x+y-2)^\alpha$ and $f(x,y) = xy$ are all special escalating for $x \geq y \geq 2$ and $\alpha > 1$. Now, Theorem 1.1 follows from Theorem 2.1. ■

3. The proof of Theorem 1.2

Similarly as in Section 2, we shall prove a more general result, namely, the function version for Theorem 1.2. To do this, we need to introduce more notations:

Definition 3.1 ([10]). Let $\pi = (x_1, x_2, \ldots, x_n)$ and $\pi' = (x'_1, x'_2, \ldots, x'_n)$ be two different non-increasing sequences of nonnegative real numbers, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^n x_i = \sum_{i=1}^n x'_i$, and $\sum_{i=1}^j x_i \leq \sum_{i=1}^j x'_i$ for all $j = 1, 2, \ldots, n$.

The function $f(x)$ defined on a convex set D is called a *strictly convex function* if

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda)f(y) \tag{3.1}$$

for $\lambda \in (0,1)$ and $x, y \in D$ with $x \neq y$.

Lemma 3.1 ([10]). *Suppose that $\pi = (x_1, x_2, \ldots, x_n)$ and $\pi' = (x'_1, x'_2, \ldots, x'_n)$ are two non-increasing sequences of nonnegative real numbers. If $\pi \lhd \pi'$, then for any strictly convex function $f(x)$, we have $\sum_{i=1}^n f(x_i) < \sum_{i=1}^n f(x'_i)$.*

A symmetric bivariate function $f(x,y)$ defined on positive real numbers is called *good symmetric* if $f(x,y)$ satisfies the following (i), (ii) and (iii):
(i) $f(x_1+2, y_1) + f(x_1-2, y_1) \geq 2f(x_1, y_1)$ holds for any $x_1 \geq 4$ and $y_1 \geq 2$,
(ii) $f(x_1+2, 2) > f(x_1-2, 2) + 4$ holds for any $x_1 \geq 4$,
(iii) $f(x_1+2, y_1-2) + f(x_1-2, y_1+2) \geq 2f(x_1, y_1) - 16$ holds for any $x_1 \geq 4$ and $y_1 \geq 4$.
The following example shows that good symmetric function does exist:

Example 3.1. Let $f(x,y) = (x+y)^\alpha$ and $\Phi(z) = z^\alpha$, where $z \geq 0$. When $\alpha > 1$, since $\Phi''(z) \geq 0$ and $\Phi''(z) = 0$ if and only if $z = 0$, $\Phi(z)$ is a strictly convex function. If $x_1 \geq 4$, then $(x_1, 4) \lhd (x_1+4, 0)$, and hence Lemma 3.1 implies that

$$f(x_1+2, 2) = (x_1+4)^\alpha > x_1^\alpha + 4^\alpha > x_1^\alpha + 4 = f(x_1-2, 2) + 4.$$

Furthermore, when $\alpha > 1$, it is easy to see that

$$f(x_1+2, y_1-2) + f(x_1-2, y_1+2) = 2(x_1+y_1)^\alpha > 2(x_1+y_1)^\alpha - 16 = 2f(x_1, y_1) - 16$$

holds for any $x_1 \geq 4$ and $y_1 \geq 4$. Consequently, $f(x,y) = (x+y)^\alpha$ is a good symmetric function for $\alpha > 1$ and $x \geq y \geq 2$.

Theorem 3.1. *Let G be a cactus of $\mathcal{G}_{n,k}$, where $k \geq 3$ and $n \geq 3$. If $f(x,y)$ is a good symmetric function, then $BID(G) \leq 2nf(2n,2) + n(k-2)f(2,2)$ with equality holding if and only if $G \cong W_{n,k}$.*

Proof. Let G be a cactus of $\mathcal{G}_{n,k}$ such that $BID(G)$ is as large as possible. Let $C_k^{(1)} : u_1u_2\cdots u_ku_1$ and $C_k^{(2)} : w_1w_2\cdots w_kw_1$ be two pendent polygons such that $dist_G(C_k^{(1)}, C_k^{(2)})$ is as large as possible, where u_1 and w_1 are the cut-vertices of $C_k^{(1)}$ and $C_k^{(2)}$, respectively.

If $G \cong W_{n,k}$, then $BID(G) = 2nf(2n,2) + n(k-2)f(2,2)$ and hence the equality holds. Otherwise, $G \ncong W_{n,k}$. Then, $u_1 \neq w_1$. Let $G_1 = G - w_1w_2 - w_1w_k + u_1w_2 + u_1w_k$ and let $G_2 = G - u_1u_2 - u_1u_k + w_1u_2 + w_1u_k$. We consider the following two cases:

Case 1. $u_1w_1 \notin E(G)$. By an elementary computation, we have

$$\begin{aligned} BID(G_1) - BID(G) = &\sum_{v \in N_G(w_1)} \big(f(d_G(w_1)-2, d_G(v)) - f(d_G(w_1), d_G(v))\big) \\ &+ \sum_{w \in N_G(u_1)} \big(f(d_G(u_1)+2, d_G(w)) - f(d_G(u_1), d_G(w))\big) \\ &+ 2f(d_G(u_1)+2, 2) - 2f(d_G(w_1)-2, 2), \text{ and} \end{aligned}$$

$$\begin{aligned} BID(G_2) - BID(G) = &\sum_{v \in N_G(w_1)} \big(f(d_G(w_1)+2, d_G(v)) - f(d_G(w_1), d_G(v))\big) \\ &+ \sum_{w \in N_G(u_1)} \big(f(d_G(u_1)-2, d_G(w)) - f(d_G(u_1), d_G(w))\big) \\ &+ 2f(d_G(w_1)+2, 2) - 2f(d_G(u_1)-2, 2). \end{aligned}$$

Recall that $f(x, y)$ is a good symmetric function and u_1 and w_1 are the cut-vertices of $C_k^{(1)}$ and $C_k^{(2)}$, respectively. Thus, $d_G(u_1) \geq 4$ and $d_G(w_1) \geq 4$, and hence

$$\begin{aligned}
&f\big(d_G(w_1)-2, d_G(v)\big)+f\big(d_G(w_1)+2, d_G(v)\big)-2f\big(d_G(w_1), d_G(v)\big)\geq 0,\\
&f\big(d_G(u_1)-2, d_G(w)\big)+f\big(d_G(u_1)+2, d_G(w)\big)-2f\big(d_G(u_1), d_G(w)\big)\geq 0,\\
\text{and } &f\big(d_G(u_1)+2, 2\big)+f\big(d_G(w_1)+2, 2\big)-f\big(d_G(w_1)-2, 2\big)-f\big(d_G(u_1)-2, 2\big)>8,
\end{aligned}$$

which is contrary with $BID(G_1)+BID(G_2)-2BID(G)\leq 0$.

Case 2. $u_1w_1 \in E(G)$. By an elementary computation, we have

$$\begin{aligned}
BID(G_1)-BID(G) = &\sum_{v\in N_G(w_1)\setminus\{u_1\}}\big(f\big(d_G(w_1)-2, d_G(v)\big)-f\big(d_G(w_1), d_G(v)\big)\big)\\
&+\sum_{w\in N_G(u_1)\setminus\{w_1\}}\big(f\big(d_G(u_1)+2, d_G(w)\big)-f\big(d_G(u_1), d_G(w)\big)\big)\\
&+2f\big(d_G(u_1)+2, 2\big)-2f\big(d_G(w_1)-2, 2\big)\\
&+f\big(d_G(w_1)-2, d_G(u_1)+2\big)-f\big(d_G(w_1), d_G(u_1)\big),\ \text{and}
\end{aligned}$$

$$\begin{aligned}
BID(G_2)-BID(G) = &\sum_{v\in N_G(w_1)\setminus\{u_1\}}\big(f\big(d_G(w_1)+2, d_G(v)\big)-f\big(d_G(w_1), d_G(v)\big)\big)\\
&+\sum_{w\in N_G(u_1)\setminus\{w_1\}}\big(f\big(d_G(u_1)-2, d_G(w)\big)-f\big(d_G(u_1), d_G(w)\big)\big)\\
&+2f\big(d_G(w_1)+2, 2\big)-2f\big(d_G(u_1)-2, 2\big)\\
&+f\big(d_G(w_1)+2, d_G(u_1)-2\big)-f\big(d_G(w_1), d_G(u_1)\big).
\end{aligned}$$

Recall that $f(x, y)$ is a good symmetric function. Thus,

$$\begin{aligned}
&f\big(d_G(w_1)-2, d_G(v)\big)+f\big(d_G(w_1)+2, d_G(v)\big)-2f\big(d_G(w_1), d_G(v)\big)\geq 0,\\
&f\big(d_G(u_1)-2, d_G(w)\big)+f\big(d_G(u_1)+2, d_G(w)\big)-2f\big(d_G(u_1), d_G(w)\big)\geq 0,\\
&f\big(d_G(u_1)+2, 2\big)+f\big(d_G(w_1)+2, 2\big)-f\big(d_G(w_1)-2, 2\big)-f\big(d_G(u_1)-2, 2\big)>8,\\
\text{and } &f\big(d_G(w_1)+2, d_G(u_1)-2\big)+f\big(d_G(w_1)-2, d_G(u_1)+2\big)\geq 2f\big(d_G(w_1), d_G(u_1)\big)-16,
\end{aligned}$$

which is contrary with $BID(G_1)+BID(G_2)-2BID(G)\leq 0$. This completes the proof of the theorem. ■

The proof of Theorem 1.2. By Example 3.1, when $x \geq y \geq 2, f(x, y) = (x + y)^\alpha$ is a good symmetric function for $\alpha > 1$, and it is easy to see that $f(x, y) = xy$ is a good symmetric function. Thus, the statements for $M_2(G)$ and $\chi_\alpha(G)$ follow from Theorem 3.1.

Let $f(x, y) = (x + y - 2)^\alpha$ and $\Phi(z) = z^\alpha$, where $z \geq 0$. By Example 3.1, $\Phi(z)$ is a strictly convex function for $\alpha > 1$. If $x_1 \geq 6$, then $(x_1 - 2, 4) \lhd (x_1 + 2, 0)$. Otherwise, $4 \leq x_1 \leq 6$. In the later case, we have $(4, x_1 - 2) \lhd (x_1 + 2, 0)$. In both cases, by Lemma 3.1, it follows that

$$f(x_1 + 2, 2) = (x_1 + 2)^\alpha > (x_1 - 2)^\alpha + 4^\alpha > (x_1 - 2)^\alpha + 4 = f(x_1 - 2, 2) + 4$$

holds for any $x_1 \geq 4$. Furthermore, it is easy to see that

$$f(x_1 + 2, y_1 - 2) + f(x_1 - 2, y_1 + 2) = 2\big(x_1 + y_1 - 2\big)^\alpha > 2\big(x_1 + y_1 - 2\big)^\alpha - 16 = 2f(x_1, y_1) - 16$$

holds for any $x_1 \geq 4$ and $y_1 \geq 4$.

Consequently, $f(x, y) = (x + y - 2)^\alpha$ is also a good symmetric function for $\alpha > 1$ and $x \geq y \geq 2$. Thus, the statement for $Pl_\alpha(G)$ also follows from Theorem 3.1. ■

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Some Extremal Results for Vertex–Degree–Based Invariants

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Abstract

For a symmetric bivariable function $f(x, y)$, let the connectivity function of a connected graph G be $M_f(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where $d(u)$ is the degree of vertex u. As an application of majorization theory, we present a uniform method to some extremal results together with its corresponding extremal graphs for vertex-degree-based invariants among the class of trees, unicyclic graphs and bicyclic graphs with fixed number of independence number and/or matching number, respectively. As a consequence, several known results in chemical graph theory has been obtained.

1 Introduction

In this paper, we only consider simple connected undirected graph, and $G = (V, E)$ is a connected graph with n vertices and m edges. If $m = n + c - 1$, then G is called a *c-cyclic graph*. Especially, when $c = 0$, 1 or 2, then G is called a *tree*, *unicyclic graph* or *bicyclic graph*, respectively. As usual, denote $d(u)$ the degree of u. A vertex of degree one is called a *pendent vertex* of G, and the number of pendent vertices of G will be referred as $p(G)$. In contrast with pendent vertex, a vertex of degree being at least two is called

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a *non-pendent vertex*. Furthermore, a vertex with degree k will be referred as a k-vertex. Suppose the degree of vertex v_i equals d_i for $i = 1, 2, \ldots, n$, then $\pi(G) = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G. In the following discussions we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. Consequently, $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ holds, where $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π. When G is a c-cyclic graph with degree sequence π, then

$$\sum_{i=1}^{n} d_i = 2(n + c - 1). \tag{1}$$

A subset S of $V(G)$ is said to be an *independent set* of G if each pair of vertices of S are not adjacent. The number of vertices in a maximum independent set of G is called the *independence number* of G and denoted by $\alpha(G)$. If G is a connected graph with $n \geq 3$ vertices, then it is easy to see that the class of pendent vertices form an independent vertex set of G. Thus, we have

$$p(G) \leq \alpha(G). \tag{2}$$

A *matching* in a graph G is a set of pairwise nonadjacent edges. The maximum size of a matching set of G is called the *matching number* of G and denoted by $\beta(G)$ hereafter. For any connected graph G, since each edge of any matching has at least one end vertex being a non-pendent vertex, we have

$$p(G) \leq n - \beta(G). \tag{3}$$

Among all the vertex-degree-based graph invariants, the *first Zagreb index* $M_1(G)$ and *second Zagreb index* $M_2(G)$ [2] are two famous topological indices, where

$$M_1(G) = \sum_{v \in V(G)} (d(u))^2, \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In what follows, γ denotes a real number. As a generalization of $M_1(G)$, Li and Zheng [4] introduced the notation of *general Randić index* $R_\gamma(G)$ (sometimes also referred as "zeroth-order general Randić index"), where

$$R_\gamma(G) = \sum_{v \in V(G)} (d(v))^\gamma.$$

Furthermore, $R_{-1}(G)$ is called the *inverse degree* of graph G and denoted by $ID(G)$ (See [12]).

Since $\sum_{uv\in E(G)}(d(u)+d(v)) = \sum_{v\in V(G)}(d(v))^2$, as another extension to $M_1(G)$, the *general sum-connectivity index* [14] $\chi_\gamma(G)$ of G is constructed as

$$\chi_\gamma(G) = \sum_{uv\in E(G)} (d(u)+d(v))^\gamma .$$

The *reformulated Zagreb index* $Z_2(G)$ of G [9] is a slight modification to $\chi_2(G)$, where

$$Z_2(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^2 .$$

As an extension of $Z_2(G)$, we define $Z_\gamma(G)$ as follows:

$$Z_\gamma(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^\gamma .$$

In order to study on vertex-degree-based invariants of a graph, Wang [10] recently proposed the concept of escalating function as follows: A symmetric bivariate function $f(x,y)$ defined on positive real numbers is called *escalating* if

$$f(x_1,x_2)+f(y_1,y_2) \geq f(x_2,y_1)+f(x_1,y_2) \tag{4}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (4) is strict if $x_1 > y_1$ and $x_2 > y_2$. Furthermore, an escalating function $f(x,y)$ is called *good escalating* if $f(x,y)$ satisfies

$$\frac{\partial f(x,y)}{\partial x} > 0, \quad \frac{\partial^2 f(x,y)}{\partial x^2} \geq 0,$$

and

$$f(x_1+1,x_2)+f(x_1+1,y_1-1) \geq f(x_2,y_1)+f(x_1,y_1)$$

holds for any $x_1 \geq y_1$ and $x_2 \geq 1$. To extend these above definitions of vertex-degree-based invariants, Wang [10] defined *connectivity function* of a connected graph G associated with a symmetric bivariate function $f(x,y)$ as

$$M_f(G) = \sum_{uv\in E(G)} f\left(d(u),d(v)\right). \tag{5}$$

In this paper, we will employ the majorization theorem as a tool to give a uniform method for some extremal results together with its corresponding extremal graphs of vertex-degree-based invariants among the class of trees, unicyclic graphs and bicyclic graphs with fixed number of independence number and/or matching number, respectively.

2 Some useful preliminaries

As stated in [6, 13], the majorization theorem is an important and effective tool to deal with extremal problem of graph spectrum and topological index theory. In this section, we shall introduce some majorization theorems for vertex-degree-based invariants. Firstly, we introduce the definition of *majorization*.

Definition 2.1 (See [6, 8]) Let $\pi = (a_1, a_2, \ldots, a_n)$ and $\pi' = (a'_1, a'_2, \ldots, a'_n)$ be two different non-increasing sequences of nonnegative real numbers, we write $\pi \trianglelefteq \pi'$ if and only if $\sum_{i=1}^{n} a_i = \sum_{i=1}^{n} a'_i$, and $\sum_{i=1}^{j} a_i \leq \sum_{i=1}^{j} a'_i$ for all $j = 1, 2, \ldots, n$. Furthermore, we write $\pi \triangleleft \pi'$ if and only if $\pi \trianglelefteq \pi'$ and $\pi \neq \pi'$. The ordering $\pi \trianglelefteq \pi'$ is sometimes called *majorization*.

A real valued function $f(x)$ defined on a convex set D is said to be strictly convex if

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda) f(y)$$

holds for all $0 \leq \lambda \leq 1$ and all $x, y \in D$. The following majorization theorem for a strictly convex function had been discovered long time ago [3].

Theorem 2.1 [3] *Let $\pi = (a_1, a_2, \ldots, a_n)$ and $\pi' = (b_1, b_2, \ldots, b_n)$ be two non-increasing sequences of nonnegative real numbers. If $\pi \triangleleft \pi'$ and φ is a strictly convex function, then $\sum_{i=1}^{n} \varphi(a_i) < \sum_{i=1}^{n} \varphi(b_i)$.*

Note that $\varphi(x) = x^r$ is a strictly convex function for either $r > 1$ or $r < 0$, and $\varphi(x) = -x^r$ is a strictly convex function for $0 < r < 1$. Thus, Theorem 2.1 implies the following corollary.

Corollary 2.1 *Let $\pi = (a_1, a_2, \ldots, a_n)$ and $\pi' = (b_1, b_2, \ldots, b_n)$ be two non-increasing sequences of nonnegative real numbers. If $\pi \triangleleft \pi'$, then $\sum_{i=1}^{n} a_i^r < \sum_{i=1}^{n} b_i^r$ holds for either $r > 1$ or $r < 0$, and $\sum_{i=1}^{n} a_i^r > \sum_{i=1}^{n} b_i^r$ holds for $0 < r < 1$.*

For a given degree sequence π and a good escalating function $f(x, y)$, if G has the maximum connectivity function in $\Gamma(\pi)$, then G is called an *extremal graph* of $\Gamma(\pi)$.

Theorem 2.2 *Let π and π' be two different non-increasing degree sequences with $\pi \triangleleft \pi'$.*
(i) [5] *If $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, then $R_\gamma(G) < R_\gamma(G')$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(G) > R_\gamma(G')$ holds for $0 < \gamma < 1$.*
(ii) [7] *Let G and G' be an extremal c-cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is a good escalating function, then $M_f(G) < M_f(G')$ holds for $c \in \{0, 1, 2\}$.*

Theorem 2.3 [7] *The second Zagreb index $M_2(G)$ is good escalating, $Z_\gamma(G)$ and $\chi_\gamma(G)$ are also good escalating for $\gamma > 1$.*

3 Extremal results with given independence number

Denote by $\mathcal{R}(G)$ the reduced graph obtained from G by recursively deleting pendent vertices of the resultant graph until no pendent vertices remain. If G is a c-cyclic graph with $c \geq 1$, it is easy to see that $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a c-cyclic graph. Hereafter, let $\pi_1 = (2c+p, 2^{(n-p-1)}, 1^{(p)})$, $\pi_2 = (2c+p-2, 3^{(2)}, 2^{(n-p-3)}, 1^{(p)})$ and $\pi_3 = (2c+p-4, 4, 3^{(2)}, 2^{(n-p-4)}, 1^{(p)})$.

Lemma 3.1 *Let G be a c-cyclic graph with n vertices, p pendent vertices and degree sequence π. If $\pi \neq \pi_1$, then $\pi \lhd \pi_1$. Furthermore, $(2c+p, 2^{(n-p-1)}, 1^{(p)}) \lhd (2c+p+1, 2^{(n-p-2)}, 1^{(p+1)})$.*

Proof. By Definition 2.1, it is easy to check that $(2c+p, 2^{(n-p-1)}, 1^{(p)}) \lhd (2c+p+1, 2^{(n-p-2)}, 1^{(p+1)})$. Now, we turn to prove $\pi \lhd \pi_1$. To do this, let $\pi_1 = (d'_1, d'_2, \ldots, d'_{n-p}, 1^{(p)})$ and $\pi = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-p} \geq 2$. Then,

$$d_1 = 2(n+c-1) - p - d_2 - d_3 - \cdots - d_{n-p} \leq 2(n+c-1) - p - 2(n-p-1) = 2c+p.$$

If $d_1 = 2c+p$, then $d_2 = d_3 = \cdots = d_{n-p} = 2$, and hence $\pi = \pi_1$, a contradiction. Thus, $d_1 < 2c+p$. Since $d_j \geq 2$ holds for $2 \leq j \leq n-p$,

$$\sum_{i=1}^{j} d_i = 2(n+c-1) - p - d_{j+1} - \cdots - d_{n-p} \leq 2(n+c-1) - p - 2(n-p-j) = \sum_{i=1}^{j} d'_i$$

holds for $2 \leq j \leq n-p$. Thus, $\pi \lhd \pi_1$. ■

As usual, let P_n, C_n and K_n be the path, cycle and complete graph with n vertices, respectively. An s-rose graph is a graph with exactly s cycles that all meet in one vertex.

Lemma 3.2 *Let G be a c-cyclic graph with n vertices, p pendent vertices and degree sequence π such that every vertex of $\mathcal{R}(G)$ is adjacent to at least one pendent vertex.*

(i) If $\pi \neq \pi_2$ and $c \geq 1$, then $\pi \lhd \pi_2$. (ii) If $\pi \neq \pi_3$ and $c \geq 2$, then $\pi \lhd \pi_3$.

Proof. Let $\pi(G) = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-p} \geq 2$. Since $c \geq 1$, G contains at least one cycle such that every vertex of this cycle is adjacent to at least one pendent vertex. Thus, we have $d_1 \geq d_2 \geq d_3 \geq 3$ and hence $\pi \lhd \pi_2$ by (1). So, (i) holds.

Now, we turn to prove (ii). Since $c \geq 2$, we may suppose that C_s and C_t are two cycles of G. Thus, each vertex of C_s and C_t is adjacent to at least one pendent vertex, and hence the degree of every vertex on C_s or C_t is at least three. Furthermore, since G is connected, there is at least one vertex with degree being at least four. In this case, we may suppose that $\pi = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \cdots \geq d_k \geq 4 > d_{k+1} = d_{k+2} = \cdots = d_q = 3 > d_{q+1} = d_{q+2} = \cdots = d_{n-p} = 2$. By the former argument, $k \geq 1$ and $q \geq 4$.

If $k = 1$, then $\mathcal{R}(G)$ is a c-rose graph (since every vertex of $\mathcal{R}(G)$ is adjacent to at least one pendent vertex). Thus, $\pi = (d_1, 3^{(q-1)}, 2^{(n-p-q)}, 1^{(p)})$ and $q \geq s + t - 1 \geq 5$. In this case,

$$d_1 = 2(n + c - 1) - p - 3(q - 1) - 2(n - p - q) = 2c + p - q + 1 \leq 2c + p - 4$$

and $$d_1 + d_2 = 2(n + c - 1) - p - 3(q - 2) - 2(n - p - q) = 2c + 4 + p - q < 2c + p.$$

Now, it is easy to check that $\pi \lhd \pi_3$, as $d_3 \geq d_4 \geq 3$. Otherwise, $k \geq 2$. In this case, $\pi(B) = (d_1, d_2, \ldots, d_k, 3^{(q-k)}, 2^{(n-p-q)}, 1^{(p)})$. Since $q \geq 4$, $k \geq 2$ and $\pi \neq \pi_3$, we have $\pi \lhd \pi_3$. ■

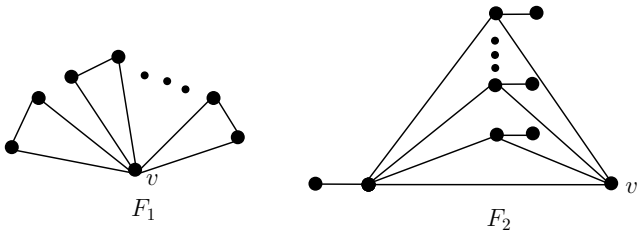
Lemma 3.3 *Let G be a c-cyclic graph with n vertices and degree sequence $\pi = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$ such that $d_3 \geq 3$. If $\pi \neq \pi_2$ and $c \geq 2$, then $\pi \lhd \pi_2$.*

Proof. We may suppose that $d_1 \geq d_2 \geq \cdots \geq d_q \geq 3 > d_{q+1} = d_{q+2} = \cdots = d_{n-p} = 2$. Since $d_3 \geq 3$, we have $q \geq 3$ and hence

$$\pi \trianglelefteq (2c + 1 + p - q, 3^{(q-1)}, 2^{(n-p-q)}, 1^{(p)}) \lhd \pi_2.$$

This completes the proof of this result. ■

Let v be a vertex of a graph G. Suppose $P_s = u_1 u_2 \cdots u_s$, where $u_i \notin V(G)$ for $1 \leq i \leq s$. If we obtain G' by identifying the vertex v with u_1, then we say that G' is obtained from G by *attaching the path P_s to v of G*. As shown in Figure 1, let F_1 and F_2 be two c-cyclic graphs, where $c \geq 1$. Hereafter, let $S_1(c; a, b)$ (resp., $S_2(c; a, b)$) define the c-cyclic graph obtained by attaching a paths of lengths two and b paths of lengths one, respectively, to the vertex v of F_1 (resp., F_2). If $c = 0$, then we agree with $a + b \geq 2$ and we define $S_1(0; a, b)$ as the tree obtained by attaching a paths of lengths two and b paths of lengths one, respectively, to one common vertex.



