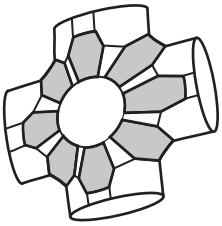

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Ante Graovac and Chemical Graph Theory

Ante Graovac (Split, Croatia, July 15, 1945 – Zagreb, Croatia, November 13, 2012), a theoretical physicist, was a member of the Advisory Board of our journal from its inception in 2008. In 2014, a book about his life and work was published in Kragujevac, Serbia [2]. His technical work speaks for itself. We can only add that Ante was a larger than life character, known amongst mathematical chemists for his enthusiasm, kindness, and readiness to collaborate. He had a real talent for bringing colleagues together, formally and informally.

Ante Graovac also has a special place in field of this journal. Only now that we look back, can we see how significant was his role in the development of mathematical chemistry/chemical graph theory in Slovenia, his native Croatia, other countries of former Yugoslavia and beyond. Together with mathematician Dragoš Cvetković, chemists Ivan Gutman, Nenad Trinajstić and physicist Milan Randić he was a pioneer in the field of chemical graph theory, mainly in connection with applications of linear algebra to chemically motivated problems. One of the earliest systematic treatments of this graph-theoretical or 'topological' approach to conjugated molecules was a volume in the Springer Lecture Notes Series co-authored by Graovac, Gutman and Trinajstić [1]. In the seventies and early eighties, his favourite graphs were benzenoids and other planar molecular graphs arising from hydrocarbons. Later, like many in the field who were inspired by the revolution in carbon chemistry and physics that led to the award of the fullerene and graphene Nobel prizes, respectively, to Curl, Kroto and Smalley (Chemistry, 1996) and to Geim and Novoselov (Physics, 2010), Ante turned to exploration of features of many other types of carbon framework.

In particular, in the eighties, after the discovery of buckminsterfullerene by Kroto, Smalley and Rice, he became fascinated with fullerenes. It was Ante who brought the late Harry Kroto by train from Zagreb to Ljubljana, a few months before Harry shared the Nobel Prize. In the nineties, Ante worked with us and others on the remarkable property of some graphs that they 'know' how to draw themselves. In addition to our many pairwise interactions, the three of us (AG, TP and PWF) have a single paper in common. This deals with a generalisation of the face-spiral approach for description and enumeration of cubic polyhedra, especially fullerenes.

In 1985 W. Imrich, the late T. D. Parsons (thesis advisor of TP) and TP organised an international conference in Dubrovnik at which Ante also took part. The success of the conference motivated Ante to start, a year later, a series of unusual, but very successful annual summer schools, workshops and conferences Math/Chem/Comp which charted the territory of chemical graph theory.

Ante was among the founding members of the International Academy of Mathematical Chemistry. He served as its secretary until his untimely death. Although he spent most of his working life at the Ruđer Bošković Institute in Zagreb and the University of Split, his work in Mathematical Chemistry inspired many younger colleagues at home and abroad to take up this interdisciplinary subject. Let us mention just Damir Vukičević and Tomislav Došlić. Throughout his life Ante maintained a strong friendship with Ivan Gutman. Ivan, with his editorship of the journal MATCH, and Ante with his Math/Chem/Comp meetings were important sources of inspiration for mathematicians starting up this field in several countries.

Algebraic and Topological Graph Theory, IUC, Dubrovnik, 1985, organised by Imrich, Parsons and Pisanski. Ante Graovac with glasses in the last row. The meeting was an inspiration for Ante's Math/Chem/Comp meetings. (Photo: Vladimir Batagelj)

Although mathematical chemistry is a prime application of combinatorics, and dates back to the 19th century with the first treatments of enumeration problems of alkanes, it received important new impetus from Hückel theory in the early 20th century with the explicit connection of quantum mechanics to linear algebra. Kekulé structures alias perfect matchings continue to inspire applications of graph theory. Numerous graph invariants, also known as topological indices of molecular graphs have been devised to represent, with varying degrees of success, physical and chemical properties of molecules from calculable properties of the molecular graph. In the last decade, graph theory in chemistry has received another fillip, from its new-found applicability to the theory of molecular conduction, another field represented in this volume.

It seems fair to say that mathematical chemistry of the mid-twentieth century was a subject practiced mostly by theoretical chemists and was looked upon with a certain scepticism by mathematicians. One aim in editing this volume was to show that discrete mathematical chemistry does offer questions worthy of serious mathematical study