F_1 F_2

Figure 1. The c-cyclic graphs F_1 and F_2.

In what follows, let $\pi_4 = (2c + a + b, 2^{(a+2c)}, 1^{(a+b)})$ and $\pi_5 = (c + 1 + a + b, c + 2, 3^{(c)}, 2^{(a)}, 1^{(a+b+c+1)})$. It is easy to see that $S_1(c; a, b) \in \Gamma(\pi_4)$ and $S_2(c; a, b) \in \Gamma(\pi_5)$.

Lemma 3.4 *Let G be a c-cyclic graph such that $G \in \Gamma(\pi_4)$, where $c \geq 0$ and $2c+a+b \geq 2$. If exactly $2c$ vertices of degrees two are not adjacent to any pendent vertex in G, then $G \cong S_1(c; a, b)$.*

Proof. We may suppose that $c \geq 1$, as the case of $c = 0$ can be proved similarly. Since G is a c-cyclic graph with $d_2 = 2$, $\mathcal{R}(G)$ is just a c-rose graph. Thus, each vertex of $V(\mathcal{R}(G)) \setminus \{v_1\}$ is not adjacent to any pendent vertex. Since exactly $2c$ vertices of degrees two of G are not adjacent to any pendent vertex, we can conclude that each cycle of G is a triangle, and hence each vertex of $V(G) \setminus V(\mathcal{R}(G))$ is adjacent to at least one pendent vertex.

Let u be a 2-vertex of G such that $u \notin V(\mathcal{R}(G))$. Since u is adjacent to at least one pendent vertex, we can conclude that u is adjacent to exactly one pendent vertex (Otherwise, G is disconnected, a contradiction). If u is adjacent to another 2-vertex (say v), then v is adjacent to a pendent vertex and u, which implies that G is disconnected, a contradiction. Thus, u is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $G \cong S_1(c; a, b)$. ■

Lemma 3.5 *Let G be a c-cyclic graph such that $G \in \Gamma(\pi_5)$, where $c \geq 1$ and $a + b \geq 1$. If every non-pendent vertex of G is adjacent to at least one pendent vertex, then $G \cong S_2(c; a, b)$.*

Proof. Since every non-pendent vertex of G is adjacent to at least one pendent vertex and $G \in \Gamma(\pi_5)$, then the degree of each vertex of $V(\mathcal{R}(G))$ is at least three. By the definition of π_5, $\mathcal{R}(G)$ is a c-cyclic graph with at most $c+2$ vertices and the third maximum degree vertex of $\mathcal{R}(G)$ is a 2-vertex. Thus, $\mathcal{R}(G) \cong \mathcal{R}(F_2)$.

Since every non-pendent vertex of G is adjacent to at least one pendent vertex, similar with the proof of Lemma 3.4, we can conclude that every 2-vertex of G is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $G \cong S_2(c; a, b)$. ■

Let $B_1(a, b)$ be the bicyclic graph obtained from $S_1(1; a, b)$ by adding one edge between two 2-vertices in $V(S_1(1; a, b))\backslash V(C_3)$, where $a \geq 2$ and let $B_2(a, b)$ be the bicyclic graph obtained from $S_1(1; a, b)$ by adding one edge between one 2-vertex of $V(C_3)$ and one 2-vertex of $V(S_1(1; a, b))\backslash V(C_3)$, where $a \geq 1$. In what follows, let $\pi_6 = (a + b + 2, 3^{(2)}, 2^{(a)}, 1^{(a+b)})$ and let $K_4 - e$ be a bicyclic graph obtained by deleting one edge from K_4.

Lemma 3.6 *Let B be a bicyclic graph such that $B \in \Gamma(\pi_6)$, where $a + b \geq 1$. If all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3, then either $B \cong B_1(a, b)$ or $B \cong B_2(a, b)$.*

Proof. Suppose that C_s and C_t are two cycles of B with $t \geq s \geq 3$, and suppose that $\pi_6 = (d_1, d_2, \ldots, d_n)$. Since except for at most three non-pendent vertices, each of the other non-pendent vertices of B is adjacent to at least one pendent vertex, there are at least $|V(C_s \cup C_t)| - 3$ vertices with degree being at least three. Note that $d_2 = 3$ and $d_4 = 2$. Thus, $4 \leq |V(C_s) \cup V(C_t)| \leq 6$ and $1 \leq |V(C_s) \cap V(C_t)| \leq 3$.

We firstly consider the case of $|V(C_s) \cap V(C_t)| = 1$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3. Combining this with $d_2 = 3$ and $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 5$ and $s = t = 3$. By the hypothesis, v_2 and v_3 are two adjacent 3-vertices in the same triangle of B, and v_2 and v_3 are adjacent to exactly one pendent vertex, respectively. Furthermore, the other two adjacent 2-vertices in the same triangle of B are not adjacent to any pendent vertex. Let u be a 2-vertex of B such that $u \notin V(\mathcal{R}(B))$. Then, u is adjacent to at least one pendent vertex. Since B is connected, u is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $B \cong B_1(a, b)$ with $a \geq 2$.

We secondly consider the case of $|V(C_s) \cap V(C_t)| = 2$. In this case, we have $(s, t) \in \{(3, 3), (3, 4), (3, 5), (4, 4)\}$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3. Combining this with $d_2 = 3$ and $d_4 = 2$, we have $\mathcal{R}(B) \cong K_4 - e$. Now, since $d_2 = 3$ and $d_4 = 2$, one 3-vertex and one 2-vertex of $K_4 - e$ cannot be adjacent to any pendent vertex. Since B is connected, each of the other

2-vertices not in $K_4 - e$ is adjacent with exactly one pendent vertex and the maximum degree vertex. Now, by the definition of B and π_6, we have $B \cong B_2(a, b)$ with $a \geq 1$.

We thirdly consider the case of $|V(C_s) \cap V(C_t)| = 3$. In this case, $(s, t) \in \{(4, 4), (4, 5)\}$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3. Thus, we have $d_4 \geq 3$, a contradiction. ■

For convenience, we rewrite $S_1(0; n-1-\alpha, 2\alpha+1-n)$ as $T(n, \alpha)$, $S_1(1; n-\alpha-2, 2\alpha+1-n)$ as $U_1(n, \alpha)$, $S_2(1; n-\alpha-3, 2\alpha+1-n)$ as $U_2(n, \alpha)$, $B_1(n-\alpha-2, 2\alpha+1-n)$ as $Z_1(n, \alpha)$, $B_2(n-\alpha-2, 2\alpha+1-n)$ as $Z_2(n, \alpha)$, $S_1(2; n-\alpha-3, 2\alpha+1-n)$ as $Z_3(n, \alpha)$, and rewrite $S_2(2; n-\alpha-4, 2\alpha+1-n)$ as $Z_4(n, \alpha)$.

Theorem 3.1 *Let T be a tree with n (≥ 3) vertices and independence number α. If $T \ncong T(n, \alpha)$, then (i) $R_\gamma(T) < R_\gamma(T(n, \alpha))$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(T) > R_\gamma(T(n, \alpha))$ holds for $0 < \gamma < 1$, and (ii) $M_f(T) < M_f(T(n, \alpha))$ holds for any good escalating function $f(x, y)$.*

Proof. Since T is a bipartite graph, we have $\alpha \geq \lceil \frac{n}{2} \rceil$. We suppose that T contains p pendent vertices and suppose the degree sequence of T is π. By (2) and since $n \geq 3$, we have $2 \leq p \leq \alpha$. Let $\pi' = (\alpha, 2^{(n-\alpha-1)}, 1^{(\alpha)})$.

Suppose that $T \in \Gamma(\pi')$. Since $p = \alpha$, the class of pendent vertices of T form a maximum independent vertex set of T, and hence every non-pendent vertex must be adjacent to at least one pendent vertex. By Lemma 3.4, we have $T \cong T(n, \alpha)$, and hence

$$\Gamma(\pi') = \Big\{T(n, \alpha)\Big\}. \tag{6}$$

By (6), we have $\pi \neq \pi'$.

If $p = \alpha$ and $\pi \neq \pi'$, then $\pi \lhd \pi'$ by Lemma 3.1.

Otherwise, $p \leq \alpha - 1$. In this case, Lemma 3.1 implies that $\pi \trianglelefteq (\alpha-1, 2^{(n-\alpha)}, 1^{(\alpha-1)}) \lhd \pi'$.

In both cases, the results follow from Theorem 2.2 and (6). ■

Corollary 3.1 *Let T be a tree with n (≥ 3) vertices and independence number α. If $T \ncong T(n, \alpha)$, then (i) [11] $\chi_\gamma(T) < \chi_\gamma(T(n, \alpha))$ holds for $\gamma \geq 1$, (ii) [1] $M_1(T) < M_1(T(n, \alpha))$ and $M_2(T) < M_2(T(n, \alpha))$, and (iii) [12] $ID(T) < ID(T(n, \alpha))$.*

Proof. By Theorems 2.3 and 3.1, the results hold. ■

Theorem 3.2 *Let U be a unicyclic graph with n vertices and independence number α, where $3 \leq \alpha \leq n-3$. If $U \notin \Big\{U_1(n, \alpha), U_2(n, \alpha)\Big\}$, then (i) $R_\gamma(U) < \max\Big\{R_\gamma(U_1(n, \alpha)),$*

$R_\gamma(U_2(n,\alpha))\Big\}$ *for* $\gamma < 0$ *or* $\gamma > 1$ *and* $R_\gamma(U) > \min\Big\{R_\gamma(U_1(n,\alpha)),\, R_\gamma(U_2(n,\alpha))\Big\}$ *for* $0 < \gamma < 1$, *and* (ii) $M_f(U) < \max\Big\{M_f(U_1(n,\alpha)), M_f(U_2(n,\alpha))\Big\}$ *holds for any good escalating function* $f(x,y)$.

Proof. In the proof of this result, denote by $\pi' = (\alpha+1, 2^{(n-\alpha)}, 1^{(\alpha-1)})$ and $\pi'' = (\alpha, 3^{(2)}, 2^{(n-\alpha-3)}, 1^{(\alpha)})$. Since the deletion of any edge of the unique cycle of U forms a tree, we have $\alpha \geq \lceil \frac{n-1}{2} \rceil$. We suppose that the degree sequence of U is π, C_g is the unique cycle of U, and U contains p pendent vertices. By (2), $p \leq \alpha$.

Let U be a unicyclic graph of $\Gamma(\pi')$. If $g \geq 4$, then all the pendent vertices combining with at least two vertices of C_g will form an independent vertex set of size being at least $\alpha+1$, a contradiction. Thus, the unique cycle of U is a triangle. Since U contains exactly $\alpha - 1$ pendent vertices, except for two adjacent 2-vertices in the triangle of U, each of the other 2-vertices is adjacent to at least one pendent vertex. By Lemma 3.4, we have $U \cong U_1(n,\alpha)$.

Let U be a unicyclic graph of $\Gamma(\pi'')$. Then, the class of pendent vertices of U form an independent vertex set of U, and hence every non-pendent vertex is adjacent to at least a pendent vertex. By Lemma 3.5, we have $U \cong U_2(n,\alpha)$.

Now, we can conclude that

$$\Gamma(\pi') = \Big\{U_1(n,\alpha)\Big\} \text{ and } \Gamma(\pi'') = \Big\{U_2(n,\alpha)\Big\}. \tag{7}$$

Since $U \notin \Big\{U_1(n,\alpha), U_2(n,\alpha)\Big\}$, we have $\pi \notin \Big\{\pi', \pi''\Big\}$.

If $p \leq \alpha - 1$, then $\pi \lhd \pi'$ by Lemma 3.1.

Otherwise, $p = \alpha$. Since $p = \alpha$, each non-pendent vertex is adjacent to at least a pendent vertex. By Lemma 3.2 (i), we have $\pi \lhd \pi''$.

By Theorem 2.2 and (7), the results hold. ■

Corollary 3.2 *Let* U *be a unicyclic graph with* n *vertices and independence number* α $(\leq n-3)$ *such that* $U \ncong U_1(n,\alpha)$. (i) *If* $\gamma > 1$ *and* $\alpha \geq 4$, *then* $\chi_\gamma(U) < \chi_\gamma(U_1(n,\alpha))$ *and* $Z_\gamma(U) < Z_\gamma(U_1(n,\alpha))$. (ii) *If* $\alpha \geq 4$, *then* $M_1(U) < M_1(U_1(n,\alpha))$. (iii) *If* $n \geq 9$ *and* $\alpha \geq 3$, *then* $M_2(U) < M_2(U_1(n,\alpha))$.

Proof. By an elementary computation, it follows that

$$\begin{aligned}\chi_\gamma(U_1(n,\alpha)) =& (n-\alpha)(\alpha+3)^\gamma + (2\alpha-n+1)(\alpha+2)^\gamma + 4^\gamma + (n-\alpha-2)3^\gamma,\\ \chi_\gamma(U_2(n,\alpha)) =& 2(\alpha+3)^\gamma + (n-\alpha-3)(\alpha+2)^\gamma + (2\alpha-n+1)(\alpha+1)^\gamma + 6^\gamma\end{aligned}$$

$$+ 2 \times 4^{\gamma} + (n-\alpha-3)3^{\gamma}.$$

When $\gamma > 1$ and $\alpha \geq 4$, we have

$$\begin{aligned}\chi_{\gamma}(U_1(n,\alpha)) - \chi_{\gamma}(U_2(n,\alpha)) &= (\alpha+3)^{\gamma} + (n-\alpha-3)\Big((\alpha+3)^{\gamma} - (\alpha+2)^{\gamma}\Big) \\ &\quad +(2\alpha-n+1) \times \Big((\alpha+2)^{\gamma} - (\alpha+1)^{\gamma}\Big) - 6^{\gamma} - 4^{\gamma} + 3^{\gamma} \\ &> 7^{\gamma} - 6^{\gamma} - 4^{\gamma} + 3^{\gamma} > 0\end{aligned}$$

by Corollary 2.1. With the similar reason, we have $Z_{\gamma}(U_1(n,\alpha)) > Z_{\gamma}(U_2(n,\alpha))$.
Thus, (i) follows from Theorems 2.2 and 3.2.
It is easy to check that

$$M_1(U_1(n,\alpha)) - M_1(U_2(n,\alpha)) = 2(\alpha-3) > 0$$

when $\alpha \geq 4$, and hence (ii) also follows from Theorems 2.2 and 3.2.

Now, we turn to prove (iii). Since

$$\begin{aligned}M_2(U_1(n,\alpha)) &= 2(\alpha+1)(n-\alpha) + 4 + 2(n-\alpha-2) + (\alpha+1)(2\alpha+1-n) \\ &= n\alpha + 3n - \alpha + 1, \\ \text{and } M_2(U_2(n,\alpha)) &= 2 \times 3\alpha + 15 + 2\alpha(n-\alpha-3) + 2(n-\alpha-3) + \alpha(2\alpha+1-n) \\ &= n\alpha + 2n - \alpha + 9.\end{aligned}$$

For $n \geq 9$, we have

$$M_2(U_1(n,\alpha)) - M_2(U_2(n,\alpha)) = n - 8 > 0,$$

and hence (iii) follows from Theorems 2.2 and 3.2. ■

Theorem 3.3 *Let B be a bicyclic graph with n vertices and independence number α, where $4 \leq \alpha \leq n-4$.*
(i) If $B \notin \Big\{Z_1(n,\alpha),\ Z_2(n,\alpha),\ Z_3(n,\alpha),\ Z_4(n,\alpha)\Big\}$, then

$$R_{\gamma}(B) < \max\Big\{R_{\gamma}(Z_2(n,\alpha)),\ R_{\gamma}(Z_3(n,\alpha)),\ R_{\gamma}(Z_4(n,\alpha))\Big\}$$

holds for $\gamma < 0$ or $\gamma > 1$, and

$$R_{\gamma}(B) > \min\Big\{R_{\gamma}(Z_2(n,\alpha)),\ R_{\gamma}(Z_3(n,\alpha)),\ R_{\gamma}(Z_4(n,\alpha))\Big\}$$

holds for $0 < \gamma < 1$.
(ii) If $B \notin \Big\{Z_2(n,\alpha),\ Z_3(n,\alpha),\ Z_4(n,\alpha)\Big\}$ and $f(x,y)$ is a good escalating function, then

$$M_f(B) < \max\Big\{M_f(Z_2(n,\alpha)),\ M_f(Z_3(n,\alpha)),\ M_f(Z_4(n,\alpha))\Big\}.$$

Proof. Suppose C_s and C_t are two cycles of B, the degree sequence of B is $\pi = (d_1, d_2, \ldots, d_n)$ and B contains p pendent vertices. By (2), $p \leq \alpha$. In the proof of this result, denote by $\pi' = (\alpha, 4, 3^{(2)}, 2^{(n-\alpha-4)}, 1^{(\alpha)})$, $\pi'' = (\alpha+1, 3^{(2)}, 2^{(n-\alpha-2)}, 1^{(\alpha-1)})$ and $\pi''' = (\alpha+2, 2^{(n-\alpha+1)}, 1^{(\alpha-2)})$.

Firstly, we suppose that $\pi = \pi'$. Since $p = \alpha$, every non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.5, we have $B \cong Z_4(n, \alpha)$.

Secondly, we suppose that $\pi = \pi'''$. Since $d_2 = 2$, we have $|V(C_s) \cap V(C_t)| = 1$. Then, there is an independent set of size at least $\alpha - 2 + \lfloor \frac{s}{2} \rfloor + \lfloor \frac{t}{2} \rfloor$, and hence $s = t = 3$. Now, it is easy to see that there are exactly four 2-vertices being not adjacent to any pendent vertex in B. By Lemma 3.4, $B \cong Z_3(n, \alpha)$.

Thirdly, we suppose that $\pi = \pi''$. Since $p = \alpha - 1$, all the non-pendent vertices being not adjacent to any pendent vertex must induce a complete graph K_q. Recall that $\mathcal{R}(B)$ is also a bicyclic graph. Thus, $q \in \{0, 1, 2, 3\}$. We assume that $q \in \{0, 1\}$. Since $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 4$ and there is exactly one non-pendent vertex being not adjacent to any pendent vertex, that is, $q = 1$. In this case, $\mathcal{R}(B) \cong K_4 - e$, and either $d_2 \geq 4$ or $d_4 \geq 3$ (since there is exactly one non-pendent vertex of B being not adjacent to any pendent vertex), a contradiction. Thus, $q \in \{2, 3\}$, that is, all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3. By Lemma 3.6, $B \in \Big\{Z_1(n, \alpha), Z_2(n, \alpha)\Big\}$.

By an elementary computation, it follows that

$$M_f(Z_2(n, \alpha)) - M_f(Z_1(n, \alpha)) = f(3, 2) + f(2, 1) - f(2, 2) - f(3, 1) > 0$$

when $f(x, y)$ is a good escalating function. Combining this with the above arguments, we may suppose that $\pi \notin \Big\{\pi', \pi'', \pi'''\Big\}$. By Theorem 2.2, it suffices to show

$$\pi \lhd \pi' \text{ or } \pi \lhd \pi'' \text{ or } \pi \lhd \pi'''. \tag{8}$$

If $p \leq \alpha - 2$, then $\pi \lhd \pi'''$ by Lemma 3.1 and hence (8) holds.

If $p = \alpha$, then every non-pendent vertex is adjacent to at least one pendent vertex. Now, Lemma 3.2 (ii) implies that $\pi \lhd \pi'$ and hence (8) holds.

If $p = \alpha - 1$, then all non-pendent vertices of B being not adjacent to any pendent vertex induce a complete graph K_q. Since $\mathcal{R}(B)$ is also a bicyclic graph, $q \in \{0, 1, 2, 3\}$. When $q \in \{0, 1\}$ or $|V(C_s) \cup V(C_t)| \geq 6$, then $d_3 \geq 3$. When $|V(C_s) \cup V(C_t)| = 5$ and $q \in \{2, 3\}$, we also have $d_3 \geq 3$. Otherwise, $|V(C_s) \cup V(C_t)| = 4$ and $q \in \{2, 3\}$. In this case, $\mathcal{R}(B) \cong K_4 - e$ and hence $d_3 \geq 3$. Now, Lemma 3.3 implies that $\pi \lhd \pi''$ and hence (8) holds. ■

Corollary 3.3 *Let B be a bicyclic graph with n vertices and independence number α such that $B \ncong Z_3(n,\alpha)$. If $\gamma > 1$ and $5 \le \alpha \le n-4$, then $\chi_\gamma(B) < \chi_\gamma(Z_3(n,\alpha))$ and $Z_\gamma(B) < Z_\gamma(Z_3(n,\alpha))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned}
\chi_\gamma(Z_2(n,\alpha)) &= 2(\alpha+4)^\gamma + (\alpha+3)^\gamma(n-\alpha-2) + (\alpha+2)^\gamma(2\alpha-n+1) \\
&\quad +5^\gamma + 6^\gamma + 4^\gamma + 3^\gamma(n-\alpha-3), \\
\chi_\gamma(Z_3(n,\alpha)) &= (\alpha+4)^\gamma(n-\alpha+1) + (\alpha+3)^\gamma(2\alpha-n+1) + 3^\gamma(n-\alpha-3) + 4^\gamma \times 2, \\
\chi_\gamma(Z_4(n,\alpha)) &= (\alpha+4)^\gamma + 2(\alpha+3)^\gamma + (\alpha+2)^\gamma(n-\alpha-4) \\
&\quad +(\alpha+1)^\gamma(2\alpha-n+1) + 3^\gamma(n-\alpha-4) + 7^\gamma \times 2 + 5^\gamma + 4^\gamma \times 2.
\end{aligned}$$

For $\gamma > 1$, by Corollary 2.1 we have

$$\begin{aligned}
&\chi_\gamma(Z_3(n,\alpha)) - \chi_\gamma(Z_2(n,\alpha)) \\
= \;& (\alpha+4)^\gamma + (n-\alpha-2)\Big((\alpha+4)^\gamma - (\alpha+3)^\gamma\Big) \\
&+(2\alpha-n+1)\Big((\alpha+3)^\gamma - (\alpha+2)^\gamma\Big) + 4^\gamma - 5^\gamma - 6^\gamma \\
\ge \;& (\alpha+4)^\gamma + 4^\gamma - 5^\gamma - 6^\gamma \ge 7^\gamma + 4^\gamma - 5^\gamma - 6^\gamma > 0, \\
&\chi_\gamma(Z_2(n,\alpha)) - \chi_\gamma(Z_4(n,\alpha)) \\
= \;& (\alpha+4)^\gamma + (n-\alpha-4)\Big((\alpha+3)^\gamma - (\alpha+2)^\gamma\Big) \\
&+(2\alpha-n+1) \times \Big((\alpha+2)^\gamma - (\alpha+1)^\gamma\Big) + 3^\gamma + 6^\gamma - 7^\gamma \times 2 - 4^\gamma \\
\ge \;& (\alpha+4)^\gamma + 3^\gamma + 6^\gamma - 7^\gamma \times 2 - 4^\gamma \\
\ge \;& 9^\gamma + 6^\gamma + 3^\gamma - 7^\gamma \times 2 - 4^\gamma > 0.
\end{aligned}$$

Thus, $\chi_\gamma(Z_4(n,\alpha)) < \chi_\gamma(Z_2(n,\alpha)) < \chi_\gamma(Z_3(n,\alpha))$.
With the similar reason,

$$Z_\gamma(Z_4(n,\alpha)) < Z_\gamma(Z_2(n,\alpha)) < Z_\gamma(Z_3(n,\alpha)).$$

Now, the result follows from Theorems 2.3 and 3.3. ■

Corollary 3.4 *Let B be a bicyclic graph with n vertices and independence number α, where $4 \le \alpha \le n-4$. If $n \ge 10$ and $B \ncong Z_3(n,\alpha)$, then $M_2(B) < M_2(Z_3(n,\alpha))$.*

Proof. From the definition, it follows that

$$M_2(Z_4(n,\alpha)) = 4\alpha + 2 \times 3\alpha + 2\alpha(n-\alpha-4) + \alpha(2\alpha-n+1) + 2(n-\alpha-4) + 34$$

$$\begin{aligned} &= \alpha n + 2n + \alpha + 26, \\ M_2(Z_3(n,\alpha)) &= 2(\alpha+2)(n-\alpha+1) + (\alpha+2)(2\alpha-n+1) + 8 + 2(n-\alpha-3) \\ &= \alpha n + \alpha + 4n + 8, \\ M_2(Z_2(n,\alpha)) &= \alpha n + 3n + \alpha + 15. \end{aligned}$$

Thus, $M_2(Z_3(n,\alpha)) - M_2(Z_2(n,\alpha)) = n - 7 > 0$ and $M_2(Z_3(n,\alpha)) - M_2(Z_4(n,\alpha)) = 2n - 18 > 0$.

Now, the result follows from Theorems 2.3 and 3.3. ■

4 Extremal results with given matching number

In this section, we will consider the extremal problem in the class of c-cyclic graph with n vertices and matching number β. To this aim, we rewrite $S_1(0;\beta-1,n+1-2\beta)$ as $T(n;\beta)$, $S_1(1;\beta-2,n+1-2\beta)$ as $U_1(n;\beta)$, $S_2(1;\beta-3,n+1-2\beta)$ as $U_2(n;\beta)$, $B_1(\beta-2,n+1-2\beta)$ as $Z_1(n;\beta)$, $B_2(\beta-2,n+1-2\beta)$ as $Z_2(n;\beta)$, $S_1(2;\beta-3,n+1-2\beta)$ as $Z_3(n;\beta)$, and rewrite $S_2(2;\beta-4,n+1-2\beta)$ as $Z_4(n;\beta)$.

Theorem 4.1 *Let T be a tree with n (≥ 3) vertices and matching number β. If $T \ncong T(n;\beta)$, then (i) $R_\gamma(T) < R_\gamma(T(n;\beta))$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(T) > R_\gamma(T(n;\beta))$ holds for $0 < \gamma < 1$, and (ii) $M_f(T) < M_f(T(n;\beta))$ for any good escalating function $f(x,y)$.*

Proof. Suppose the degree sequence of T is π and $\pi' = (n-\beta, 2^{(\beta-1)}, 1^{(n-\beta)})$. Note that T contains at least β vertices of degree being at least two and $\beta \leq \lfloor \frac{n}{2} \rfloor$. Thus, $p(T) \leq n - \beta$ and hence $\pi \trianglelefteq \pi'$ by Lemma 3.1 and (3). If $\pi = \pi'$, then T contains exactly β vertices with degree being at least two. Since the matching number of T is β, each non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.4, we have $T \cong T(n;\beta)$, a contradiction. Thus, $\pi \triangleleft \pi'$ and hence the results follow from Theorem 2.2 and $\Gamma(\pi') = \Big\{T(n;\beta)\Big\}$. ■

Corollary 4.1 *Let T be a tree with n (≥ 3) vertices and matching number β. If $T \ncong T(n;\beta)$, then (i) $\chi_\gamma(T) < \chi_\gamma(T(n;\beta))$ and $Z_\gamma(T) < Z_\gamma(T(n;\beta))$ holds for $\gamma \geq 1$, (ii) $M_1(T) < M_1(T(n;\beta))$ and $M_2(T) < M_2(T(n;\beta))$, and (iii)* [12] *$ID(T) < ID(T(n;\beta))$.*

Proof. By Theorems 2.3 and 4.1, the results hold. ■

Theorem 4.2 *Let U be a unicyclic graph with n vertices and matching number β, where $3 \leq \beta \leq n-3$. If $U \notin \Big\{U_1(n;\beta), U_2(n;\beta)\Big\}$, then (i) $R_\gamma(U) < \max\Big\{R_\gamma(U_1(n;\beta)),\ R_\gamma(U_2(n;\beta))\Big\}$ for $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(U) > \min\Big\{R_\gamma(U_1(n;\beta)),\ R_\gamma(U_2(n;\beta))\Big\}$ for $0 < \gamma < 1$, and (ii) $M_f(U) < \max\Big\{M_f(U_1(n;\beta)), M_f(U_2(n;\beta))\Big\}$ for any good escalating function.*

Proof. In the proof of this result, let $\pi' = (n-\beta, 3^{(2)}, 2^{(\beta-3)}, 1^{(n-\beta)})$ and $\pi'' = (n-\beta+1, 2^{(\beta)}, 1^{(n-\beta-1)})$. Suppose that the degree sequence of U is π, C_g is the unique cycle of U, and U contains p pendent vertices. By (3), $p(U) \leq n-\beta$.

Firstly, we suppose that $U \in \Gamma(\pi')$. Then, every non-pendent vertex is adjacent to at least one pendent vertex (since U contains exactly $n-\beta$ pendent vertices and β non-pendent vertices). By Lemma 3.5, we have $U \cong U_2(n;\beta)$, a contradiction.

Secondly, we suppose that $U \in \Gamma(\pi'')$. By the definition of π'', every vertex of $V(C_g) \setminus \{v_1\}$ cannot be adjacent to any pendent vertex. Note that there are $\beta+1$ non-pendent vertices in U and every edge in a matching has at least one non-pendent vertex as its end vertex. If $g \geq 4$, then the matching number of U is at most $\lfloor \frac{g-1}{2} \rfloor + \beta + 1 - (g-1) \leq \beta - 1$, a contradiction. Thus, $g = 3$ and hence there are exactly two 2-vertices in C_g being not adjacent to any pendent vertex. By Lemma 3.4, we have $U \cong U_1(n;\beta)$, a contradiction.

From the above arguments, it follows that

$$\Gamma(\pi') = \Big\{U_2(n;\beta)\Big\} \text{ and } \Gamma(\pi'') = \Big\{U_1(n;\beta)\Big\}. \tag{9}$$

Now, we suppose that $\pi \notin \{\pi', \pi''\}$. If $p \leq n-\beta-1$, then $\pi \lhd \pi''$ by Lemma 3.1. If $p = n-\beta$, then since every edge in a matching has at least one non-pendent vertex as its end vertex and the matching number of U is β, we can conclude that each non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.2 (i), it follows that $\pi \lhd \pi'$.

By Theorem 2.2 and (9), the results hold. ■

Corollary 4.2 *Let U be a unicyclic graph with n vertices and matching number β (≥ 3) such that $U \ncong U_1(n;\beta)$. (i) If $\gamma > 1$ and $\beta \leq n-4$, then $\chi_\gamma(U) < \chi_\gamma(U_1(n;\beta))$, $Z_\gamma(U) < Z_\gamma(U_1(n;\beta))$ and $M_1(U) < M_1(U_1(n;\beta))$. (ii) If $n \geq 9$ and $\beta \leq n-3$, then $M_2(U) < M_2(U_1(n;\beta))$.*

Proof. By an elementary computation, we have

$$\chi_\gamma(U_1(n;\beta)) = \beta(n-\beta+3)^\gamma + (n-2\beta+1)(n-\beta+2)^\gamma + 4^\gamma + (\beta-2)3^\gamma,$$

and

$$\chi_\gamma(U_2(n;\beta)) = 2(n-\beta+3)^\gamma + (\beta-3)\left((n-\beta+2)^\gamma + 3^\gamma\right) + (n-2\beta+1)(n-\beta+1)^\gamma + 6^\gamma + 2\times 4^\gamma.$$

We first prove (i). Since $\gamma > 1$ and $3 \le \beta \le n-4$,

$$\begin{aligned}\chi_\gamma(U_1(n;\beta)) - \chi_\gamma(U_2(n;\beta)) &= (n-\beta+3)^\gamma + (\beta-3)\left((n-\beta+3)^\gamma - (n-\beta+2)^\gamma\right)\\ &\quad +(n-2\beta+1)\left((n-\beta+2)^\gamma - (n-\beta+1)^\gamma\right) - 6^\gamma - 4^\gamma\\ &\quad +3^\gamma > 7^\gamma - 6^\gamma - 4^\gamma + 3^\gamma > 0\end{aligned}$$

by Corollary 2.1. With the similar reason, $Z_\gamma(U_2(n;\beta)) < Z_\gamma(U_1(n;\beta))$. It is easy to see that

$$M_1(U_1(n;\beta)) - M_1(U_2(n;\beta)) = 2(n-\beta-3) > 0.$$

Thus, (i) follows from Theorems 2.3 and 4.2.

Now, we turn to prove (ii). By Theorems 2.3 and 4.2, it suffices to show that $M_2(U_1(n;\beta)) > M_2(U_2(n;\beta))$. By an elementary computation, we have

$$\begin{aligned}M_2(U_1(n;\beta)) &= 2\beta(n-\beta+1) + 4 + 2(\beta-2) + (n-\beta+1)(n-2\beta+1)\\ &= n^2 - n\beta + \beta + 2n + 1,\\ M_2(U_2(n;\beta)) &= 2\times 3(n-\beta) + 15 + 2(n-\beta)(\beta-3) + 2(\beta-3) + (n-\beta)(n-2\beta+1)\\ &= n^2 - n\beta + \beta + n + 9.\end{aligned}$$

Thus, $M_2(U_1(n;\beta)) - M_2(U_2(n;\beta)) = n - 8 > 0$. ■

Theorem 4.3 *Let B be a bicyclic graph with n vertices and matching number β, where $4 \le \beta \le n-4$.*

(i) If $B \notin \left\{Z_1(n;\beta), Z_2(n;\beta), Z_3(n;\beta), Z_4(n;\beta)\right\}$, then

$$R_\gamma(B) < \max\left\{R_\gamma(Z_2(n;\beta)),\ R_\gamma(Z_3(n;\beta)),\ R_\gamma(Z_4(n;\beta))\right\}$$

holds for $\gamma < 0$ or $\gamma > 1$, and

$$R_\gamma(B) > \min\left\{R_\gamma(Z_2(n;\beta)),\ R_\gamma(Z_3(n;\beta)),\ R_\gamma(Z_4(n;\beta))\right\}$$

holds for $0 < \gamma < 1$.

(ii) If $B \notin \left\{Z_2(n;\beta),\ Z_3(n;\beta),\ Z_4(n;\beta)\right\}$ and $f(x,y)$ is a good escalating function, then

$$M_f(B) < \max\left\{M_f(Z_2(n;\beta)),\ M_f(Z_3(n;\beta)),\ M_f(Z_4(n;\beta))\right\}.$$

Proof. Suppose C_s and C_t are two cycles of B, the degree sequence of B is $\pi = (d_1, d_2, \ldots, d_n)$ and B contains p pendent vertices. By (3), $p \leq n - \beta$. In the proof of this result, denote by $\pi' = (n-\beta, 4, 3^{(2)}, 2^{(\beta-4)}, 1^{(n-\beta)})$, $\pi'' = (n-\beta+1, 3^{(2)}, 2^{(\beta-2)}, 1^{(n-\beta-1)})$ and $\pi''' = (n-\beta+2, 2^{(\beta+1)}, 1^{(n-\beta-2)})$.

Firstly, we suppose that $\pi = \pi'$. Since B contains exactly β non-pendent vertices and the matching number of B is equal to β, every non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.5, we have $B \cong Z_4(n;\beta)$.

Secondly, we suppose that $\pi = \pi'''$. Since $d_2 = 2$, we have $|V(C_s) \cap V(C_t)| = 1$. Note that there are at most $\lfloor \frac{s-1}{2} \rfloor + \lfloor \frac{t-1}{2} \rfloor$ independent edges induced by the vertex set $(V(C_s) \cup V(C_t)) \backslash \{v_1\}$. Thus, the matching number of B is at most

$$\beta + \left\lfloor \frac{s-1}{2} \right\rfloor + \left\lfloor \frac{t-1}{2} \right\rfloor + 2 - (s-1+t-1) \leq \beta + 2 - \left\lceil \frac{s-1}{2} \right\rceil - \left\lceil \frac{t-1}{2} \right\rceil \leq \beta,$$

and hence $s = t = 3$. Since the matching number of B is equal to β, B contains exactly four 2-vertices being not adjacent to any pendent vertex in B. By Lemma 3.4, $B \cong Z_3(n;\beta)$.

Thirdly, we suppose that $\pi = \pi''$. Since B contains $\beta+1$ non-pendent vertices and each edge of the maximum matching with β edges in B contains at least one non-pendent vertex as its end vertex, there is either at most one non-pendent vertex being not adjacent to any pendent vertex or there are exactly two adjacent non-pendent vertices being not adjacent to any pendent vertex. Now, we assume that there is at most one non-pendent vertex being not adjacent to any pendent vertex. Since $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 4$ and there is exactly one non-pendent vertex being not adjacent to any pendent vertex. In this case, it follows that $\mathcal{R}(B) \cong K_4 - e$, and hence either $d_2 \geq 4$ or $d_4 \geq 3$ (since there is exactly one non-pendent vertex of B being not adjacent to any pendent vertex), a contradiction. Thus, there are exactly two adjacent non-pendent vertices being not adjacent to any pendent vertex. By Lemma 3.6, $B \in \Big\{Z_1(n;\beta), Z_2(n;\beta)\Big\}$.

By an elementary computation, it follows that

$$M_f(Z_2(n;\beta)) - M_f(Z_1(n;\beta)) = f(3,2) + f(2,1) - f(2,2) - f(3,1) > 0$$

when $f(x,y)$ is a good escalating function. Combining this with the above arguments, we may suppose that $\pi \notin \Big\{\pi', \pi'', \pi'''\Big\}$. By Theorem 2.2, it suffices to show

$$\pi \lhd \pi' \text{ or } \pi \lhd \pi'' \text{ or } \pi \lhd \pi'''. \tag{10}$$

If $p \leq n - \beta - 2$, then $\pi \lhd \pi'''$ by Lemma 3.1 and hence (10) holds.

If $p = n-\beta$, then every non-pendent vertex is adjacent to at least one pendent vertex. Now, Lemma 3.2 (ii) implies that $\pi \lhd \pi'$ and hence (10) holds.

If $p = n-\beta-1$, then B contains exactly $\beta+1$ non-pendent vertices. In this case, either at most one non-pendent vertex being not adjacent to any pendent vertex or there exist two adjacent non-pendent vertices being not adjacent to any pendent vertex. When $|V(C_s) \cup V(C_t)| \geq 5$, then $d_3 \geq 3$. Otherwise, $|V(C_s) \cup V(C_t)| = 4$ and hence $\mathcal{R}(B) \cong K_4 - e$. Recall that either at most one non-pendent vertex is not adjacent to any pendent vertex or there exist two adjacent non-pendent vertices being not adjacent to any pendent vertex. Thus, $d_3 \geq 3$. Now, Lemma 3.3 implies that $\pi \lhd \pi''$ and hence (10) holds. ■

Corollary 4.3 *Let B be a bicyclic graph with n vertices and matching number β such that $B \ncong Z_3(n;\beta)$. If $\gamma > 1$ and $4 \leq \beta \leq n-4$, then $\chi_\gamma(B) < \chi_\gamma(Z_3(n;\beta))$ and $Z_\gamma(B) < Z_\gamma(Z_3(n;\beta))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned}
\chi_\gamma(Z_2(n,\alpha)) &= 2(n-\beta+4)^\gamma + (n-\beta+3)^\gamma(\beta-2) + (n-\beta+2)^\gamma(n-2\beta+1) \\
&\quad +5^\gamma + 6^\gamma + 4^\gamma + 3^\gamma(\beta-3), \\
\chi_\gamma(Z_3(n;\beta)) &= (n-\beta+4)^\gamma(\beta+1) + (n-\beta+3)^\gamma(n-2\beta+1) + 3^\gamma(\beta-3) \\
&\quad +4^\gamma \times 2, \\
\text{and } \chi_\gamma(Z_4(n;\beta)) &= (n-\beta+4)^\gamma + 2(n-\beta+3)^\gamma + (n-\beta+2)^\gamma(\beta-4) \\
&\quad +(n-\beta+1)^\gamma(n-2\beta+1) + 3^\gamma(\beta-4) + 7^\gamma \times 2 + 5^\gamma + 4^\gamma \times 2.
\end{aligned}$$

Since $\gamma > 1$ and $4 \leq \beta \leq n-4$, by Corollary 2.1 we have

$$\begin{aligned}
\chi_\gamma(Z_3(n;\beta)) - \chi_\gamma(Z_2(n;\beta)) &= (n-\beta+4)^\gamma + (\beta-2)\Big((n-\beta+4)^\gamma - (n-\beta+3)^\gamma\Big) \\
&\quad +(n-2\beta+1) \times \Big((n-\beta+3)^\gamma - (n-\beta+2)^\gamma\Big) + 4^\gamma \\
&\quad -5^\gamma - 6^\gamma \\
&\geq (n-\beta+4)^\gamma + 4^\gamma - 5^\gamma - 6^\gamma \geq 7^\gamma + 4^\gamma - 5^\gamma - 6^\gamma > 0, \\
\chi_\gamma(Z_3(n;\beta)) - \chi_\gamma(Z_4(n;\beta)) &= (n-\beta+4)^\gamma \times 2 + (\beta-4)\Big((n-\beta+4)^\gamma - (n-\beta+2)^\gamma\Big) \\
&\quad +(n-2\beta+1)\Big((n-\beta+3)^\gamma - (n-\beta+1)^\gamma\Big) \\
&\quad +2\Big((n-\beta+4)^\gamma - (n-\beta+3)^\gamma\Big) + 3^\gamma - 7^\gamma \times 2 - 5^\gamma \\
&\geq 2(n-\beta+4)^\gamma + 3^\gamma - 7^\gamma \times 2 - 5^\gamma \geq 8^\gamma \times 2 + 3^\gamma - 7^\gamma \times 2 \\
&\quad -5^\gamma > 0.
\end{aligned}$$

Thus, $\max\left\{\chi_\gamma(Z_2(n;\beta)), \chi_\gamma(Z_4(n;\beta))\right\} < \chi_\gamma(Z_3(n;\beta))$.
With the similar reason,

$$\max\left\{Z_\gamma(Z_2(n;\beta)), Z_\gamma(Z_4(n;\beta))\right\} < Z_\gamma(Z_3(n;\beta)).$$

Now, the result follows from Theorems 2.3 and 4.3. ■

Corollary 4.4 *Let B be a bicyclic graph with n vertices and matching number β, where $4 \le \beta \le n-4$. If $n \ge 10$ and $B \ncong Z_3(n;\beta)$, then $M_2(B) < M_2(Z_3(n;\beta))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned}
M_2(Z_2(n;\beta)) &= 6(n-\beta+1) + 2(n-\beta+1)(\beta-2) + (n-\beta+1)(n-2\beta+1) + 18 \\
&\quad +2(\beta-3) \\
&= n^2 - \beta n - \beta + 4n + 15, \\
M_2(Z_3(n;\beta)) &= 2(n-\beta+2)(\beta+1) + (n-\beta+2)(n-2\beta+1) + 8 + 2(\beta-3) \\
&= n^2 - \beta n - \beta + 5n + 8, \\
M_2(Z_4(n;\beta)) &= 4(n-\beta) + 6(n-\beta) + 2(n-\beta)(\beta-4) + (n-\beta)(n-2\beta+1) \\
&\quad 2(\beta-4) + 34 \\
&= n^2 - \beta n - \beta + 3n + 26.
\end{aligned}$$

Since $M_2(Z_3(n;\beta)) - M_2(Z_2(n;\beta)) = n - 7 > 0$ and $M_2(Z_3(n;\beta)) - M_2(Z_4(n;\beta)) = 2n - 18 > 0$, the result follows from Theorems 2.3 and 4.3. ■

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Unified Extremal Results for Vertex–Degree–Based Graph Invariants with Given Diameter

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Abstract

In this paper, we determine all unified extremal graphs for maximum (resp., minimum) first general Zagreb index $R^0_\alpha(G)$ for $\alpha < 0$ or $\alpha > 1$ (resp., $0 < \alpha < 1$), maximum (resp., minimum) general first multiplicative Zagreb index $\prod^{\alpha}(G)$ for $\alpha < 0$ (resp., $\alpha > 0$), maximum second multiplicative Zagreb index $\prod_2(G)$, and minimum first Zagreb coindex $\overline{M_1(G)}$ among the class of trees, unicyclic graphs and bicyclic graphs with given diameter, respectively.

1 Introduction

In this paper, we only consider simple connected undirected graphs. Throughout the paper, α always denotes a real number and c is a nonnegative integer. Let $G = (V, E)$ be a connected graph with n vertices and m edges. If $m = n + c - 1$, then G is called a *c-cyclic graph*. A c-cyclic graph with $c = 0, 1, 2$ is called a *tree*, *unicyclic graph* and *bicyclic graph*, respectively. As usual, $d_G(u)$ or $d(u)$ for short, denotes the degree of u in G. A *k-vertex* is a vertex with degree k. A 1-vertex is called a *pendant vertex* of G, while a k-vertex with $k \geq 2$ is called a *non-pendant vertex*. The number of pendant vertices of G will be referred as $p(G)$ throughout this paper.

Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Let $d(v_i) = d_i$ for $i = 1, 2, \ldots, n$. The non-increasing sequence $\pi(G) = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G. Denote by $\Gamma(\pi)$ the set of all connected graphs with degree sequence π. If G is a c-cyclic graph with degree sequence π, then

$$\sum_{i=1}^{n} d_i = 2(n + c - 1). \tag{1}$$

The *distance* between u and v, denoted by $\mathrm{dist}(u, v)$, is the number of edges in a shortest path from u to v. Then, the *diameter* $d(G)$ of graph G is the maximum distance over all pairs of vertices of G.

In 1972, Gutman and Trinajstić [4] introduced the first Zagreb index, where the *first Zagreb index* $M_1(G)$ of a graph G equals to the sum of the squares of the degrees of all vertices of G. This topological index has been widely studied [3]. The *first Zagreb coindex* $\overline{M_1(G)}$ of a graph G defined by Došlić [2] is

$$\overline{M_1(G)} = \sum_{uv \notin E(G)} \big(d(u) + d(v)\big).$$

As a generalization of the first Zagreb index, the *first general Zagreb index* $R_\alpha(G)$ was introduced by Li and Zheng [7] which is defined as

$$R^0_\alpha(G) = \sum_{u \in V(G)} \big(d(u)\big)^\alpha.$$

In particular, $R^0_{-1}(G)$ is called the *inverse degree* of G and denoted by $ID(G)$ (see [18]); and $R^0_2(G)$ is just the first Zagreb index.

In 2010, Todeschini and Consonni [16] put forward the notations of the *first multiplicative Zagreb index* $\prod^1(G)$ and the *second multiplicative Zagreb index* $\prod_2(G)$ of graph G, where

$$\prod^1(G) = \prod_{u \in V(G)} d^2(u), \text{ and } \prod_2(G) = \prod_{u \in V(G)} \big(d(u)\big)^{d(u)}.$$

Very recently, the *general first multiplicative Zagreb index* $\prod^\alpha(G)$ was defined in [20] as

$$\prod^\alpha(G) = \prod_{u \in V(G)} \big(d(u)\big)^\alpha.$$

It is not hard to see that $\prod^\alpha(G)$ is a generalization of the first multiplicative Zagreb index.

To unify the vertex-degree-based topological indices, the *vertex-degree-function index* $H_f(G)$ of a graph G was constructed in [20], where

$$H_f(G) = \sum_{v \in V(G)} f\big(d(v)\big)$$

for a function $f(x)$ defined on positive real numbers.

Definition 1.1 *For a graph family $\mathcal{G}$, a graph $G \in \mathcal{G}$ is called a* good extremal graph *of $\mathcal{G}$ if*

(i) $R^0_\alpha(G)$ is maximum for $\alpha < 0$ or $\alpha > 1$, and $R^0_\alpha(G)$ is minimum for $0 < \alpha < 1$.

(ii) $\overset{\alpha}{\prod}(G)$ is maximum for $\alpha < 0$, and $\overset{\alpha}{\prod}(G)$ is minimum for $\alpha > 0$.

(iii) $\underset{2}{\prod}(G)$ is maximum and $\overline{M_1(G)}$ is minimum.

Extremal ordering problem is an important topic on topological indices. As observed in some literatures ([10,19] for instance), many topological indices share the same extremal graphs. Thus, it is rather interesting for us to determine unified extremal graphs for as many topological indices as possible in a given graph family [8, 19, 20]. As extremal ordering problem for some topological indices in the class of c-cyclic graphs with a given diameter always attract much attention [6, 9, 17, 21], we shall identify all good extremal graphs in the class of c-cyclic graphs with given diameter for $c \in \{0, 1, 2\}$. Theorems 2.1, 2.2 and 2.3 are main results in this paper.

2 The main results

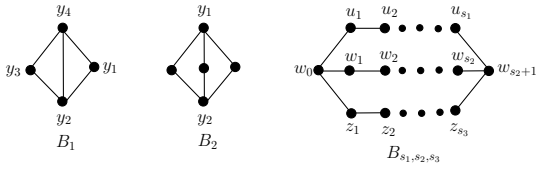


Figure 1. The bicyclic graphs B_1, B_2 and B_{s_1,s_2,s_3}

In this section, we shall introduce the main results of this paper, and we need to introduce more notations. As usual, the cycle and path with n vertices will be referred as C_n and P_n, respectively. Let G be a connected graph with $v \in V(G)$, and let P_k be a

path on k vertices such that G and P_k are vertex-disjoint. Let G^* be a graph obtained from G and P_k by adding one edge between v and one end vertex of P_k. In this way, we say that G^* is obtained by *attaching* the path P_k to vertex v of G.

Hereafter, we suppose that d is the diameter of G. Let $x_0, x_d \in V(G)$ with $dist(x_0, x_d) = d$ and $P_{d+1} = x_0x_1 \dots x_d$ denote a shortest path from x_0 to x_d. Define by $T_j(n,d)$ the tree obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to x_j, where $1 \le j \le d-1$.

Theorem 2.1 *A tree T with n vertices and diameter d is a good extremal tree if and only if $T \in \Big\{T_1(n,d), T_2(n,d), \dots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\}$.*

If U is a unicyclic graph, then we let $C_g = z_1z_2 \dots z_gz_1$ be the unique cycle of U. For $1 \le j \le d-2$, let $U_{1,j}(n,d)$ be the unicyclic graph obtained from C_3 by attaching $n-d-2$ isolated vertices together with the path P_j with j vertices to z_1, and then attaching another path P_{d-j-1} with $d-j-1$ vertices to z_2. For $1 \le j \le d-3$, let $U_{2,j}(n,d)$ be the unicyclic graph obtained from C_4 by attaching $n-d-2$ isolated vertices together with the path P_j with j vertices to z_1, and then attaching another path P_{d-j-2} with $d-j-2$ vertices to z_3.

Theorem 2.2 *Let U be a unicyclic graph in the class of unicyclic graphs with n vertices and diameter d. If $4 \le d \le n-2$, then U is a good extremal unicyclic graph if and only if $U \in \big\{U_{1,1}(n,d), U_{1,2}(n,d), \dots, U_{1,d-2}(n,d), U_{2,1}(n,d), U_{2,2}(n,d), \dots, U_{2,d-3}(n,d)\big\}$.*

Hereafter, denote by B_1, B_2 and B_{s_1,s_2,s_3} the three bicyclic graphs as shown in Fig. 1. Let $B_{1,j}(n,d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-2$ isolated vertices together with a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_3, where $1 \le j \le d-3$. Let $B_{2,j}(n,d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-2$ isolated vertices to y_2, a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_3, where $1 \le j \le d-3$. Let $B_{3,j}(n,d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-3$ isolated vertices together with a path with j vertices to y_2 and then attaching another path with $d-j-1$ vertices to y_4, where $1 \le j \le d-2$. Let $B_{4,j}(n,d)$ be the bicyclic graph obtained from B_2 by attaching $n-d-3$ isolated vertices together with a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_2, where $1 \le j \le d-3$.

Theorem 2.3 *If $4 \leq d \leq n-3$ and B is a good extremal bicyclic graph in the class of bicyclic graphs with n vertices and diameter d, then either $B \in \big\{B_{1,i}(n,d), B_{2,j}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq j \leq \lfloor \frac{d}{2} \rfloor - 1\big\}$ or $B \in \big\{B_{3,k}(n,d), B_{4,i}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq k \leq d-2\big\}$.*

3 Some preliminaries

Let $\mathbf{s} = (s_1, s_2, ..., s_n)$ and $\mathbf{t} = (t_1, t_2, ..., t_n)$ be two non-increasing sequences of real numbers. We write $\mathbf{s} \trianglelefteq \mathbf{t}$ if and only if $\sum_{i=1}^{n} s_i = \sum_{i=1}^{n} t_i$, and $\sum_{i=1}^{j} s_i \leq \sum_{i=1}^{j} t_i$ for all $j = 1, 2, ..., n$. Furthermore, we write $\mathbf{s} \triangleleft \mathbf{t}$ if and only if $\mathbf{s} \trianglelefteq \mathbf{t}$ and $\mathbf{s} \neq \mathbf{t}$. The ordering $\mathbf{s} \trianglelefteq \mathbf{t}$ is always referred to as *majorization* [5, 12, 15].

A *strictly convex function* is a real valued function $g(x)$ defined on a convex set D such that

$$g\big(px + (1-p)y\big) < pg(x) + (1-p)g(y)$$

for all $0 < p < 1$ and all x, $y \in D$. Among all majorization theorems, the following one was discovered long time ago, and it is not restricted to graphical invariants.

Theorem 3.1 [15] *Let $\mathbf{s} = (s_1, s_2, ..., s_n)$ and $\mathbf{t} = (t_1, t_2, ..., t_n)$ be two non-increasing sequences of real numbers. If $\mathbf{s} \triangleleft \mathbf{t}$, then for any strictly convex function $g(x)$, we have $\sum_{i=1}^{n} g(s_i) < \sum_{i=1}^{n} g(t_i)$.*

Note that $-f(x)$ is a strictly convex function if and only if $f(x)$ is a strictly concave function. Thus, the following theorem easily follows from Theorem 3.1.

Theorem 3.2 [14,20] *Let π and π' be two different non-increasing degree sequences with $\pi \triangleleft \pi'$, and G and G' be two graphs with $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$.*

(i) If $f(x)$ is a strictly convex function on $x \geq 1$, then $H_f(G) < H_f(G')$;

(ii) If $f(x)$ is a strictly concave function on $x \geq 1$, then $H_f(G) > H_f(G')$.

The following two results can be deduced from Theorems 3.1 and 3.2:

Theorem 3.3 [14,20] *In a given graph family $\mathcal{G}$, if $H_f(G)$ is maximum for any strictly convex function on $x \geq 1$, then $R_\alpha^0(G)$ is maximum for $\alpha > 1$ or $\alpha < 0$, $\overset{\alpha}{\prod}(G)$ is maximum for $\alpha < 0$, $\underset{2}{\prod}(G)$ is maximum, and $\overline{M_1(G)}$ is minimum.*

Theorem 3.4 [14, 20] *In a given graph family $\mathcal{G}$, if $H_f(G)$ is minimum for any strictly concave function on $x \geq 1$, then $R^0_\alpha(G)$ is minimum for $0 < \alpha < 1$, and $\overset{\alpha}{\prod}(G)$ is minimum for $\alpha > 0$.*

4 The proof of Theorem 2.1

Let $\mathbb{C}(n, d, p; c)$ be the set of c-cyclic graphs with n vertices, p pendant vertices and diameter d. We will use the symbol $p^{(q)}$ to define q copies of the real number p. In what follows, denote by

$$\pi_1 = \left(n-d+1, 2^{(d-2)}, 1^{(n-d+1)}\right), \pi_2 = \left(n-d+1, 3, 2^{(d-2)}, 1^{(n-d)}\right),$$
$$\pi_3 = \left(n-d+1, 3^{(3)}, 2^{(d-4)}, 1^{(n-d)}\right), \text{and } \pi_4 = \left(n-d+1, 4, 2^{(d-1)}, 1^{(n-d-1)}\right).$$

Lemma 4.1 *If $T \in \mathbb{C}(n, d, p; 0)$, then $p \leq n-d+1$, where the equality holds if and only if T is obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to some vertices of $\{x_1, x_2, \ldots, x_{d-1}\}$.*

Proof. If $T \in \mathbb{C}(n, d, p; 0)$, that is, T is a tree with n vertices, p pendant vertices and diameter d, then since there are at least $d-1$ non-pendant vertices on P_{d+1}, we have $p \leq n-d+1$. From this fact, it is straightly to verify this lemma. ■

Lemma 4.2 *Let $T \in \mathbb{C}(n, d, p; 0)$. If $\pi \neq \pi_1$ and $d \geq 2$, then $\pi \lhd \pi_1$.*

Proof. Let $\pi = \left(d_1, d_2, \ldots, d_{n-p}, 1^{(p)}\right)$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-p} \geq 2$. Recall that $\pi_1 = \left(n-d+1, 2^{(d-2)}, 1^{(n-d+1)}\right)$. We assume that $\pi_1 = \left(d'_1, d'_2, \ldots, d'_{d-1}, 1^{(n-d+1)}\right)$, that is, $d'_1 = n-d+1$ and $d'_i = 2$ for $2 \leq i \leq d-1$.

Since T is a tree, by Lemma 4.1, we have

$$d_1 = 2(n-1) - p - d_2 - d_3 - \cdots - d_{n-p} \leq 2(n-1) - p - 2(n-p-1) = p \leq n-d+1.$$

If $d_1 = n-d+1$, then $d_2 = d_3 = \cdots = d_{n-p} = 2$, and hence $\pi = \pi_1$, a contradiction. Consequently, $d_1 < n-d+1$.

For $2 \leq j \leq d-1$, since $d_j \geq 2$ and $p \leq n-d+1$, by Lemma 4.1, we have

$$\sum_{i=1}^{j} d_i = 2(n-1) - p - d_{j+1} - \cdots - d_{n-p}$$
$$\leq 2(n-1) - p - 2(n-p-j) = p + 2j - 2 \leq n-d-1+2j = \sum_{i=1}^{j} d'_i.$$

For $d \leq j \leq n$, since $d'_d = 1 \leq d_d$, we have $\sum_{i=1}^{j} d_i \leq 2(n-1) - (n-j) = n + j - 2 = \sum_{i=1}^{j} d'_i$. Combining the above arguments, we have $\pi \lhd \pi_1$. ■

For simplification, let $\mathbb{T}(n,d)$ be the set of trees with n vertices, diameter d and degree sequence π_1, and $\mathbb{U}(n,d)$ be the set of unicyclic graphs with n vertices, diameter d and degree sequence π_2. Define $\mathbb{B}_1(n,d)$ $\big($resp., $\mathbb{B}_2(n,d)\big)$ as the set of bicyclic graphs with n vertices, diameter d and degree sequence π_3 $\big($resp., $\pi_4\big)$.

Lemma 4.3 *If $d \geq 2$, then $\mathbb{T}(n,d) = \Big\{T_1(n,d), T_2(n,d), \ldots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\}$.*

Proof. From the definition of $T_i(n,d)$, where $1 \leq i \leq d-1$,

$$\Big\{T_1(n,d), T_2(n,d), \ldots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\} \subseteq \mathbb{T}(n,d),$$

and so it suffices to show that $\mathbb{T}(n,d) \subseteq \Big\{T_1(n,d), T_2(n,d), \ldots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\}$.

Suppose that $T \in \mathbb{T}(n,d)$. By Lemma 4.1, T is obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to some vertices of $\big\{x_1, x_2, \ldots, x_d\big\}$. Since $d_1 = n-d+1$ by the definition of π_1, then all these $n-d-1$ isolated vertices are adjacent to the same vertex x_i, where $1 \leq i \leq d-1$. Since $T_i(n,d) = T_{d-i}(n,d)$, we can conclude that $T = T_j(n,d)$ for some $j \in \big\{1, 2, \ldots, \lfloor \frac{d}{2} \rfloor\big\}$. ■

Now it is ready to present the following proof of Theorem 2.1.

Proof of Theorem 2.1. In view of Theorems 3.3 and 3.4, it suffices to show that T has the maximum (resp., minimum) $H_f(T)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \geq 1$. We suppose that the degree sequence of T is π. By Lemma 4.2, $\pi \lhd \pi_1$ unless $\pi = \pi_1$. Combining this with Lemma 4.3, the result follows from Theorem 3.2. ■

5 The Proof of Theorem 2.2

Denote by $\mathcal{R}(G)$ the *reduced graph* obtained from G by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. Let H be a subgraph of G and let N_H be the set of non-pendant vertices of H in G. Recall that $P_{d+1} = x_0 x_1 \ldots x_d$ is a shortest path from x_0 to x_d. It is not hard to see that

$$d - 1 \leq |N_{P_{d+1}}| \leq d + 1. \tag{2}$$

Lemma 5.1 *If u and v are two vertices of $V\big(P_{d+1}\big) \cap V\big(\mathcal{R}(G)\big)$, then all the vertices of $V\big(P_{d+1}\big)$ between u and v belong to $V\big(\mathcal{R}(G)\big)$.*

Proof. Let u_0 and v_0 be two vertices of $V\big(P_{d+1}\big) \cap V\big(\mathcal{R}(G)\big)$ with maximum distance, that is, $dist\big(u_0, v_0\big) = \max\big\{dist(u,v) : \{u,v\} \subseteq V\big(\mathcal{R}(G)\big) \cap V\big(P_{d+1}\big)\big\}$. It suffices to show that all the vertices of $V\big(P_{d+1}\big)$ between u_0 and v_0 belong to $V\big(\mathcal{R}(G)\big)$. Suppose not, and let y be a vertex of $V\big(P_{d+1}\big)$ between u_0 and v_0 and $y \notin V\big(\mathcal{R}(G)\big)$. Then, there is a path $P_{u_0v_0}$ in $\mathcal{R}(G) \subseteq G-y$ connecting u_0 and v_0. Let x be the last vertex before y in P_{d+1} such that $x \in P_{u_0v_0}$, and let z be the first vertex after y in P_{d+1} such that $z \in P_{u_0v_0}$. In this case, there is another path P_{xz} connecting x and z such that $V\big(P_{xz}\big) \cap V\big(P_{u_0v_0}\big) = \{x, z\}$ and $y \in P_{xz}$, which means that x, y, z are in the same cycle of G, and thus $y \in V\big(\mathcal{R}(G)\big)$, a contradiction. ■

Corollary 5.2 *For any cycle C_g, at least $\lceil \frac{g}{2} \rceil - 1$ vertices of C_g are not on P_{d+1}.*

Proof. As $g > \lceil \frac{g}{2} \rceil$, the result holds for $|V(C_g) \cap V(P_{d+1})| \leq 1$. Thus, we may suppose that $|V(C_g) \cap V(P_{d+1})| \geq 2$. In this case, the distance of any two different vertices in C_g is at most $\lfloor \frac{g}{2} \rfloor$, so at most $\lfloor \frac{g}{2} \rfloor + 1$ vertices of C_g are contained in $V\big(P_{d+1}\big)$ by Lemma 5.1. Consequently, at least $g - \big(\lfloor \frac{g}{2} \rfloor + 1\big) = \lceil \frac{g}{2} \rceil - 1$ vertices of C_g are not on P_{d+1}. ■

Lemma 5.3 *If $G \in \mathbb{C}(n,d,p;c)$ and $c \geq 1$, then $p \leq n-d$, where the equality implies that x_0 and x_d are two pendant vertices of G, and either $g \in \{3,4\}$ and $\mathcal{R}(G) = C_g$ with $|V\big(P_{d+1}\big) \cap V(C_g)| = g-1$ or $\mathcal{R}(G) = B_1$ with $V\big(P_{d+1}\big) \cap V(B_1) = \big\{y_1, y_2, y_3\big\}$.*

Proof. Let C_g be an induced subgraph of G, as $c \geq 1$. By Corollary 5.2, there are at least $\lceil \frac{g}{2} \rceil - 1$ vertices of C_g that are not on P_{d+1}. Combining this with $g \geq 3$ and (2), it follows that

$$p \leq n - |N_{P_{d+1}}| - \left(\left\lceil \frac{g}{2} \right\rceil - 1\right) \leq n - \big(d-1\big) - \left(\left\lceil \frac{g}{2} \right\rceil - 1\right) = n - d + 2 - \left\lceil \frac{g}{2} \right\rceil \leq n - d, \quad (3)$$

as required.

We now suppose that $p = n-d$, that is, the equality holds in (3). In this case, P_{d+1} contains exactly $d-1$ non-pendant vertices by (3), and so x_0 and x_d are two pendant vertices of G. Since P_{d+1} contains exactly $d-1$ non-pendant vertices in G and since P_{d+1} cannot contain all vertices of C_g by Corollary 5.2, we conclude that $\mathcal{R}(G)$ contains exactly one vertex, say w_0, not on P_{d+1}, and we may suppose that $u_1u_2 \ldots u_{|V(\mathcal{R}(G))|-1}$ are the sub-path of P_{d+1} in $\mathcal{R}(G)$.

As P_{d+1} is a shortest path from x_0 to x_d, we have $N_G(u_1) \cap \big\{u_2, u_3, \ldots, u_{|V(\mathcal{R}(G))|-1}\big\} = \big\{u_2\big\}$ and $N_G\big(u_{|V(\mathcal{R}(G))|-1}\big) \cap \big\{u_1, u_2, \ldots, u_{|V(\mathcal{R}(G))|-2}\big\} = \big\{u_{|V(\mathcal{R}(G))|-2}\big\}$. Combining this

with $\{u_1, u_{|V(\mathcal{R}(G))|-1}\} \subseteq V(\mathcal{R}(G))$, it follows that $w_0u_1 \in E(G)$ and $w_0u_{|V(\mathcal{R}(G))|-1} \in E(G)$. Now, since P_{d+1} is a shortest path from x_0 to x_d and since $u_1w_0u_{|V(\mathcal{R}(G))|-1}$ is a path of length two from u_1 to $u_{|V(\mathcal{R}(G))|-1}$, we have $|V(\mathcal{R}(G))| \in \{3, 4\}$, as $w_0 \notin V(P_{d+1})$.

If $|V(\mathcal{R}(G))| = 3$, then $\mathcal{R}(G) = C_3$ and $|V(P_{d+1}) \cap V(C_3)| = 2$. Otherwise, $|V(\mathcal{R}(G))| = 4$.

If $u_2w_0 \in E(G)$, then $\mathcal{R}(G) = B_1$ and we may suppose that $V(P_{d+1}) \cap V(B_1) = \{y_1, y_2, y_3\}$ and $w_0 = y_4$. If $u_2w_0 \notin E(G)$, then $\mathcal{R}(G) = C_4$ and $|V(P_{d+1}) \cap V(C_4)| = 3$. ■

Lemma 5.4 *Suppose that* $1 \leq c \leq 2$ *and* $2c \leq d \leq n-2$. *(i) Let* $G \in \mathbb{C}(n, d, n-d; c)$ *with degree sequence* π. *If* $\pi \neq \pi' = (n-d+1, 3^{(2c-1)}, 2^{(d-2c)}, 1^{(n-d)})$, *then* $\pi \lhd \pi'$. *(ii) If* $G \in \mathbb{C}(n, d, p; 1)$ *and* $\pi \neq \pi_2$, *then* $\pi \lhd \pi_2$.

Proof. We first prove (i). Since $p = n-d$ by $G \in \mathbb{C}(n, d, n-d; c)$, the degree sequence of G is equal to $\pi = (d_1, d_2, \ldots, d_d, 1^{(n-d)})$, where $d_1 \geq d_2 \geq \cdots \geq d_j \geq 3 > d_{j+1} = \cdots = d_d = 2$. By Lemma 5.3, x_0 and x_d are two pendant vertices of G and $j \geq 2c$. Note that $\pi \neq \pi'$, we have

$$\pi \trianglelefteq (n-d+2c-j+1, 3^{(j-1)}, 2^{(d-j)}, 1^{(n-d)}) \lhd \pi',$$

and so (i) holds.

To prove (ii), if $p = n-d$, then (ii) follows from (i). If $p \leq n-d-1$ and $c = 1$, then

$$\pi \trianglelefteq (p+2, 2^{(n-p-1)}, 1^{(p)}) \trianglelefteq (n-d+1, 2^{(d)}, 1^{(n-d-1)}) \lhd \pi_2,$$

completing the proof of (ii). ■

Lemma 5.5 *If* $4 \leq d \leq n-2$, *then*

$$\mathbb{U}(n, d) = \Big\{U_{1,1}(n, d), U_{1,2}(n, d), \ldots, U_{1,d-2}(n, d), U_{2,1}(n, d), U_{2,2}(n, d), \ldots, U_{2,d-3}(n, d)\Big\}.$$

Proof. It is not hard to see that $\{U_{1,1}(n, d), U_{1,2}(n, d), \ldots, U_{1,d-2}(n, d), U_{2,1}(n, d), U_{2,2}(n, d), \ldots, U_{2,d-3}(n, d)\} \subseteq \mathbb{U}(n, d)$. It suffices to show that $\mathbb{U}(n, d) \subseteq \{U_{1,1}(n, d), U_{1,2}(n, d), \ldots, U_{1,d-2}(n, d), U_{2,1}(n, d), U_{2,2}(n, d), \ldots, U_{2,d-3}(n, d)\}$. Let $U \in \mathbb{U}(n, d)$.

By Lemma 5.3, x_0 and x_d are two pendant vertices of U, so $|N_{P_{d+1}}| = d-1$. Besides, $g \in \{3, 4\}$ and $|V(P_{d+1}) \cap V(C_g)| = g-1$. Let $z_1z_2 \ldots z_{g-1}$ be the sub-path of P_{d+1} in

C_g. Since P_{d+1} is a shortest path from x_0 to x_d, $d(z_1) \geq 3$ and $d(z_{g-1}) \geq 3$. Since $d_3 = 2$ by the definition of π_2, we may suppose that $d(z_1) = n - d + 1$ and $d(z_{g-1}) = 3$.

In the case of $g = 3$, z_1z_2 is the sub-path of P_{d+1} in C_3, $d(z_1) = n-d+1$ and $d(z_2) = 3$. Since x_0 and x_d are two pendant vertices of U, U is obtained from C_3 by attaching one path with j vertices together with $n-d-2$ isolated vertices to z_1, one path with $d-j-1$ vertices to z_2, where $1 \leq j \leq d-2$. Thus, $U = U_{1,j}(n, d)$ for some j, where $1 \leq j \leq d-2$. The case of $g = 4$ can be proceeded similarly and thus will be omitted here. ■

Proof of Theorem 2.2. In view of Theorems 3.3 and 3.4, it suffices to show that U has the maximum (resp., minimum) $H_f(U)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \geq 1$. Let π be the degree sequence of U. If $\pi \neq \pi_2$, then $\pi \lhd \pi_2$ by Lemma 5.4. Combining this with Lemma 5.5, the result follows from Theorem 3.2. ■

6 The proof of Theorem 2.3

In what follows, if $c \geq 2$, then let $\mathcal{B}$ be a bicycle subgraph of $\mathcal{R}(G)$, and suppose that C_s and C_t are two cycles of $\mathcal{B}$ such that $|V(C_s) \cap V(C_t)| = r$. Furthermore, we always suppose that $V(C_s) \cap V(C_t) = \{w_0, w_1, \ldots, w_{r-1}\}$ when $r \geq 1$, and we define

$$dist\big(u'_0, v'_0\big) = \max\big\{dist(u, v) : \{u, v\} \subseteq V(\mathcal{B}) \cap V\big(P_{d+1}\big)\big\}$$

when $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \geq 2$.

Lemma 6.1 *Let $G \in \mathbb{C}(n, d, n-d-1; c)$ with degree sequence $(d_1, d_2, \ldots, d_n)$. If $c \geq 2$, then either $d_2 \geq 4$ or $d_3 \geq 3$. Furthermore, (i) If $r \geq 2$ and $|\{w_0, w_{r-1}\} \cap \big\{u'_0, v'_0\big\}| = 2$, then $d_2 \geq 4$ and x_0 and x_d are two pendant vertices of G; (ii) If either $r \geq 2$ with $|\{w_0, w_{r-1}\} \cap \big\{u'_0, v'_0\big\}| \leq 1$ or $r \leq 1$, then $d_3 \geq 3$.*

Proof. Since $G \in \mathbb{C}(n, d, n-d-1; c)$, G contains exactly $d+1$ non-pendant vertices. If $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \leq 1$, note that $|N_{P_{d+1}}| \geq d-1$ by (2), then

$$|N_G| \geq |N_{P_{d+1}}| + |V(\mathcal{B})| - 1 \geq d - 1 + 3 = d + 2,$$

a contradiction. Therefore, $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \geq 2$. Next, we consider three cases according to the value of r.

Case 1. $r \geq 2$.

In this case, we may suppose that $\mathcal{B} \cong B_{s_1,s_2,s_3}$, where $\min\{s_1,\, s_3\} \geq s_2 \geq 0$ and $\min\{s_1,\, s_3\} \geq 1$ (see Fig. 1). By the definition of r and the choices of u_0' and v_0', we have $r = s_2 + 2$, either $\{u_0', v_0'\} \subseteq V(C_{s_1+s_2+2})$, or $\{u_0', v_0'\} \subseteq V(C_{s_2+s_3+2})$ or $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$.

Recall that $\mathcal{B}$ contains at least one vertex that is not on P_{d+1} by Corollary 5.2, and G contains exactly $d+1$ non-pendant vertices. Thus, $|N_{P_{d+1}}| \leq d$, and so $d-1 \leq |N_{P_{d+1}}| \leq d$ by (2).

We first suppose that $|N_{P_{d+1}}| = d-1$. Since P_{d+1} contains exactly $d-1$ non-pendant vertices of G and so x_0 and x_d are two pendant vertices of G, verifying that $\min\{d(u_0'),\, d(v_0')\} \geq 3$. If $\{u_0', v_0'\} = \{w_0, w_{s_2+1}\}$, then $d_1 \geq d_2 \geq \min\{d(u_0'), d(v_0')\} \geq 4$. Otherwise, $|\{w_0, w_{s_2+1}\} \cap \{u_0', v_0'\}| \leq 1$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as required.

We secondly assume that $|N_{P_{d+1}}| = d$. That is, P_{d+1} contains exactly d non-pendant vertices of G. We claim that $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$. Otherwise, by the symmetry of s_1 and s_3, we suppose that $\{u_0', v_0'\} \subseteq V(C_{s_1+s_2+2})$. Then $C_{s_1+s_2+2}$ contains at least $\lceil \frac{s_1+s_2}{2} \rceil$ vertices that are not on P_{d+1} by Corollary 5.2. Since G contains exactly $d+1$ non-pendant vertices and since each vertex of $\mathcal{B}$ is a non-pendant vertex, by (2) and $\min\{s_1,\, s_3\} \geq 1$, we have

$$d = |N_{P_{d+1}}| \leq d+1-\left\lceil \frac{s_1+s_2}{2} \right\rceil - s_3 \leq d+1-\left\lceil \frac{s_1+s_2}{2} \right\rceil - 1 \leq d-1,$$

a contradiction. This completes our claim.

Since $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$, $C_{s_1+s_3+2}$ contains at least $\lceil \frac{s_1+s_3}{2} \rceil$ vertices that are not on P_{d+1} by Corollary 5.2. Combining this with $|N_{P_{d+1}}| = d$ and $\min\{s_1,\, s_3\} \geq 1$, we have

$$d = |N_{P_{d+1}}| \leq d+1-\left\lceil \frac{s_1+s_3}{2} \right\rceil - s_2 \leq d+1-\left\lceil \frac{s_1+s_3}{2} \right\rceil \leq d,$$

and so $s_1 = s_3 = 1$ and $s_2 = 0$, that is, $\mathcal{B} \cong B_1$ with $y_2 = w_1$.

If $|\{u_0', v_0'\} \cap \{w_0, w_1\}| = 0$, then $\{u_0', v_0'\} = \{y_1, y_3\}$ (see Fig. 1). Note that $|N_{P_{d+1}}| = d$, then either $d(y_1) \geq 3$ or $d(y_3) \geq 3$, and hence $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, $|\{u_0', v_0'\} \cap \{w_0, w_1\}| \geq 1$. We may suppose that $u_0' = w_0 = y_4$. In this case, $v_0' \in \{y_1, y_2, y_3\}$, and hence $|N_G| \geq |N_{P_{d+1}}| + |\{y_1, y_2, y_3\} \setminus \{v_0'\}| = d+2$, a contradiction.

Case 2. $r = 1$.

In this case, $V(C_s) \cap V(C_t) = \{w_0\}$ and at least $\lceil \frac{s}{2} \rceil + \lceil \frac{t}{2} \rceil - 2$ vertices are not on P_{d+1} by Corollary 5.2. Combining this with (2), it follows that

$$d-1 \leq |N_{P_{d+1}}| \leq d+1-\left(\left\lceil \frac{s}{2} \right\rceil + \left\lceil \frac{t}{2} \right\rceil - 2\right) \leq d-1, \tag{4}$$

and hence $|N_{P_{d+1}}| = d-1$. Thus, x_0 and x_d are two pendant vertices of G. If $w_0 \notin \{u_0', v_0'\}$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, u_0' and v_0' lie on the same cycle of $\mathcal{B}$. Without loss of generality, we suppose that $\{u_0', v_0'\} \subset V(C_t)$. By Corollary 5.2 and $|N_{P_{d+1}}| = d-1$ by (4), $|N_G| \geq |N_{P_{d+1}}| + s - 1 + \lceil \frac{t}{2} \rceil - 1 \geq d+2$, a contradiction.

Case 3. $r = 0$.

Since $\mathcal{B}$ is connected, there must be a path, say $P_k = u_1 u_2 \cdots u_k$, connecting C_s and C_t, where $u_1 \in V(C_s)$, $u_k \in V(C_t)$ and $k \geq 2$. Thus, $d(u_1) \geq 3$ and $d(u_k) \geq 3$.

By Corollary 5.2, at least $\lceil \frac{s}{2} \rceil + \lceil \frac{t}{2} \rceil - 2$ vertices are not on $V(P_{d+1})$. Similarly with (4), we have $|N_{P_{d+1}}| = d-1$ and hence x_0 and x_d are also two pendant vertices of G. If $|\{u_0', v_0'\} \cap \{u_1, u_k\}| \leq 1$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, $|\{u_0', v_0'\} \cap \{u_1, u_k\}| = 2$. Since $|N_{P_{d+1}}| = d-1$, and so $|N_G| \geq |N_{P_{d+1}}| + s - 1 + t - 1 \geq d+3$, a contradiction. ■

Lemma 6.2 *Let $B \in \mathbb{C}(n, d, p; 2)$. If $\pi \notin \{\pi_3, \pi_4\}$ and $4 \leq d \leq n-3$, then $\pi \lhd \pi_3$ or $\pi \lhd \pi_4$.*

Proof. Let $\pi = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \cdots \geq d_k \geq 4 > d_{k+1} = \cdots = d_j = 3 > d_{j+1} = \cdots = d_{n-p} = 2$. By Lemma 5.3, we have $p \leq n-d$. If $p = n-d$, then $\pi \lhd \pi_3$ by Lemma 5.4. Thus, we may assume that $p \leq n-d-1$ in the following, and we will prove that $\pi \lhd \pi_4$.

Case 1. $p = n-d-1$. By Lemma 6.1, $k \geq 2$ or $j \geq 3$.

If $k \geq 2$, since $\pi \neq \pi_4$ and $j \geq k \geq 2$,

$$\pi \trianglelefteq (n-d-k-j+5, 4^{(k-1)}, 3^{(j-k)}, 2^{(d+1-j)}, 1^{(n-d-1)}) \lhd \pi_4.$$

Otherwise, $j \geq 3$. Since $\pi \neq \pi_4$, we have

$$\pi \trianglelefteq (n-d-j+4, 3^{(j-1)}, 2^{(d+1-j)}, 1^{(n-d-1)}) \trianglelefteq (n-d+1, 3^{(2)}, 2^{(d-2)}, 1^{(n-d-1)}) \lhd \pi_4.$$

Case 2. $p \leq n-d-2$. It is not hard to see that

$$\pi \trianglelefteq (p-j+5, 3^{(j-1)}, 2^{(n-p-j)}, 1^{(p)}) \trianglelefteq (n-d-j+3, 3^{(j-1)}, 2^{(d+2-j)}, 1^{(n-d-2)}). \quad (5)$$

Next, we prove that

$$\text{If } p = n-d-2, \text{ then } j \geq 2. \quad (6)$$

Recall that C_s and C_t are two cycles of $\mathcal{B}$ such that $|V(C_s)\cap V(C_t)| = r$. We may suppose that $s \geq t \geq 3$. If $r \neq 1$, then $j \geq 2$ and hence (6) holds. Thus, we may assume that $r = 1$ in the following.

By contradiction, we assume that $j = 1$. Thus $\pi = \big(n-d+2, 2^{(d+1)}, 1^{(n-d-2)}\big)$. Let $V(C_s)\cap V(C_t) = \{w_0\}$. If $|V\big(P_{d+1}\big)\cap V(\mathcal{R}(B))| \leq 1$, then $|N_B| \geq |N_{P_{d+1}}|+s+t-2 \geq d+3$ by (2), a contradiction. Otherwise, $|V\big(P_{d+1}\big) \cap V(\mathcal{R}(B))| \geq 2$.

As in Lemma 5.1, let u_0 and v_0 be two vertices of $V\big(P_{d+1}\big) \cap V\big(\mathcal{R}(B)\big)$ with the maximum distance. Since $d_2 = 2$ and $d_1 = n-d+2$, B is obtained from $\mathcal{R}(B)$ by attaching $n-d-2$ paths to the 4-vertex of $\mathcal{R}(B)$. Combining this with $|V\big(P_{d+1}\big) \cap V(\mathcal{R}(B))| \geq 2$, we have $|\{u_0, v_0\} \cap \{x_0, x_d\}| \geq 1$ verifying that $|N_{P_{d+1}}| \geq d$.

If $w_0 \in \{u_0, v_0\}$, without loss of generality, we may assume that $w_0 = u_0$, and so $d(v_0) = 2$. In this case, $v_0 \in \{x_0, x_d\}$. Since $|N_{P_{d+1}}| \geq d$, by Corollary 5.2, we have $|N_B| \geq |N_{P_{d+1}}| + t - 1 + \lceil \frac{s}{2} \rceil - 1 \geq d+3$, a contradiction. Thus, $w_0 \notin \{u_0, v_0\}$.

Recall that B is obtained from $\mathcal{R}(B)$ by attaching $n-d-2$ paths to the 4-vertex of $\mathcal{R}(B)$ and $d_2 = 2$. Thus, $\big\{u_0, v_0\big\} = \big\{x_0, x_d\big\}$ and $|N_{P_{d+1}}| = d+1$. Again, Corollary 5.2 implies that $|N_B| \geq |N_{P_{d+1}}| + \lceil \frac{s}{2} \rceil - 1 + \lceil \frac{t}{2} \rceil - 1 \geq d+3$, a contradiction. This completes the proof of (6).

By combining (5) and (6), we have $\pi \trianglelefteq \big(n-d+1, 3, 2^{(d)}, 1^{(n-d-2)}\big) \lhd \pi_4$, as $\pi \neq \pi_4$. ■

Lemma 6.3 *If $4 \leq d \leq n-3$, then $\mathbb{B}_1(n,d) = \big\{B_{1,i}(n,d), B_{2,j}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq j \leq \lfloor \frac{d}{2} \rfloor - 1\big\}$ and $\mathbb{B}_2(n,d) = \big\{B_{3,k}(n,d), B_{4,i}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq k \leq d-2\big\}$.*

Proof. For $1 \leq i \leq d-3$, $1 \leq j \leq \lfloor \frac{d}{2} \rfloor - 1$ and $1 \leq k \leq d-2$, it is not hard to see that $B_{1,j} \in \mathbb{B}_1(n,d)$, $B_{2,j} \in \mathbb{B}_1(n,d)$, $B_{3,i} \in \mathbb{B}_2(n,d)$ and $B_{4,j} \in \mathbb{B}_2(n,d)$. Let B be a bicyclic graph of $\mathbb{B}_1(n,d) \cup \mathbb{B}_2(n,d)$.

Case 1. $B \in \mathbb{B}_1(n,d)$**.**

By Lemma 5.3, x_0 and x_d are two pendant vertices of B and $\mathcal{R}(B) = B_1$ with $V\big(P_{d+1}\big) \cap V(B_1) = \big\{y_1, y_2, y_3\big\}$ and so $\min\big\{d(y_1), d(y_2), d(y_3)\big\} \geq 3$. Since B contains exactly d non-pendant vertices by the definition of π_3, $\{x_1, x_2, \ldots, x_{d-1}, y_4\}$ are all these non-pendant vertices of B. Note that $\big\{y_1, y_2, y_3, y_4\big\}$ are the four vertices with degree at least three in B, and $d_1 = n-d+1 \geq 3 = d_2 = d_3 = d_4 > d_5$. Thus, y_1 is symmetric with y_3 and y_2 is symmetric with y_4, and either $d(y_1) = n-d+1$ or $d(y_2) = n-d+1$.

Here, we only consider the case of $d(y_2) = n-d+1$, as the case of $d(y_1) = n-d+1$ can be proved similarly. Since x_0 and x_d are two pendant vertices of B and since $d(y_2) = n-d+1$, B is obtained from B_1 by attaching $n-d-2$ isolated vertices to y_2, one path with q vertices to y_1, and another path with $d-q-2$ vertices to y_3, where $1 \leq q \leq d-3$. It is easily checked that $B_{2,q}(n,d) = B_{2,d-2-q}$, and so $B = B_{2,j}$, where $1 \leq j \leq \lfloor \frac{d}{2} \rfloor - 1$.

Case 2. $B \in \mathbb{B}_2(n,d)$**.**

Recall that C_s and C_t are two cycles of $\mathcal{B}$ with $|V(C_s) \cap V(C_t)| = r$. By Lemma 6.1, $r \geq 2$ and hence we may suppose that $V(C_s) \cap V(C_t) = \{w_0, w_1, \ldots, w_{r-1}\}$, $s \geq t \geq 2(r-1)$ and $\min\{d(w_0), d(w_{r-1})\} = 4$, as x_0 and x_d are two pendant vertices of G and $\{w_0, w_{r-1}\} = \{u_0', v_0'\}$ (see Lemma 6.1). Since $\{w_0, w_{r-1}\} = \{u_0', v_0'\}$ and $s \geq t \geq 2(r-1)$, at least $s+t-2r$ vertices of $V(\mathcal{R}(B))$ are not on P_{d+1}. Combining this with (2),

$$d-1+(s+t-2r) \leq |N_{P_{d+1}}| + (s+t-2r) \leq |N_B| = d+1, \tag{7}$$

and hence $2(r-1) \leq t \leq r+1$. Thus, $2 \leq r \leq 3$.

Combining with $t \geq 3$, we have $t = r+1$. By (7) and $s \geq t = r+1$, we have $d+1 = |N_B| \geq d-1+2(r+1)-2r = d+1$, which implies that $s = t = r+1$. Recall that $|V(C_s) \cap V(C_t)| = r \in \{2,3\}$. Thus, $\mathcal{R}(B) \in \{B_1, B_2\}$. In view of the definition of π_4 and since $\min\{d(w_0), d(w_{r-1})\} = 4$, we may suppose that $d(w_0) = n-d+1$.

We first suppose that $\mathcal{R}(B) = B_1$ and we may assume that $y_2 = w_0$ by symmetry. Since x_0 and x_d are two pendant vertices of B, B is obtained from B_1 by attaching one path with k vertices together with $n-d-3$ isolated vertices to y_2, and one path with $d-k-1$ vertices to y_4, where $1 \leq k \leq d-2$, this implying that $B = B_{3,k}(n,d)$ for some $1 \leq k \leq d-2$. Now, we suppose that $\mathcal{R}(B) = B_2$. In a similar way, we can conclude that $B = B_{4,i}(n,d)$ for $1 \leq i \leq d-3$, and so complete the proof of this result. ■

Proof of Theorem 2.3. In view of Theorems 3.3 and 3.4, it suffices to show that B has the maximum (resp., minimum) $H_f(B)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \geq 1$. Suppose that the degree sequence of B is π. If $\pi \in \{\pi_3, \pi_4\}$, then Lemma 6.3 implies that $B \in \mathbb{B}_1(n,d) \cup \mathbb{B}_2(n,d)$. Otherwise, $\pi \notin \{\pi_3, \pi_4\}$. Since $4 \leq d \leq n-3$, $\pi \lhd \pi_3$ or $\pi \lhd \pi_4$ by Lemma 6.2. Now, the result follows from Theorem 3.2. ■

Remark 6.4 Actually, in this paper, we have determined all the extremal graphs with maximum (resp., minimum) vertex-degree-function index $H_f(G)$ for any strictly convex

(resp., concave) function $f(x)$ defined on $x \geq 1$ among the class of trees, unicyclic graphs and bicyclic graphs with given diameter, respectively.

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Unified extremal results of topological indices and spectral invariants of graphs☆

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ABSTRACT

Identifying graphs with extremal properties is an extensively studied topic in both topological graph theory and spectral graph theory. As observed in the literature, for many graph categories the extremal graphs with respect to some prescribed topological index or spectral invariant are the same. Therefore, it is an interesting problem to find a unified method to identify the extremal graphs for a set of topological or spectral invariants. Here we consider the majorization theorem to obtain extremal graphs in the class of trees, unicyclic graphs and bicyclic graphs with given order and fixed maximum degree, independence number, matching number, domination number, and/or number of pendant vertices, respectively.

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1. Introduction

In this paper we consider simple undirected graphs. Let $G = (V, E)$ be a connected graph with n vertices and m edges. If $m = n+c-1$, then G is said to be a c-cyclic graph. In particular, when $c = 0$, 1 or 2, G is called a tree, unicyclic graph or bicyclic graph, respectively. As usual, $d(u)$ or $d_G(u)$ when G is needed to be indicated, denotes the degree of u, and a vertex of degree k is called a k-vertex. A 1-vertex is said to be a pendant vertex of G. Evidently, vertices of degree at least 2 are said to be non-pendant, and those adjacent to a pendant vertex will be called quasi-pendant. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let $d_i = d(v_i)$, for $i = 1, 2, \ldots, n$, then $\pi = (d_1, d_2, \ldots, d_n)$ is the degree sequence of G. In the sequel we list the degrees in non-increasing order, that is, $d_1 \geq d_2 \geq \cdots \geq d_n$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π. Clearly, if $G \in \Gamma(\pi)$, and G is a c-cyclic graph, then

$$\sum_{i=1}^{n} d_i = 2(n + c - 1). \tag{1.1}$$

A subset D of $V(G)$ is said to be a dominating set of G if each vertex of $V(G)\backslash D$ is adjacent to at least a vertex of D. The number of vertices in a dominating set of G with minimum cardinality is called the domination number of G, and it

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is denoted by $\gamma(G)$. It is easy to see that when G is a connected graph with n vertices, then

$$\gamma(G) \leq \frac{n}{2}. \tag{1.2}$$

A subset S of $V(G)$ is said to be an independent set of G if each pair of vertices of S are not adjacent, and a matching in a graph G is a set of pairwise non-incident edges. The number of vertices in a maximum independent set of G is called the independence number of G, and the maximum size of a matching set of G is called the matching number of G.

For all notations not given here, we refer the reader to [4].

1.1. The degree-based invariants of graphs

Among all (vertex) degree-based graph invariants, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ [7] are two famous topological indices. They are defined as

$$M_1(G) = \sum_{v\in V(G)} (d(v))^2, \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d(u)d(v).$$

Later, Došlić [6] defined the first Zagreb coindex $\overline{M_1(G)}$ and the second Zagreb coindex $\overline{M_2(G)}$ of G as

$$\overline{M_1(G)} = \sum_{uv\notin E(G)} (d(u)+d(v)), \qquad \text{and} \qquad \overline{M_2(G)} = \sum_{uv\notin E(G)} d(u)d(v).$$

In 2010, Todeschini et al. [23] introduced the concepts of multiplicative Zagreb indices, as

$$\prod\nolimits_1^1(G) = \prod_{u\in V(G)} (d(u))^2, \text{ and } \prod\nolimits_2^1(G) = \prod_{u\in V(G)} (d(u))^{d(u)}.$$

Throughout this paper, a denotes a real number. As a generalization of $M_2(G)$, Bollobás and Erdős [3] gave the definition of general Randić index $R_a(G)$, where

$$R_a(G) = \sum_{uv\in E(G)} (d(u)d(v))^a.$$

Similarly, Li and Zheng [11] generalized the first Zagreb index to the zeroth-order general Randić index $R_a^0(G)$, where

$$R_a^0(G) = \sum_{u\in V(G)} (d(u))^a.$$

In particular, $R_{-1}^0(G)$ in [28] is called the inverse degree $ID(G)$ of G, $R_2^0(G)$ is just equal to $M_1(G)$, and $R_{-\frac{1}{2}}(G)$ in [22] is called the Randić index $R(G)$ of G.

Since $\sum_{uv\in E(G)}(d(u)+d(v)) = \sum_{v\in V(G)}(d(v))^2$, as a generalization of $M_1(G)$, in [36] the authors defined the general sum-connectivity index $\chi_a(G)$ of G as

$$\chi_a(G) = \sum_{uv\in E(G)} (d(u)+d(v))^a.$$

The reformulated first Zagreb index $EM_1(G)$ of G [21] is a slight modification to $\chi_2(G)$, where

$$EM_1(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^2.$$

Recently, Ali and Dimitrov in [1] generalized $EM_1(G)$ to the general Platt index $Pl_a(G)$ of G. Similarly, we can generalize $\prod_1^1(G)$ to $\prod_1^a(G)$, where

$$\prod\nolimits_1^a(G) = \prod_{u\in V(G)} (d(u))^a, \text{ and } Pl_a(G) = \sum_{uv\in E(G)} (d(u)+d(v)-2)^a.$$

In order to study on degree-based invariants of a graph, Wang in [25] proposed the concept of escalating function in the following way: a symmetric bivariate function $\varphi(x,y)$ defined on positive real numbers is said to be escalating (de-escalating) if

$$\varphi(x_1,x_2)+\varphi(y_1,y_2) \geq \ (resp.\ \leq)\ \varphi(x_2,y_1)+\varphi(x_1,y_2) \tag{1.3}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (1.3) is strict whenever $x_1 > y_1$ and $x_2 > y_2$. Furthermore, an escalating function $\varphi(x,y)$ is said to be a good escalating function [19], if $\varphi(x,y)$ satisfies

$$\frac{\partial\varphi(x,y)}{\partial x} > 0, \quad \frac{\partial^2\varphi(x,y)}{\partial x^2} \geq 0,$$

and

$$\varphi(x_1+1,x_2)+\varphi(x_1+1,y_1-1)\geq\varphi(x_2,y_1)+\varphi(x_1,y_1)$$

holds for any $x_1\geq y_1>0$ and $x_2\geq 1$. To extend the above definitions of degree-based invariants, Hollas [8] defined a new invariant $BID(G)$ of G as

$$BID(G)=\sum_{uv\in E(G)}\varphi(d(u),d(v)).$$

In the literature, $BID(G)$ denotes the Bond Incident Degree index of G in [1], and it is called the connectivity function of G in [25].

Let $f(x)$ be a function defined on positive real numbers. Inspired by the definition of $BID(G)$, we establish the notion of degree-function index $H_f(G)$ associated with $f(x)$, where

$$H_f(G)=\sum_{v\in V(G)}f(d(v)).$$

1.2. The distance-based invariants of graphs

The distance between u and v, denoted by $dist(u,v)$, is the number of edges in a shortest path from u to v. Among distance-based graph invariants of a graph G, the Wiener index $W(G)$, the hyper-Wiener index $WW(G)$, and the Harary index $H(G)$ are three famous topological indices (e.g., [29]), where

$$W(G)=\sum_{\{u,v\}\subseteq V(G)}dist(u,v),\quad H(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{dist(u,v)},\quad\text{and}$$
$$WW(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{2}(dist(u,v)+(dist(u,v))^2).$$

When $\psi(x)$ is a function defined on positive real numbers, then the (hyper-)Wiener and Harary indices can be unified [5] as the Q-index $W_\psi(G)$ of G, where

$$W_\psi(G)=\sum_{\{u,v\}\subseteq V(G)}\psi(dist(u,v)).$$

1.3. The general matrix of graphs

Let $A(G)$ and $D(G)$ be, respectively, the adjacency matrix and the diagonal matrix of a graph G. The signless Laplacian matrix of G is defined as $Q(G)=D(G)+A(G)$. Let $\rho(G)$ and $\mu(G)$ denote the largest eigenvalues of $A(G)$ and $Q(G)$, respectively. The spectral invariants $\rho(G)$ and $\mu(G)$ are widely known as the spectral radius and signless Laplacian spectral radius of G, respectively. Throughout this paper, b is a nonnegative real number. Following [17], we define $A(G)+bD(G)$ as the general matrix of G and we denote its largest eigenvalue by $\Theta(G,b)$. In the sequel, $\Theta(G,b)$ is also called the general spectral radius of G. Clearly, we have $\Theta(G,0)=\rho(G)$, and $\Theta(G,1)=\mu(G)$, as special instances of the general spectral radius.

1.4. The majorization theorem

Let $(x)=(x_1,x_2,\ldots,x_n)$ and $(y)=(y_1,y_2,\ldots,y_n)$ be two non-increasing sequences of real numbers. We write $(x)\trianglelefteq(y)$ if and only if $\sum_{i=1}^n x_i=\sum_{i=1}^n y_i$, and $\sum_{i=1}^j x_i\leq\sum_{i=1}^j y_i$ for all $j=1,2,\ldots,n$. Furthermore, we write $(x)\triangleleft(y)$ if and only if $(x)\trianglelefteq(y)$ and $(x)\neq(y)$. The ordering $\pi\trianglelefteq\pi'$ is called majorization [9,17,20].

Let $\Phi(G)$ be an invariant defined on G. If $\Phi(G)$ is maximum (resp., minimum) among all graphs in a given graph category $\mathcal{G}$, then we call G as a maximum (resp., minimum) extremal graph of $\mathcal{G}$. In what follows, when G and G' are two maximum (resp., minimum) extremal graphs of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, if $\pi\triangleleft\pi'$ implies that relationship $\Phi(G)<\Phi(G')$ (resp., $\Phi(G)>\Phi(G')$), then we say that $\Phi(G)$ satisfies the majorization theorem.

Hereafter, unless otherwise stated, as a (good) extremal graph we refer to one of the following definitions.

Definition 1.1. For a graph category $\mathcal{G}$, we say that G is an extremal graph of $\mathcal{G}$, if G satisfies either one of the following items:

(i) $BID(G)$ is maximum in $\mathcal{G}$ when $\varphi(x,y)$ is an escalating function;
(ii) $BID(G)$ is minimum in $\mathcal{G}$ when $\varphi(x,y)$ is a de-escalating function;
(iii) $\Theta(G,b)$ is maximum in $\mathcal{G}$ when $b\geq 0$;
(iv) $W_\psi(G)$ is maximum in $\mathcal{G}$ when $\psi(x)$ is a strictly nonnegative decreasing function;

(v) $W_\psi(G)$ is minimum in $\mathcal{G}$ when $\psi(x)$ is a strictly nonnegative increasing function;
(iv) $\overline{M_2(G)}$ is minimum in $\mathcal{G}$.

Definition 1.2. For a graph category $\mathcal{G}$, we say that G is a good extremal graph of $\mathcal{G}$, if G satisfies all of the following items:

(1) $\Theta(G, b)$ is largest in $\mathcal{G}$ for $b \geq 0$ when G is either a tree or a unicyclic graph;
(2) $\rho(G)$ is largest in $\mathcal{G}$ when G is a bicyclic graph;
(3) $\mu(G)$ is largest in $\mathcal{G}$ when G is a bicyclic graph;
(4) $BID(G)$ is maximum in $\mathcal{G}$ when $\varphi(x, y)$ is a good escalating function;
(5) $W_\psi(G)$ is maximum in $\mathcal{G}$ when $\psi(x)$ is a strictly nonnegative decreasing function;
(6) $W_\psi(G)$ is minimum in $\mathcal{G}$ when $\psi(x)$ is a strictly nonnegative increasing function;
(7) $H_f(G)$ is maximum in $\mathcal{G}$ when $f(x)$ is a strictly convex function on $x \geq 1$;
(8) $H_f(G)$ is minimum in $\mathcal{G}$ when $f(x)$ is a strictly concave function on $x \geq 1$;
(9) $\overline{M_1(G)}$ and $\overline{M_2(G)}$ are minimum in $\mathcal{G}$.

Extremal problems are an important topic in both topological graph theory and spectral graph theory. As observed in the literature (see, for instance, [13,29]), in many graph categories, several topological indices and spectral graph invariants share the same extremal graph(s). Therefore, a natural question arises:

Problem 1.1. Which is the unified method to identify the extremal graph(s) for as many as possible topological indices and spectral graph invariants in a given graph category?

As stated in [13,17,18] and here in the sequel, the majorization theorem is a strong and effective tool to deal with Problem 1.1. In this paper, we will apply the majorization theorem to determine a unified good extremal graph in the class of trees, unicyclic graphs and bicyclic graphs with fixed maximum degree, independence number, matching number, domination number and/or number of pendant vertices, respectively.

The organization of this paper is as follows. In Section 2, we give a survey on the recently appeared majorization theorems. In Section 3, we introduce the extremal c-cyclic graph in the class of graphs with given degree sequence π for $c \in \{0, 1, 2\}$. In Sections 4 and 5 we give the main results of this paper. In particular, in Section 4 we give a unified good extremal graph in the class of trees, unicyclic graphs and bicyclic graphs with fixed maximum degree, independence number, matching number, number of pendant vertices, respectively. In Section 5, we determine the unique unified good extremal graph in the class of trees, unicyclic graphs and bicyclic graphs with given domination number. Finally, in the last section we comment the results and we present three problems for further study in this topic.

2. Majorization theorems for graph invariants

A strictly convex function is a real valued function $g(x)$ defined on a convex set D such that

$$g(px + (1-p)y) < pg(x) + (1-p)g(y)$$

for all $0 < p < 1$ and all $x, y \in D$. Among all majorization theorems, the following one was given a long time ago in [20], and it is not restricted to graph invariants.

Theorem 2.1. *Let $(s) = (s_1, s_2, \ldots, s_n)$ and $(t) = (t_1, t_2, \ldots, t_n)$ be two non-increasing sequences of real numbers. If $(s) \lhd (t)$, then for any strictly convex function $g(x)$, we have $\sum_{i=1}^n g(s_i) < \sum_{i=1}^n g(t_i)$.*

Note that $-f(x)$ is a strictly convex function if and only if $f(x)$ is a strictly concave function. The subsequent result is an easy consequence of Theorem 2.1.

Theorem 2.2. *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$, and G and G' be two graphs with $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$.*

(i) If $f(x)$ is a strictly convex function on $x \geq 1$, then $H_f(G) < H_f(G')$;
(ii) If $f(x)$ is a strictly concave function on $x \geq 1$, then $H_f(G) > H_f(G')$.

Corollary 2.3. *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. If G and G' are two graphs with $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, then*

(i) $R^0_a(G) < R^0_a(G')$ holds for $a < 0$ or $a > 1$, and $R^0_a(G) > R^0_a(G')$ holds for $0 < a < 1$ (cf. [15]).
(ii) $\prod_a(G) < \prod_a(G')$ holds for $a < 0$, and $\prod_a(G) > \prod_a(G')$ holds for $a > 0$.
(iii) $\prod_2(G) < \prod_2(G')$ and $\overline{M_1(G)} > \overline{M_1(G')}$ (for the latter, see [14]).

Proof. Since (i) is proved in [15], it is sufficient to show (ii) and (iii).

Consider first (ii). Let $f(x) = a\ln(x)$. Then, $H_f(G) = \sum_{i=1}^{n} a\ln(d_i)$. It is easy to see that $\prod^{a}(G) < \prod^{a}(G')$ if and only if $H_f(G) < H_f(G')$. When $x \geq 1$, since $f''(x) = -\frac{a}{x^2}$, we conclude that $f(x)$ is a strictly convex function for $a < 0$, and it is a strictly concave function for $a > 0$. Now, the result follows from Theorem 2.2.

Consider next (iii). Since $\overline{M_1(G)} > \overline{M_1(G')}$ comes from [14], we only need to show that $\prod_{2}(G) < \prod_{2}(G')$. Let $f(x) = x\ln(x)$ and let $H_f(G) = \sum_{i=1}^{n} d_i\ln(d_i)$. Then, $\prod_{2}(G) < \prod_{2}(G')$ if and only if $H_f(G) < H_f(G')$. When $x \geq 1$, since $f''(x) = \frac{1}{x} > 0$, $f(x)$ is also a strictly convex function. Now, by Theorem 2.2, we can get the desired inequality. ■

Remark 2.4. When $\pi \lhd \pi'$, since $a = 2 > 0$, it follows from Corollary 2.3 (ii) that $\prod^{1}(G) > \prod^{1}(G')$ holds for any graphs $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$.

Theorem 2.5. *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. Let G and G' be a maximum extremal c-cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively.*

(i) For $c \in \{0, 1, 2\}$, if $\varphi(x, y)$ is a good escalating function, then $BID(G) < BID(G')$ (see [19]);
(ii) If $b \geq 0$ is a real number, then $\Theta(G, b) < \Theta(G', b)$ holds for $c \in \{0, 1\}$ (see [17]);
(iii) If $c = 2$, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$ (see [9,10]);
(iv) If $\psi(x)$ is a nonnegative and strictly decreasing function and $c = 0$, then $W_\psi(G) < W_\psi(G')$ (see [13,24,35]).

Theorem 2.6. *Let π and π' be two different non-increasing degree sequences with $\pi \lhd \pi'$. Let G and G' be a minimum extremal c-cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively.*

(i) If $\psi(x)$ is a nonnegative and strictly increasing function and $c = 0$, then $W_\psi(G) > W_\psi(G')$ (see [13,24,35]);
(ii) If $c \in \{0, 1, 2\}$, then $\overline{M_2(G)} > \overline{M_2(G')}$ (see [14]).

Remark 2.7. In [19], the authors show that the second Zagreb index $M_2(G)$ is good escalating, while $Pl_a(G)$ and $\chi_a(G)$ are good escalating for $a > 1$. Combining this with Theorem 2.5 (i), we conclude that $M_2(G)$, $Pl_a(G)$ and $\chi_a(G)$ satisfy the majorization theorem for $a > 1$.

Remark 2.8. As shown in the following (i)–(iv), there are many escalating and de-escalating graph invariants:

(i) $Pl_a(G)$ and $\chi_a(G)$ are escalating for $a > 1$ or $a < 0$ (see [19]);
(ii) $Pl_a(G)$ and $\chi_a(G)$ are de-escalating for $0 < a < 1$ (see [19]);
(iii) $R_a(G)$ is escalating for any real number $a \neq 0$ (see [19]);
(iv) the Atom-Bond Connectivity index defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

is de-escalating (see [34]).

Remark 2.9. Let G be a connected graph with m edges, n vertices and degree sequence π. Since $\overline{M_2(G)} = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$ and $\overline{M_1(G)} = 2m(n-1) - M_1(G)$ [6], $\overline{M_1(G)}$ is constant for any graph G of $\Gamma(\pi)$ and $\overline{M_2(G)}$ is minimum if $M_2(G)$ is maximum in $\Gamma(\pi)$.

3. The extremal graphs with given degree sequence

We begin this section by introducing the notion of *BFS*-graphs:

Definition 3.1 (*[12,33]*)**.** Let G be a connected graph. We say that G is a *BFS*-graph if there exists a vertex ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(G)$ satisfying:

(i) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i) = dist(v_i, v_1)$;
(ii) let $v \in N(u)\backslash N(w)$ and $z \in N(w)\backslash N(u)$ such that $h(v) = h(u) + 1$ and $h(z) = h(w) + 1$. If $u \prec w$, then $v \prec z$.

Hereafter, we use the symbol $p^{(q)}$ to define q copies of the real number p. In [32] the authors show that for any tree degree sequence π there exists a unique *BFS*-tree, here denoted by $T_M(\pi)$. The *BFS*-trees are also called greedy trees in the literature, e.g. [24].

In fact, we can also construct a unique unicyclic *BFS*-graph $U_M(\pi)$ by the following breadth-first-search method for any unicyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$ [2,16]: The unique cycle of $U_M(\pi)$ is a

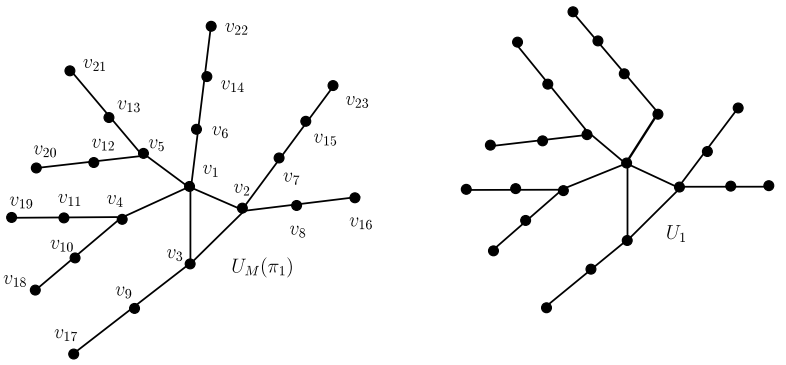


Fig. 3.1. The unicyclic graphs $U_M(\pi_1)$ and U_1.

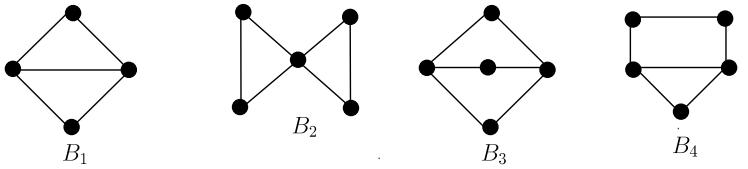


Fig. 3.2. The bicyclic graphs B_1, B_2, B_3 and B_4.

triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Select the vertex v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices v_2, v_3, v_4, v_5,..., v_{d_1+1} as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$. Let $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$ and $N(v_3) = \{v_1, v_2, v_{d_1+d_2}, \ldots, v_{d_1+d_2+d_3-3}\}$. Then, append $d_4 - 1$ vertices to v_4 such that $N(v_4) = \{v_1, v_{d_1+d_2+d_3-2}, \ldots, v_{d_1+d_2+d_3+d_4-4}\}$, and so on. Informally, the *BFS*-unicyclic graph is constructed as a *BFS*-tree by allowing an edge between v_2 and v_3. As an example, consider the unicyclic degree sequence $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, $U_M(\pi_1)$ is depicted in Fig. 3.1 [16].

In what follows, we introduce the extremal c-cyclic graphs in the class of c-cyclic graphs with given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ for $c \in \{0, 1, 2\}$. When $c \in \{0, 1\}$, by Remarks 2.7 and 2.9, we have the following two theorems:

Theorem 3.1. *In the class of trees with given degree sequence π*

(i) $T_M(\pi)$ is the unique extremal tree with largest general spectral radius for $b \geq 0$ (cf. [17]);
(ii) $T_M(\pi)$ is an extremal tree of BID(G) (cf. [19,25]), $W_\psi(G)$ (cf. [13,24,35]), and $\overline{M_2(G)}$, respectively.

Theorem 3.2. *In the class of unicyclic graphs with given degree sequence π, if $d_n = 1$ then:*

(i) $U_M(\pi)$ is the unique extremal unicyclic graph with largest general spectral radius for $b \geq 0$ (cf. [17]);
(ii) $U_M(\pi)$ is an extremal unicyclic graph of BID(G) and $\overline{M_2(G)}$, respectively (cf. [19,31]).

Denote by $\mathcal{R}(G)$ the reduced graph obtained from G by recursively deleting pendant vertices to the resultant graph until no pendant vertices remain. If $c \geq 1$ and G is a (connected) c-cyclic graph, then $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a (connected) c-cyclic graph.

Some paths P_{l_1}, P_{l_2}, ..., P_{l_k} are said to have almost equal lengths if their lengths pairwise differ at most by 1, that is, $|l_i - l_j| \leq 1$ for $1 \leq i < j \leq k$. Let B_1, B_2, B_3 and B_4 be the four bicyclic graphs depicted in Fig. 3.2. If $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence with $d_n = 1$, then $\sum_{i=1}^{n} d_i = 2n + 2$ by (1.1), which implies that π should be one of the following two cases. When $d_n = 1$, we construct a special bicyclic graph $B_M(\pi)$ of $\Gamma(\pi)$ as follows:

(i) If $d_n = 1$ and $d_1 \geq d_2 \geq 3$, then let $B_M(\pi)$ be a *BFS*-graph such that $\mathcal{R}(B_M(\pi)) = B_1$ and the remaining vertices appear in a *BFS*-ordering.
(ii) If $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$, then let $B_M(\pi)$ be the bicyclic graph with n vertices obtained from B_2 by attaching $d_1 - 4$ paths of almost equal lengths to the 4-vertex of B_2.

For extremal bicyclic graphs, we have the following theorem:

Theorem 3.3. *In the class of bicyclic graphs with given degree sequence π, if $d_n = 1$, then:*

(i) $B_M(\pi)$ is the unique extremal graph with largest general spectral radius for $b \geq 0$ (cf. [17]);
(ii) $B_M(\pi)$ is an extremal bicyclic graph of BID(G) and $\overline{M_2(G)}$, respectively (cf. [19]).

In [17,19], the structure of extremal graphs in the class of c-cyclic graphs for $c \geq 0$ has been studied, as well. At the end of this section, we would like to point out that the *BFS*-graph is just an extremal graph of $BID(G)$, but it is not the unique one. We recall the example given in [16]: for $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, it is easy to see that $M_2(U_1) = M_2(U_M(\pi_1))$ and $U_1 \neq U_M(\pi_1)$, where U_1 and $U_M(\pi_1)$ are depicted in Fig. 3.1.

4. The good extremal graphs with given graph invariants

Let $\mathcal{G}$ be a graph category. If $\pi_{\max}$ is the degree sequence of a graph $G \in \mathcal{G}$ such that $\pi \lhd \pi_{\max}$ holds for any other degree sequence π of these graphs in $\mathcal{G}$, then $\pi_{\max}$ is called the largest degree sequence of $\mathcal{G}$.

Let $S_n^{(0)}$ be the star with n vertices, $S_n^{(1)}$ be the unicyclic graph obtained by adding an edge to $S_n^{(0)}$, and let $S_n^{(2)}$ be the bicyclic graph obtained from B_1 by attaching $n-4$ isolated vertices to one 3-vertex of B_1 (or, by adding two incident edges to $S_n^{(0)}$).

Theorem 4.1. *If $n \geq 4$ and $c \in \{0, 1, 2\}$, then $S_n^{(c)}$ is the unique good extremal c-cyclic graph among all c-cyclic graphs with n vertices.*

Proof. In view of (1.1), it is easy to see that $\pi = (n-1, 1^{(n-1)})$, $\pi' = (n-1, 2^{(2)}, 1^{(n-3)})$ and $\pi'' = (n-1, 3, 2^{(2)}, 1^{(n-4)})$ are the largest sequences among all the degree sequences of trees, unicyclic graphs and bicyclic graphs on n vertices, respectively. Furthermore, it is easy to check that

$$\Gamma(\pi) = \{S_n^{(0)}\}, \quad \Gamma(\pi') = \{S_n^{(1)}\}, \quad \text{and } \Gamma(\pi'') = \{S_n^{(2)}\}.$$

Hence, the result follows from Theorems 2.2–2.6 and Remarks 2.7 and 2.9. ■

Let $F_n^{(0)}(k)$ (resp., $F_n^{(1)}(k)$, $F_n^{(2)}(k)$) be the tree (resp., unicyclic graph, bicyclic graph) with n vertices and k pendant vertices obtained by attaching k paths of almost equal lengths to an isolated vertex (resp., a vertex of C_3, the 4-vertex of B_2).

Theorem 4.2. *If $k \geq 1$ and $c \in \{0, 1, 2\}$, then $F_n^{(c)}(k)$ is a good extremal c-cyclic graph among all c-cyclic graphs with n vertices and k pendant vertices such that $n \geq k + 1 + 2c$.*

Proof. In [15] it is proved that $(k + 2c, 2^{(n-k-1)}, 1^{(k)})$ is the largest degree sequence among all the degree sequences of c-cyclic graphs with n vertices and k pendant vertices. Since $\overline{M_1(G)}$ is a constant for any graph having the same degree sequence by Remark 2.9, the result follows from Theorems 2.2–2.6 and 3.1–3.3. ■

Let $V_\Delta(G)$ be the set of Δ-vertices, where Δ is the largest degree of G, and let $G[X]$ be the subgraph of G induced by $X \subseteq V(G)$. In the sequel, let $G_M(n, \Delta)$ be the graph with n vertices and maximum degree Δ satisfying the following four conditions:

(i) $G_M(n, \Delta)$ is a *BFS*-graph with the maximum degree vertex v_1 as its root. If $G_M(n, \Delta)$ is a unicyclic graph, then $\mathcal{R}(G_M(n, \Delta)) = C_3$, where $V(C_3) = \{v_1, v_2, v_3\}$; If $G_M(n, \Delta)$ is a bicyclic graph, then $\mathcal{R}(G_M(n, \Delta)) = B_1$;
(ii) All pendant vertices of $G_M(n, \Delta)$ lie on the last or the second last layer;
(iii) If $V(\mathcal{R}(G_M(n, \Delta))) \not\subseteq V_\Delta(G)$, then all the vertices of $G_M(n, \Delta)$ outside $\mathcal{R}(G_M(n, \Delta))$ are pendant vertices. Furthermore, if $v_2 \notin V_\Delta(G)$, then $d_{G_M(n,\Delta)}(v_3) = 2$ and $G[\{v_1, v_2, v_3\}] \cong C_3$; If $v_2 \in V_\Delta(G)$, $v_3 \notin V_\Delta(G)$ and $G_M(n, \Delta)$ is a bicyclic graph, then $d_{G_M(n,\Delta)}(v_4) = 2$;
(iv) All vertices of $V(G) \setminus (V(\mathcal{R}(G_M(n, \Delta))) \cup V_\Delta(G))$, except for at most one d-vertex, are pendant vertices. Furthermore, if such a d-vertex exists, then it must belong to the second last layer, where $1 < d < \Delta$.

Theorem 4.3. *In the class of c-cyclic graphs with n vertices and maximum degree Δ, if $\Delta \geq 3$ and $c \in \{0, 1, 2\}$, then $G_M(n, \Delta)$ is a good extremal graph.*

Proof. It has been shown that the degree sequence of $G_M(n, \Delta)$ is the largest among all degree sequences of c-cyclic graphs, with $c \in \{0, 1, 2\}$, n vertices and maximum degree Δ (see Corollary 3.7 of [32] for $c = 0$, Theorem 4.2 of [33] for $c = 1$ and Corollary 3.12 of [9] for $c = 2$). Furthermore, $\overline{M_1(G)}$ is a constant for any graph with the same degree sequence by Remark 2.9. Hence, the result follows from Theorems 2.2–2.6 and 3.1–3.3. ■

Let G be a connected graph with $v \in V(G)$, and let P_k be a path on k vertices such that G and P_k are vertex-disjoint. Let G^* obtained from G and P_k by adding one edge between v and one end vertex of P_k. If so, we say that G^* is obtained by attaching the path P_k to vertex v of G. As shown in Fig. 4.1, let F_1 and F_2 be two c-cyclic graphs, where $c \geq 1$. Hereafter, let $S_1(c; s, t)$ (resp., $S_2(c; s, t)$) be the c-cyclic graph obtained by attaching s paths of lengths one and t isolated vertices, respectively, to the vertex v_1 of F_1 (resp., F_2). If $c = 0$, then $s + t \geq 2$ and $S_1(0; s, t)$ is the tree obtained by attaching s paths of lengths one and t isolated vertices, respectively, to a single common vertex. As an example, the graph $S_1(0; 3, 2)$ is depicted in Fig. 4.1.

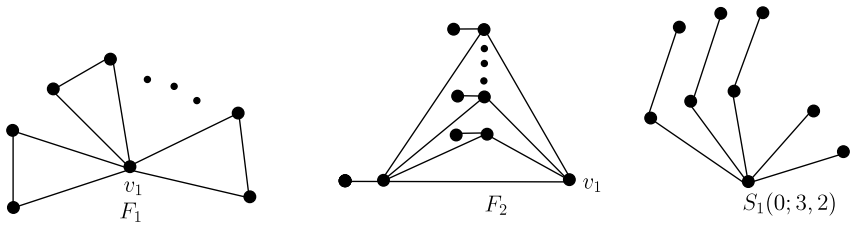


Fig. 4.1. The c-cyclic graphs F_1 and F_2, and the tree $S_1(0;3,2)$.

For $s \geq 2$, let $B_1(s,t)$ be the bicyclic graph obtained from $S_1(1;s,t)$ by adding one edge between two 2-vertices in $V(S_1(1;s,t))\backslash V(C_3)$. For $s \geq 1$, let $B_2(s,t)$ be the bicyclic graph obtained from $S_1(1;s,t)$ by adding one edge between one 2-vertex of $V(C_3)$ and one 2-vertex of $V(S_1(1;s,t))\backslash V(C_3)$.

Similarly to [30], we simplify the notation by writing $T(n,\alpha)$, $U_1(n,\alpha)$ and $U_2(n,\alpha)$ instead of $S_1(0;n-1-\alpha,2\alpha+1-n)$, $S_1(1;n-\alpha-2,2\alpha+1-n)$ and $S_2(1;n-\alpha-3,2\alpha+1-n)$, respectively. For the same reason, $B_1(n-\alpha-2,2\alpha+1-n)$, $B_2(n-\alpha-2,2\alpha+1-n)$, $S_1(2;n-\alpha-3,2\alpha+1-n)$ and $S_2(2;n-\alpha-4,2\alpha+1-n)$ are denoted by $Z_1(n,\alpha)$, $Z_2(n,\alpha)$, $Z_3(n,\alpha)$ and $Z_4(n,\alpha)$, respectively.

Theorem 4.4. *In the class of c-cyclic graphs with n vertices and independence number $\alpha \geq \frac{n}{2}$, let G be a good extremal graph, then*

(i) $G = T(n,\alpha)$ *when* $c = 0$ *and* $n \geq 3$;
(ii) $G \in \{U_1(n,\alpha),\ U_2(n,\alpha)\}$ *when* $c = 1$ *and* $3 \leq \alpha \leq n-3$;
(iii) $G \in \{Z_1(n,\alpha),\ Z_2(n,\alpha),\ Z_3(n,\alpha),\ Z_4(n,\alpha)\}$ *when* $c = 2$ *and* $4 \leq \alpha \leq n-4$.

Proof. Let $\pi_1 = (\alpha, 2^{(n-\alpha-1)}, 1^{(\alpha)})$, $\pi_2 = (\alpha+1, 2^{(n-\alpha)}, 1^{(\alpha-1)})$, $\pi_3 = (\alpha, 3^{(2)}, 2^{(n-\alpha-3)}, 1^{(\alpha)})$, $\pi_4 = (\alpha+1, 3^{(2)}, 2^{(n-\alpha-2)}, 1^{(\alpha-1)})$, $\pi_5 = (\alpha+2, 2^{(n-\alpha+1)}, 1^{(\alpha-2)})$, and $\pi_6 = (\alpha, 4, 3^{(2)}, 2^{(n-\alpha-4)}, 1^{(\alpha)})$. Let $\pi^{(c)}_{\max}$ be the largest degree sequence among all the degree sequences of graphs in the class of c-cyclic graphs with n vertices and independence number α. In [30], it is shown that $\pi^{(0)}_{\max} = \pi_1$, $\pi^{(1)}_{\max} \in \{\pi_2, \pi_3\}$ and $\pi^{(2)}_{\max} \in \{\pi_4, \pi_5, \pi_6\}$. Let $\Gamma(\pi,\alpha)$ be the set of connected graphs with n vertices, independence number α and degree sequence π. From [30], we have that $\Gamma(\pi_1,\alpha) = \{T(n,\alpha)\}$, $\Gamma(\pi_2,\alpha) = \{U_1(n,\alpha)\}$, $\Gamma(\pi_3,\alpha) = \{U_2(n,\alpha)\}$, $\Gamma(\pi_4,\alpha) = \{Z_1(n,\alpha), Z_2(n,\alpha)\}$, $\Gamma(\pi_5,\alpha) = \{Z_3(n,\alpha)\}$, and $\Gamma(\pi_6,\alpha) = \{Z_4(n,\alpha)\}$.

In what follows, we restrict the proof to the bicyclic case, as the cases for trees and unicyclic graphs can be similarly proved.

Let B be a bicyclic graph with degree sequence π and independence number α. Since $\alpha \geq \frac{n}{2}$, and in view of Theorem 3.3, the graphs $Z_2(n,\alpha)$, $Z_3(n,\alpha)$ and $Z_4(n,\alpha)$ are extremal graphs of $\Gamma(\pi_4)$, $\Gamma(\pi_5)$ and $\Gamma(\pi_6)$, respectively. Clearly, $\Gamma(\pi_4,\alpha) \subseteq \Gamma(\pi_4)$, $\Gamma(\pi_5,\alpha) \subseteq \Gamma(\pi_5)$ and $\Gamma(\pi_6,\alpha) \subseteq \Gamma(\pi_6)$, and hence $Z_2(n,\alpha)$, $Z_3(n,\alpha)$ and $Z_4(n,\alpha)$ are also extremal graphs of $\Gamma(\pi_4,\alpha)$, $\Gamma(\pi_5,\alpha)$ and $\Gamma(\pi_6,\alpha)$, respectively.

If $\pi \notin \{\pi_4, \pi_5, \pi_6\}$, since $\pi^{(2)}_{\max} \in \{\pi_4, \pi_5, \pi_6\}$, by Theorems 2.2–2.6 we get that B is not a good extremal graph. Hence, all good extremal graphs belong to $\{\Gamma(\pi_4,\alpha),\ \Gamma(\pi_5,\alpha),\ \Gamma(\pi_6,\alpha)\}$. Recall that $\Gamma(\pi_4,\alpha) = \{Z_1(n,\alpha), Z_2(n,\alpha)\}$, $\Gamma(\pi_5,\alpha) = \{Z_3(n,\alpha)\}$, and $\Gamma(\pi_6,\alpha) = \{Z_4(n,\alpha)\}$. This completes the proof. ■

In order to simplify the notation, let $S_1(0;\beta-1,n+1-2\beta)$, $S_1(1;\beta-2,n+1-2\beta)$, $S_2(1;\beta-3,n+1-2\beta)$, $B_1(\beta-2,n+1-2\beta)$, $B_2(\beta-2,n+1-2\beta)$, $S_1(2;\beta-3,n+1-2\beta)$ and $S_2(2;\beta-4,n+1-2\beta)$ be denoted by $T(n;\beta)$, $U_1(n;\beta)$, $U_2(n;\beta)$, $Z_1(n;\beta)$, $Z_2(n;\beta)$, $Z_3(n;\beta)$ and $Z_4(n;\beta)$, respectively.

Theorem 4.5. *In the class of c-cyclic graphs with n vertices and matching number β, let G be a good extremal graph. Then*

(i) $G = T(n;\beta)$ *when* $c = 0$ *and* $n \geq 3$;
(ii) $G \in \{U_1(n;\beta),\ U_2(n;\beta)\}$ *when* $c = 1$ *and* $3 \leq \beta \leq n-3$;
(iii) $G \in \{Z_1(n;\beta),\ Z_2(n;\beta),\ Z_3(n;\beta),\ Z_4(n;\beta)\}$ *when* $c = 2$ *and* $4 \leq \beta \leq n-4$.

Proof. Let $\pi_1 = (n-\beta, 2^{(\beta-1)}, 1^{(n-\beta)})$, $\pi_2 = (n-\beta+1, 2^{(\beta)}, 1^{(n-\beta-1)})$, $\pi_3 = (n-\beta, 3^{(2)}, 2^{(\beta-3)}, 1^{(n-\beta)})$, $\pi_4 = (n-\beta+1, 3^{(2)}, 2^{(\beta-2)}, 1^{(n-\beta-1)})$, $\pi_5 = (n-\beta+2, 2^{(\beta+1)}, 1^{(n-\beta-2)})$ and $\pi_6 = (n-\beta, 4, 3^{(2)}, 2^{(\beta-4)}, 1^{(n-\beta)})$, and let $\pi^{(c)}_{\max}$ be the largest degree sequence among all the degree sequences of graphs in the class of c-cyclic graphs with n vertices and matching number β. Again from [30], we get that $\pi^{(0)}_{\max} = \pi_1$, $\pi^{(1)}_{\max} \in \{\pi_2, \pi_3\}$ and $\pi^{(2)}_{\max} \in \{\pi_4, \pi_5, \pi_6\}$.

For $1 \leq i \leq 6$, let $\Gamma(\pi_i,\beta)$ be the connected graphs with n vertices, matching number β and degree sequence π_i. In [30], it is shown that $\Gamma(\pi_1,\beta) = \{T(n;\beta)\}$, $\Gamma(\pi_2,\beta) = \{U_1(n;\beta)\}$, $\Gamma(\pi_3,\beta) = \{U_2(n;\beta)\}$, $\Gamma(\pi_4,\beta) = \{Z_1(n;\beta), Z_2(n;\beta)\}$, and $\Gamma(\pi_5,\beta) = \{Z_3(n;\beta)\}$, and $\Gamma(\pi_6,\beta) = \{Z_4(n;\beta)\}$.

In view of Theorems 3.1–3.3 and by $\beta \leq \lfloor \frac{n}{2} \rfloor$, we can conclude that $T(n;\beta)$, $U_1(n;\beta)$, $U_2(n;\beta)$, $Z_2(n;\beta)$, $Z_3(n;\beta)$ and $Z_4(n;\beta)$ are extremal graphs of $\Gamma(\pi_1)$, $\Gamma(\pi_2)$, $\Gamma(\pi_3)$, $\Gamma(\pi_4)$, $\Gamma(\pi_5)$ and $\Gamma(\pi_6)$, respectively. By Theorems 2.2–2.6, all good extremal graphs belong to $\Gamma(\pi_1,\beta)$, $\Gamma(\pi_2,\beta)$, $\Gamma(\pi_3,\beta)$, $\Gamma(\pi_4,\beta)$, $\Gamma(\pi_5,\beta)$ and $\Gamma(\pi_6,\beta)$. This completes the proof. ■

Remark 4.6. In [30], the proofs of the main results, namely, Theorems 3.1–3.3 and 4.1–4.3, are not complete. For the complete proofs we refer the reader to the proofs of Theorems 4.4 and 4.5. Furthermore, the condition $\alpha \geq \frac{n}{2}$ should be added, as well.

5. The good extremal graphs with given domination number

In some graph categories $\mathcal{G}$, thought we have the majorization theorem for the graph invariant $\Phi(G)$, it is difficult to identify the corresponding extremal graph (not restricted to Definition 1.1) for $\Phi(G)$ in $\mathcal{G}$. The main reason is that neither $\pi_{\max}$, nor the extremal graph of $\Phi(G)$ in $\Gamma(\pi_{\max})$ are easily identified. From the subsequent proofs, we will see that trees, unicyclic graphs or bicyclic graphs with fixed domination number are such graph categories. Throughout this section, let $\pi_1 = (2c+p, 2^{(n-p-1)}, 1^{(p)})$, $\pi_2 = (2c+p-2, 3^{(2)}, 2^{(n-p-3)}, 1^{(p)})$ and $\pi_3 = (2c+p-4, 4, 3^{(2)}, 2^{(n-p-4)}, 1^{(p)})$. The following Lemmas 5.1–5.4 can be found in [30].

Lemma 5.1. *Let G be a c-cyclic graph with n vertices, p pendant vertices and degree sequence π. If $\pi \neq \pi_1$, then $\pi \lhd \pi_1$. Furthermore,*

$$(2c+p, 2^{(n-p-1)}, 1^{(p)}) \lhd (2c+p+1, 2^{(n-p-2)}, 1^{(p+1)}).$$

Lemma 5.2. *Let G be a c-cyclic graph with n vertices, p pendant vertices and degree sequence π such that every vertex of $\mathcal{R}(G)$ is a quasi-pendant vertex. Then, the following holds:*

(i) If $\pi \neq \pi_2$ and $c \geq 1$, then $\pi \lhd \pi_2$.
(ii) If $\pi \neq \pi_3$ and $c \geq 2$, then $\pi \lhd \pi_3$.

Lemma 5.3. *Let G be a tree with degree sequence $(s+t, 2^{(s)}, 1^{(s+t)})$, where $s+t \geq 2$. If every 2-vertex of G is a quasi-pendant vertex, then $G \cong S_1(0; s, t)$.*

Lemma 5.4. *Let G be a c-cyclic graph with degree sequence $(c+1+s+t, c+2, 3^{(c)}, 2^{(s)}, 1^{(s+t+c+1)})$, where $c \geq 1$ and $s+t \geq 1$. If every non-pendant vertex of G is a quasi-pendant vertex, then $G \cong S_2(c; s, t)$.*

Lemma 5.5. *For any connected graph G on at least 3 vertices, G has at least one minimum dominating set D containing no pendant vertices.*

Proof. To achieve the proof of the lemma, it is sufficient to show the following claim:

Claim 1. *Let D be a minimum dominating set of G. If D contains exactly p (≥ 1) pendant vertices, then G also has a minimum dominating set D' containing precisely $p-1$ pendant vertices.*

Proof of Claim 1. Let D be an arbitrary minimum dominating set of G such that D contains exactly p (≥ 1) pendant vertices. Let u be a pendant vertex of D, and suppose that $N(u) = \{v\}$. Evidently, we have $v \notin D$, otherwise $D\backslash\{u\}$ is also another dominating set of G, a contradiction to the choice of D. Therefore, $D' = (D\backslash\{u\}) \cup \{v\}$ is another dominating set of G such that D' contains precisely $p-1$ pendant vertices. That is, Claim 1 holds. ■

By Lemma 5.5, the number of non-pendant vertices of a graph G is at least $\gamma(G)$. Thus, if G contains exactly p pendant vertices, then

$$\gamma(G) \leq n - p. \tag{5.1}$$

Lemma 5.6. *If G is a connected graph with n vertices, p pendant vertices and domination number γ, then $p = n - \gamma$ if and only if every non-pendant vertex is a quasi-pendant vertex.*

Proof. If $p = n - \gamma$, then the number of non-pendant vertices is equal to $n - p = \gamma$. Thus, the class of non-pendant vertices form a dominating set, say D, of G. Let u be a non-pendant vertex, where u is not a quasi-pendant vertex. In this case, all the neighbor vertices of u must be non-pendant vertices. Then, $D\backslash\{u\}$ is a dominating set of G and we have $|D\backslash\{u\}| = n - p - 1 < \gamma$, a contradiction.

Conversely, assume that every non-pendant vertex is a quasi-pendant vertex. By Lemma 5.5, G contains a minimum dominating set D, where D has no pendant vertex. Since all pendant vertices must be dominated, then D must contain all quasi-pendant vertices, that is, $\gamma = |D| = n - p$. ■

Lemma 5.7. *If G is a connected graph with n vertices, p pendant vertices and domination number γ, then $p = n - \gamma - 1$ if and only if each of the other non-pendant vertices is a quasi-pendant vertex, except for exactly one non-pendant vertex.*

Proof. Let S be the set of non-pendant vertices of G. Assume that except for exactly one non-pendant vertex, each of non-pendant vertices is a quasi-pendant vertex, then any dominating set containing no pendant vertex has at least $n-p-1$ vertices, that is, $\gamma \geq n - p - 1$ by Lemma 5.5. Let u_0 be the non-pendant vertex of G such that u_0 is not a quasi-pendant vertex. Since u_0 must be adjacent to some vertices of $S\backslash\{u_0\}$, $S\backslash\{u_0\}$ is a dominating set of G. Thus, $\gamma \leq |S\backslash\{u_0\}| = n-p-1$, and hence $\gamma = n - p - 1$.

In what follows, we suppose that $p = n - \gamma - 1$. Then, G contains exactly $\gamma + 1$ non-pendant vertices, and we suppose that G contains exactly t non-pendant vertices which are not quasi-pendant vertices.

Case 1. $t \geq 2$

Let u and v be two non-pendant vertices such that both u and v are not quasi-pendant vertices. Since $d(u) \geq 2$ and $d(v) \geq 2$, $N(u) \setminus \{v\} \neq \emptyset$ and $N(v) \setminus \{u\} \neq \emptyset$. In this case, $S\backslash\{u, v\}$ is a dominating set of G, and $|S\backslash\{u, v\}| = \gamma - 1$, a contradiction.

Case 2. $t = 0$

In this case, every vertex of S is a quasi-pendant vertex. Thus, to dominate these pendant vertices, we need at least $\gamma + 1 = |S|$ vertices. By Lemma 5.5, any minimum dominating set of G contains at least $\gamma + 1$ vertices, a contradiction.

Consequently, $t = 1$ and the result follows. ■

Hereafter, denote by $\pi_4 = (n - \gamma, 2^{(\gamma-1)}, 1^{(n-\gamma)})$, $\pi_5 = (n - \gamma, 3^{(2)}, 2^{(\gamma-3)}, 1^{(n-\gamma)})$, $\pi_6 = (n - \gamma, 4, 3^{(2)}, 2^{(\gamma-4)}, 1^{(n-\gamma)})$ $\pi_7 = (n - \gamma, 3, 2^{(\gamma+1)}, 1^{(n-\gamma-3)})$, and $\pi_8 = (n - \gamma, 4, 2^{(\gamma)}, 1^{(n-\gamma-2)})$.

Lemma 5.8. *Let U be a unicyclic graph with n vertices, p pendant vertices, domination number γ and degree sequence π. If $\pi \neq \pi_5$ and $n \geq 6$, then $\pi \lhd \pi_5$.*

Proof. Suppose that the degree sequence of U is $\pi = (d_1, d_2, \ldots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-p} \geq 2$ and C_g is the unique cycle of U, where $g \geq 3$. By (5.1), we have $p \leq n - \gamma$.

If $p = n-\gamma$, then every non-pendant vertex is a quasi-pendant vertex by Lemma 5.6. In this case, $\pi \lhd \pi_5$ follows from Lemma 5.2 (i).

If $p = n - \gamma - 1$, then $\pi = (d_1, d_2, \ldots, d_{\gamma+1}, 1^{(n-\gamma-1)})$, where $d_1 \geq d_2 \geq \cdots \geq d_{g-1} \geq 3$ by Lemma 5.7. Note that $g \geq 3$. Thus,

$$\pi \trianglelefteq (n - \gamma + 3 - g, 3^{(g-2)}, 2^{(\gamma+2-g)}, 1^{(n-\gamma-1)}) \trianglelefteq (n - \gamma, 3, 2^{(\gamma-1)}, 1^{(n-\gamma-1)}) \lhd \pi_5.$$

Otherwise, $p \leq n - \gamma - 2$. By Lemma 5.1, we have $\pi \trianglelefteq (n - \gamma, 2^{(\gamma+1)}, 1^{(n-\gamma-2)}) \lhd \pi_5$. ■

Next, we consider the case of bicyclic graphs. Let B be a bicyclic graph with n vertices, p pendant vertices and domination number γ. In later discussion, we always suppose that C_s and C_t are two cycles of B, where $s \geq 3$ and $t \geq 3$, and the number of common vertices between C_s and C_t is equal to r_{st}, that is, $|V(C_s) \cap V(C_t)| = r_{st}$. Let $S_1(B) = \{v : N(v) \subseteq V(C_s) \cup V(C_t)$ and $d(v) = 1\}$, $S_2(B) = S_1(B) \cup V(C_s) \cup V(C_t)$ and $S_3(B) = V(G) \setminus S_2(B)$. For a bicyclic graph B, let D_1 be the set of non-pendant vertices not lying on any cycle of B. From these definitions, it is easy to see that

Lemma 5.9. *The vertices of $S_3(B) \setminus D_1$ are dominated by D_1 and $|D_1| \leq n - p - (s + t) + r_{st}$.*

Lemma 5.10. *If $r_{st} = 0$ and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3 in B, then $\gamma \leq n - p + q - 6$.*

Proof. Let P be the path connecting C_s and C_t such that $V(P) \cap V(C_s) = \{u_0\}$ and $V(P) \cap V(C_t) = \{v_0\}$. Then, $d_B(u_0) \geq 3$ and $d_B(v_0) \geq 3$. Let $\{z_1, z_2, \ldots, z_{q-2}\}$ be the $q - 2$ vertices of $(V(C_s) \cup V(C_t))\backslash\{u_0, v_0\}$ with degrees at least 3 in B. Suppose that $N(u_0) \cap V(C_s) = \{u_1, u_2\}$ and $N(v_0) \cap V(C_t) = \{w_1, w_2\}$. Since any vertex of $V(C_s) \cup V(C_t)$ can dominate at least two vertices, there is a dominating set, say D_2, of size at most $\lceil \frac{s-3}{3} \rceil$ for the vertices of $V(C_s)\backslash(\{u_0, u_1, u_2\} \cup D_2)$. Similarly, there is a dominating set, say D_3, of size at most $\lceil \frac{t-3}{3} \rceil$ for the vertices of $V(C_t) \setminus (\{v_0, w_1, w_2\} \cup D_3)$. Now, $D_4 = \{u_0, v_0, z_1, z_2, \ldots, z_{q-2}\} \cup D_2 \cup D_3$ is a dominating set of $B[S_2(B)]$. It is easy to see that

$$|D_4| \leq q + \left\lceil \frac{s-3}{3} \right\rceil + \left\lceil \frac{t-3}{3} \right\rceil.$$

Combining with $S_2(B) \cup S_3(B) = V(B)$ and Lemma 5.9, we can conclude that $D = D_1 \cup D_4$ is a dominating set of B such that

$$\begin{aligned}\gamma &\le |D| \le |D_1| + |D_4| \\ &= n - p - (s+t) + q + \left\lceil \frac{s-3}{3} \right\rceil + \left\lceil \frac{t-3}{3} \right\rceil \\ &= n - p + q - 2 - \left\lfloor \frac{2s}{3} \right\rfloor - \left\lfloor \frac{2t}{3} \right\rfloor \le n - p + q - 6,\end{aligned}$$

and so the result follows. ■

Lemma 5.11. *If $r_{st} = 1$ and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3 in B, then $\gamma \le n - p + q - 5$.*

Proof. We suppose that $V(C_s) \cap V(C_t) = \{w_0\}$ with $N(w_0) \cap V(C_s) = \{u_1, u_2\}$ and $N(w_0) \cap V(C_t) = \{w_1, w_2\}$. Then, $d_B(w_0) \ge 4$. We may suppose that $\{z_1, z_2, \ldots, z_{q-1}\}$ are the other vertices of $V(C_s) \cup V(C_t)$ with degrees at least 3 in B.

Since each vertex of $V(C_s) \cup V(C_t)$ can dominate at least two vertices, there is a dominating set, say D_2, of size at most $\lceil \frac{s-3}{3} \rceil$ for the vertices of $V(C_s) \setminus (\{w_0, u_1, u_2\} \cup D_2)$. Similarly, there is a dominating set, say D_3, of size at most $\lceil \frac{t-3}{3} \rceil$ for the vertices of $V(C_t) \setminus (\{w_0, w_1, w_2\} \cup D_3)$. Now, $D_4 = \{w_0, z_1, z_2, \ldots, z_{q-1}\} \cup D_2 \cup D_3$ is a dominating set of $B[S_2(B)]$. It is easy to see that

$$|D_4| \le q + \left\lceil \frac{s-3}{3} \right\rceil + \left\lceil \frac{t-3}{3} \right\rceil.$$

As $S_2(B) \cup S_3(B) = V(B)$ and Lemma 5.9, $D = D_1 \cup D_4$ is a dominating set of B and

$$\begin{aligned}\gamma &\le |D| \le |D_1| + |D_4| \\ &= n - p - (s+t) + 1 + q + \left\lceil \frac{s-3}{3} \right\rceil + \left\lceil \frac{t-3}{3} \right\rceil \\ &= n - p + q - 1 - \left\lfloor \frac{2s}{3} \right\rfloor - \left\lfloor \frac{2t}{3} \right\rfloor \le n - p + q - 5,\end{aligned}$$

which implies the claimed result. ■

We suppose that $V(B) = \{v_1, v_2, \ldots, v_n\}$, where $d(v_1) \ge d(v_2) \ge \cdots \ge d(v_n)$.

Lemma 5.12. *If $r_{st} \ge 2$ and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3, then $\gamma \le n - p + q - 4$, where the equality implies that $\mathcal{R}(B) = B_1$ and $d_G(v_1) \ge d_G(v_2) \ge 4$.*

Proof. By symmetry, we may suppose that $V(C_s) \cap V(C_t) = \{u_1, u_2, \ldots, u_{r_{st}}\}$, $s \ge t \ge 2(r_{st} - 1)$. Then, $d_B(u_1) \ge 3$ and $d_B(u_{r_{st}}) \ge 3$. By the hypothesis, we may suppose that $\{w_1, w_2, \ldots, w_{q-2}\}$ are the other vertices of $V(C_s) \cup V(C_t)$ with degrees at least 3 in B. Suppose that $N(u_1) \cap V(C_s) = \{z_1, u_2\}$, $N(u_1) \cap V(C_t) = \{z_2, u_2\}$, $N(u_{r_{st}}) \cap V(C_s) = \{z_3, u_{r_{st}-1}\}$, and $N(u_{r_{st}}) \cap V(C_t) = \{z_4, u_{r_{st}-1}\}$.

Case 1. $t \ge r_{st} + 2$.

Since each vertex of $V(C_s) \cup V(C_t)$ can dominate at least two vertices, there is a dominating set, say D_2, of size at most $\lceil \frac{s-r_{st}-2}{3} \rceil$ for the vertices of $V(C_s) \setminus (\{u_1, u_2, \ldots, u_{r_{st}}, z_1, z_3\} \cup D_2)$; there is a dominating set, say D_3, of size at most $\lceil \frac{r_{st}-2}{3} \rceil$ for the vertices of $\{u_1, u_2, \ldots, u_{r_{st}}\} \setminus (\{u_1, u_{r_{st}}\} \cup D_3)$; and there is a dominating set, say D_4, of size at most $\lceil \frac{t-r_{st}-2}{3} \rceil$ for the vertices of $V(C_t) \setminus (\{u_1, u_2, \ldots, u_{r_{st}}, z_2, z_4\} \cup D_4)$. Now, $D_5 = \{u_1, u_{r_{st}}, w_1, w_2, \ldots, w_{q-2}\} \cup D_2 \cup D_3 \cup D_4$ is a dominating set of $B[S_2(B)]$ such that

$$|D_5| \le q + \left\lceil \frac{s-r_{st}-2}{3} \right\rceil + \left\lceil \frac{t-r_{st}-2}{3} \right\rceil + \left\lceil \frac{r_{st}-2}{3} \right\rceil.$$

Combining with $S_2(B) \cup S_3(B) = V(B)$ and Lemma 5.9, we can conclude that $D = D_1 \cup D_5$ is a dominating set of B such that

$$\begin{aligned}\gamma &\le |D| \le |D_1| + |D_5| \\ &= n - p - (s+t) + r_{st} + q + \left\lceil \frac{s-r_{st}-2}{3} \right\rceil + \left\lceil \frac{t-r_{st}-2}{3} \right\rceil + \left\lceil \frac{r_{st}-2}{3} \right\rceil \\ &= n - p + q - 6 - \left\lfloor \frac{2(s-r_{st}-2)}{3} \right\rfloor - \left\lfloor \frac{2(t-r_{st}-2)}{3} \right\rfloor - \left\lfloor \frac{2(r_{st}-2)}{3} \right\rfloor \\ &\le n - p + q - 6,\end{aligned}$$

where the last inequality holds by the facts that $s \ge t \ge r_{st} + 2$ and $r_{st} \ge 2$.

Case 2. $2(r_{st}-1) \le t \le r_{st}+1$.

In this case, $2 \le r_{st} \le 3$. Combining with $2(r_{st}-1) \le t \le r_{st}+1$ and $t \ge 3$, we have $t = r_{st}+1$.

If $3 \le s \le 4$, since $s \ge t = r_{st}+1$, $\mathcal{R}(B) \in \{B_1, B_3, B_4\}$ (see Fig. 3.2). In this case, $D_6 = \{u_1, u_{r_{st}}, w_1, w_2, \ldots, w_{q-2}\}$ is a dominating set of $B[S_2(B)]$. Combining with $S_2(B) \cup S_3(B) = V(B)$ and Lemma 5.9, we can conclude that $D = D_1 \cup D_6$ is a dominating set of B such that

$$\begin{aligned}\gamma \le |D| &= |D_1| + |D_6| = n - p - (s+t) + r_{st} + q \\ &\le n - p + q - (2(r_{st}+1) - r_{st}) = n - p + q - 2 - r_{st} \le n - p + q - 4. \end{aligned} \tag{5.2}$$

If $\gamma = n - p + q - 4$, then $r_{st} = 2$ and $|D_6| = q$ by (5.2). In this case, (5.2) implies that $s = t = 3$, $d_G(u_1) \ge 4$ and $d_G(u_2) \ge 4$, as $|D_6| = q$ (Otherwise, we assume by symmetry that $d_G(u_2) = 3$. Then, $(D_1 \cup D_6)\backslash\{u_2\}$ is also a dominating set of size $\gamma - 1$ by (5.2), a contradiction). Therefore, $\mathcal{R}(B) = B_1$ and $d_G(v_1) \ge d_G(v_2) \ge 4$.

If $s \ge 5$, since each vertex of $V(C_s) \cup V(C_t)$ can dominate at least two vertices, there is a dominating set, say D_7, of size at most $\lceil \frac{s-r_{st}-2}{3} \rceil$ for the vertices of $V(C_s)\backslash(\{u_1, u_2, \ldots, u_{r_{st}}, z_1, z_3\} \cup D_7)$. Recall that $t = r_{st}+1 \in \{3, 4\}$. Thus, $D_8 = \{u_1, u_{r_{st}}, w_1, w_2, \ldots, w_{q-2}\} \cup D_7$ is a dominating set of $B[S_2(B)]$ such that

$$|D_8| \le q + \left\lceil \frac{s - r_{st} - 2}{3} \right\rceil.$$

Combining with $S_2(B) \cup S_3(B) = V(B)$ and Lemma 5.9, we can conclude that $D = D_1 \cup D_8$ is a dominating set of B such that

$$\begin{aligned}\gamma \le |D| &\le |D_1| + |D_8| = n - p - (s+t) + r_{st} + q + \left\lceil \frac{s - r_{st} - 2}{3} \right\rceil \\ &= n - p + q - t - 2 - \left\lfloor \frac{2(s - r_{st} - 2)}{3} \right\rfloor \le n - p + q - 5, \end{aligned}$$

where the last inequality holds by $t \ge 3$ and $s \ge 5 \ge r_{st} + 2$. ■

Lemma 5.13. *Let B be a bicyclic graph with degree sequence $\pi = (d_1, d_2, \ldots, d_{\gamma+3}, 1^{(n-\gamma-3)})$, where $d_{\gamma+3} \ge 2$. If $\pi \ne \pi_7$ and $n \ge 6$, then $\pi \lhd \pi_7$.*

Proof. We suppose that B contains p pendant vertices, and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3 in B. Since $p = n - \gamma - 3$, B contains exactly $\gamma + 3$ non-pendant vertices. Let $d_1 \ge d_2 \ge \cdots \ge d_j \ge 3 > d_{j+1} = \cdots = d_{\gamma+3} = 2$.

If $d_2 \ge 3$, then $j \ge 2$. In this case, since $\pi \ne \pi_7$, we have

$$\pi \lhd (n - \gamma + 2 - j, 3^{(j-1)}, 2^{(\gamma+3-j)}, 1^{(n-\gamma-3)}) \lhd \pi_7.$$

Otherwise, $d_2 = 2$ and so $\pi = (n - \gamma + 1, 2^{(\gamma+2)}, 1^{(n-\gamma-3)})$. In this case, $r_{st} = 1$ and $q = 1$. By Lemma 5.11, we have $\gamma \le n - p + q - 5 = n - p - 4 = \gamma - 1$, a contradiction. ■

Lemma 5.14. *Let B be a bicyclic graph with degree sequence $\pi = (d_1, d_2, \ldots, d_{\gamma+2}, 1^{(n-\gamma-2)})$, where $d_{\gamma+2} \ge 2$. If $\pi \ne \pi_8$ and $n \ge 8$, then $\pi \lhd \pi_8$.*

Proof. We suppose that B contains p pendant vertices, and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3 in B. Since $p = n - \gamma - 2$, B has $\gamma + 2$ non-pendant vertices. Assume that $d_1 \ge d_2 \ge \cdots \ge d_k \ge 4 > d_{k+1} = \cdots = d_j = 3 > d_{j+1} = d_{j+2} = \cdots = d_{\gamma+2} = 2$ and $\pi_8 = (d'_1, d'_2, \ldots, d'_n) = (n - \gamma, 4, 2^{(\gamma)}, 1^{(n-\gamma-2)})$. We consider the following three cases:

Case 1. $k = 0$.

In this case, $\pi = (3^{(j)}, 2^{(\gamma+2-j)}, 1^{(n-\gamma-2)})$. By (1.1), we have $3j + 2(\gamma + 2 - j) + (n - \gamma - 2) = 2(n+1)$. So, $j = n - \gamma$, and hence $\pi = (3^{(n-\gamma)}, 2^{(2\gamma-n+2)}, 1^{(n-\gamma-2)})$. Now, we turn to prove $\pi \lhd \pi_8$. Since $\gamma \le \frac{n}{2}$ by (1.2), we have

$$d_1 = 3 < 4 \le \frac{n}{2} \le n - \gamma = d'_1, \text{ and } d_1 + d_2 = 6 < 8 \le \frac{n}{2} + 4 \le n - \gamma + 4 = d'_1 + d'_2.$$

For $3 \le h \le n - \gamma$, since $d_h = 3$ and $n - \gamma \le \gamma + 2$ by the definition of π, it follows that

$$\begin{aligned}\sum_{i=1}^{h} d_i &= 2(n+1) - (n - \gamma - 2) - d_{h+1} - \cdots - d_{\gamma+2} \\ &= 2(n+1) - (n - \gamma - 2) - 2(2\gamma - n + 2) - 3(n - \gamma - h) = 3h \\ &\le n - \gamma + 2h = \sum_{i=1}^{h} d'_i. \end{aligned}$$

For $n-\gamma < h \le \gamma+2$, it is easy to see that

$$\sum_{i=1}^{h} d_i = 2(n+1)-(n-\gamma-2)-2(\gamma+2-h) = \sum_{i=1}^{h} d'_i.$$

Now, we can conclude that $\pi \lhd \pi_8$.

Case 2. $k=1$.

In this case, since $d_2 \le 3$ by $k=1$, $\gamma \le n-p+q-5$ follows from Lemmas 5.10–5.12. Thus, $\gamma-3+q = n-p+q-5 \ge \gamma$, and hence $j \ge q \ge 3$. This implies that

$$\pi \trianglelefteq (n-\gamma+3-j, 3^{(j-1)}, 2^{(\gamma+2-j)}, 1^{(n-\gamma-2)}) \trianglelefteq (n-\gamma, 3^{(2)}, 2^{(\gamma-1)}, 1^{(n-\gamma-2)}) \lhd \pi_8.$$

Case 3. $k \ge 2$.

Since $j \ge k \ge 2$, we have

$$\pi \trianglelefteq (n-\gamma+4-k-j, 4^{(k-1)}, 3^{(j-k)}, 2^{(\gamma+2-j)}, 1^{(n-\gamma-2)}) \trianglelefteq \pi_8. \tag{5.3}$$

Combining (5.3) with $\pi \ne \pi_8$, it follows that $\pi \lhd \pi_8$. ■

Lemma 5.15. *Let B be a bicyclic graph with n vertices, p pendant vertices, domination number γ and degree sequence π. If $\pi \ne \pi_6$ and $n \ge 8$, then $\pi \lhd \pi_6$.*

Proof. We suppose that B contains p pendant vertices, and exactly q vertices of $V(C_s) \cup V(C_t)$ have degrees at least 3 in B. By (5.1), we have $p \le n-\gamma$.

If $p \le n-\gamma-4$, then Lemma 5.1 implies that $\pi \trianglelefteq (n-\gamma, 2^{(\gamma+3)}, 1^{(n-\gamma-4)}) \lhd \pi_6$.

If $p = n-\gamma-3$, then $\pi \trianglelefteq \pi_7 \lhd \pi_6$ by Lemma 5.13.

If $p = n-\gamma-2$, then $\pi \trianglelefteq \pi_8 \lhd \pi_6$ by Lemma 5.14.

If $p = n-\gamma$, then Lemma 5.6 implies that every non-pendant vertex of B is a quasi-pendant vertex, and hence $\pi \lhd \pi_6$ by Lemma 5.2 (*ii*).

Otherwise, $p = n-\gamma-1$. In this case, $\pi = (d_1, d_2, \ldots, d_{\gamma+1}, 1^{(n-\gamma-1)})$, where $d_{\gamma+1} \ge 2$. By Lemma 5.7, it follows that $d_1 \ge d_2 \ge d_3 \ge 3$. Let $d_1 \ge d_2 \ge \cdots \ge d_k \ge 4 > d_{k+1} = \cdots = d_j = 3 > d_{j+1} = \cdots = d_{\gamma+1} = 2$.

Case 1. $k=1$.

By Lemmas 5.10–5.12, we have $\gamma \le n-p+q-5 = \gamma+q-4$, and hence $j \ge q \ge 4$. Since $j \ge 4$, we have

$$\pi \trianglelefteq (n-\gamma+4-j, 3^{(j-1)}, 2^{(\gamma+1-j)}, 1^{(n-\gamma-1)}) \trianglelefteq (n-\gamma, 3^{(3)}, 2^{(\gamma-3)}, 1^{(n-\gamma-1)}) \lhd \pi_6.$$

Case 2. $k \ge 2$.

Since $j \ge 3$ and $k \ge 2$, we have

$$\begin{aligned}\pi &\trianglelefteq (n-\gamma+5-k-j, 4^{(k-1)}, 3^{(j-k)}, 2^{(\gamma+1-j)}, 1^{(n-\gamma-1)})\\ &\trianglelefteq (n-\gamma, 4, 3, 2^{(\gamma-2)}, 1^{(n-\gamma-1)}) \lhd \pi_6.\end{aligned}$$

By combining the above arguments, we can conclude that $\pi \lhd \pi_6$. ■

For the sake of readability, let us denote $S_1(0;\gamma-1,n-2\gamma+1)$, $S_2(1;\gamma-3,n-2\gamma+1)$ and $S_2(2;\gamma-4,n-2\gamma+1)$ by $S(0;\gamma)$, $S(1;\gamma)$ and $S(2;\gamma)$, respectively.

Lemma 5.16. *We have $\Gamma(\pi_4,\gamma) = \{S(0;\gamma)\}$, $\Gamma(\pi_5,\gamma) = \{S(1;\gamma)\}$, and $\Gamma(\pi_6,\gamma) = \{S(2;\gamma)\}$.*

Proof. Suppose that $B \in \Gamma(\pi_4,\gamma) \cup \Gamma(\pi_5,\gamma) \cup \Gamma(\pi_6,\gamma)$ and B contains p pendant vertices. By the definitions of π_4, π_5 and π_6, B contains exactly γ non-pendant vertices. By Lemma 5.6, every non-pendant vertex is a quasi-pendant vertex, and hence the desired results follow from Lemmas 5.3 and 5.4. ■

Theorem 5.17. *If $n \ge 3c+3$ and $c \in \{0,1,2\}$, then $S(c;\gamma)$ is the unique good extremal graph in the class of c-cyclic graphs with n vertices and domination number γ.*

Proof. Let $\pi_{\max}^{(c)}$ be the largest degree sequence among all the degree sequences of graphs in the class of c-cyclic graphs with n vertices and domination number γ. In view of (5.1) and by Lemmas 5.1, 5.8 and 5.15 we get that $\pi_{\max}^{(0)} = \pi_4$, $\pi_{\max}^{(1)} = \pi_5$ and $\pi_{\max}^{(2)} = \pi_6$.

For $4 \le j \le 6$, let $\Gamma(\pi_j,\gamma)$ be the class of connected graphs with n vertices, domination number γ and degree sequence π_j. By Lemma 5.16 we have $\Gamma(\pi_4,\gamma) = \{S(0;\gamma)\}$, $\Gamma(\pi_5,\gamma) = \{S(1;\gamma)\}$ and $\Gamma(\pi_6,\gamma) = \{S(2;\gamma)\}$. From Theorems 3.1–3.3 together with $\gamma \le \lfloor \frac{n}{2} \rfloor$ by (1.2), we can conclude that $S(0;\gamma)$, $S(1;\gamma)$, and $S(2;\gamma)$ are extremal graphs of $\Gamma(\pi_4)$, $\Gamma(\pi_5)$ and $\Gamma(\pi_6)$, respectively. By Theorems 2.2–2.6 and $\Gamma(\pi_j,\gamma) \subseteq \Gamma(\pi_j)$ for $j \in \{4,5,6\}$, all good extremal graphs belong to $\Gamma(\pi_4,\gamma)$, $\Gamma(\pi_5,\gamma)$ and $\Gamma(\pi_6,\gamma)$, that is, the result holds. ■

6. Concluding remarks

As stated in [17], the main idea of the majorization theorem is to transfer the comparison of topological and spectral invariants of two graphs to the comparison of their degree sequences in the majorization ordering $\lhd$.

Assume that some graph invariant $\Phi(G)$ satisfies the majorization theorem. If we want to apply the majorization theorem to determine the extremal graphs (not restricted to Definition 1.1) of $\Phi(G)$ in some given graph category, then it is a standard procedure for us to perform the following three steps:

Step 1. Identify $\pi_{\max}$ in the majorization ordering $\lhd$ among all degree sequences of graphs in the corresponding graph category;
Step 2. Identify the corresponding extremal graph of $\Phi(G)$ in the class of connected graphs with degree sequence $\pi_{\max}$;
Step 3. Check whether the extremal graph determined after Step 2 is indeed the corresponding extremal graph of $\Gamma(\pi_{\max})$.

Remark 6.1. From the above procedure, if we detect a new graph invariant $\Phi(G)$ satisfying the majorization theorem and the extremal graphs of $\Phi(G)$ are *BFS*-graphs as stated in Theorems 3.1–3.3, then the good extremal graphs of Theorems 4.1–4.5 and 5.17 are also the extremal graphs of $\Phi(G)$ in the corresponding graph category.

Therefore, it appears natural to consider the following problem:

Problem 6.1. Establish new majorization theorems for topological and/or spectral invariants.

At present, in the class of c-cyclic graphs with fixed maximum degree (resp., independence number, matching number, domination number, and number of pendant vertices), we have determined the largest values for general spectral radius when $b \geq 0$ and $c \in \{0, 1\}$; the largest values of (signless Laplacian) spectral radius when $c = 2$; the largest value of $BID(G)$ for $c \in \{0, 1, 2\}$ when $\varphi(x, y)$ is a good escalating function; the largest (resp., smallest) value of $W_\psi(G)$ for $c = 0$ when $\psi(x)$ is a strictly nonnegative decreasing (resp., strictly increasing) function; the largest (resp., smallest) value of $H_f(G)$ for $c \in \{0, 1, 2\}$ when $f(x)$ is a strictly convex (resp., concave) function on $x \geq 1$. However, the above results are just restricted to $c \in \{0, 1, 2\}$, with the exception of the $H_f(G)$ case. The main reason is that, we only got the majorization theorem for $c \in \{0, 1, 2\}$. Actually, some graph invariants do not satisfy the majorization theorem for all $c \geq 0$ (cf. [10,17,18]). Hence, it is natural to consider the challenging problem:

Problem 6.2. Find a unified method to determine the extremal values of $\Theta(G, b)$, $BID(G)$, $W_\psi(G)$ and $H_f(G)$ in the class of c-cyclic graphs with different graph invariants for $c \geq 3$.

From the definition of $H_f(G)$, it is easy to see that $H_f(G)$ is constant for all graphs with the same degree sequence. So, when we want to apply the corresponding majorization theorem to identify the extremal graph of $H_f(G)$ in a given graph category $\mathcal{G}$, it suffices to consider the largest degree sequence of all graphs in $\mathcal{G}$, that is, the above mentioned Step 1. For instance, by the proof of Theorem 4.3, the degree sequence of $G_M(n, \Delta)$ is the largest degree sequence among all the degree sequences of c-cyclic graphs with n vertices and maximum degree Δ for $c \in \{0, 1, 2\}$. Therefore, when $c \in \{0, 1, 2\}$, it follows from Corollary 2.3 that

$$\prod_{1}(G) \geq \prod_{1}(G_M(n, \Delta)), \quad \text{and} \quad \prod_{2}(G) \leq \prod_{2}(G_M(n, \Delta)),$$

where equality holds if and only if G and $G_M(n, \Delta)$ share the same degree sequence. Actually, as a special case of $c = 0$, it is the main result of [26].

In [27], the authors also determined the smallest value of $\prod_{1}(G)$ and the largest value of $\prod_{2}(G)$ together with their corresponding extremal graphs in the class of trees with n vertices and domination number γ. It is a special case of Theorem 5.17 for $c = 0$. At the end of this paper, we would like to pose the following problem for further study.

Problem 6.3. Given a prescribed graph category, determine the extremal degree sequence(s) $\pi_{\max}$ in the majorization ordering $\lhd$.

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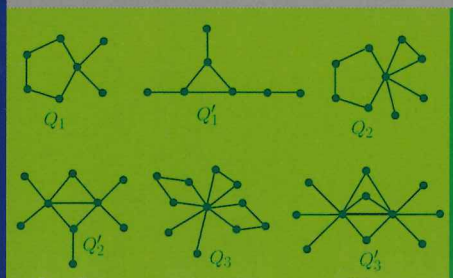
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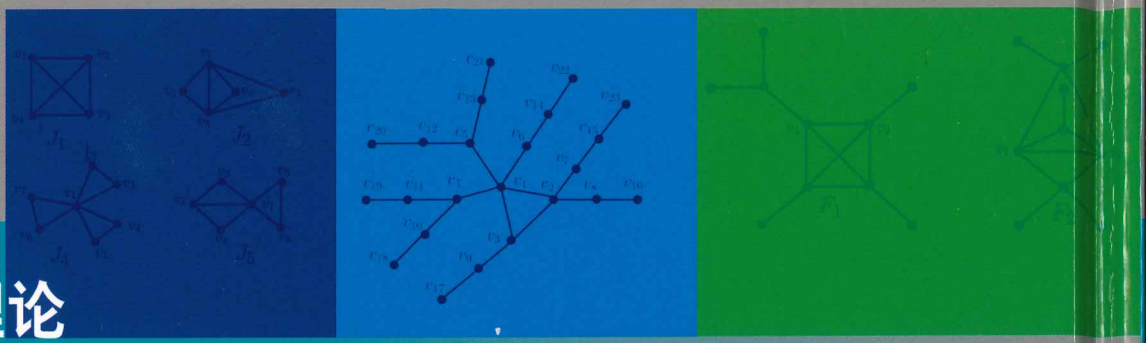
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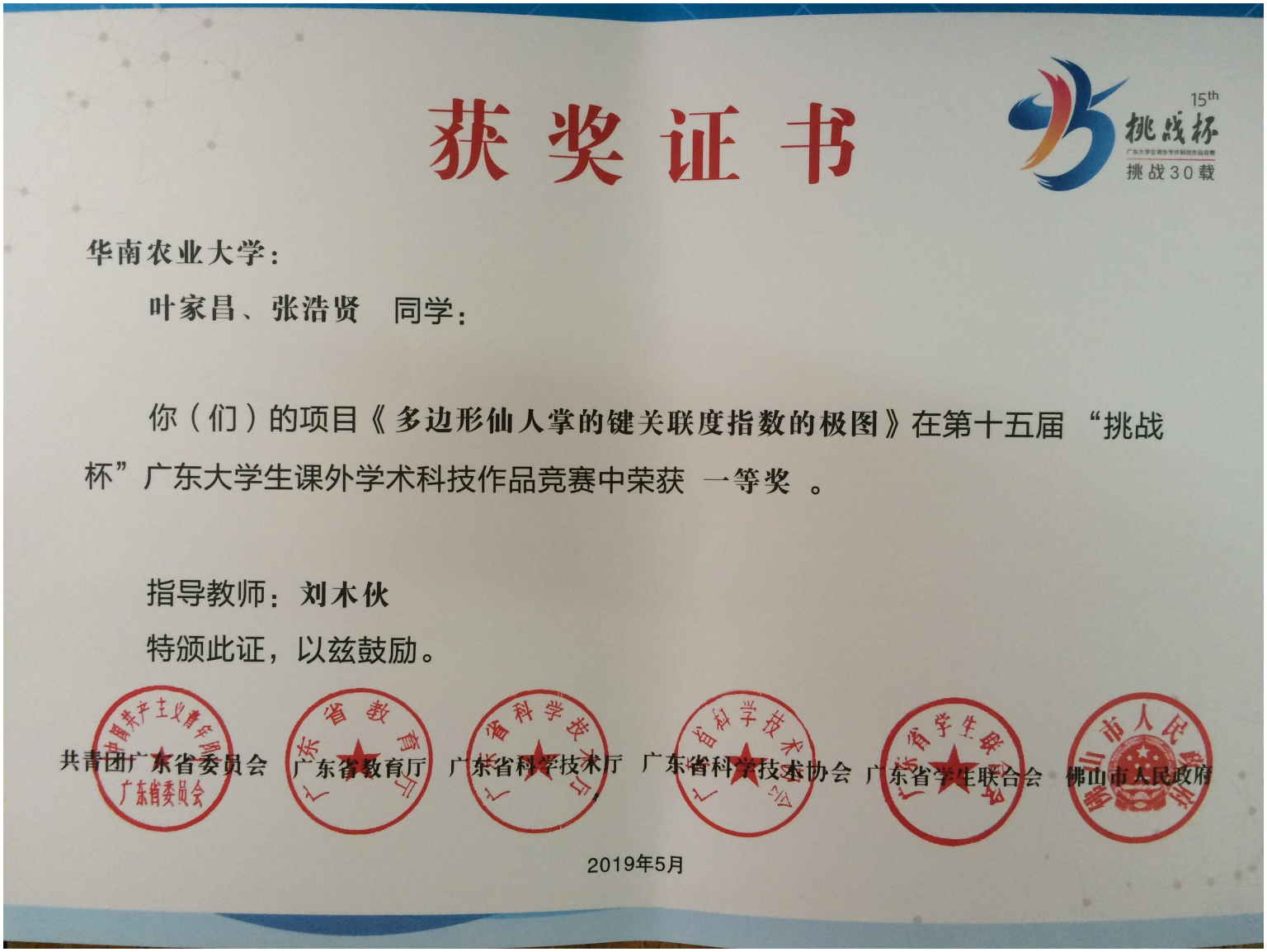
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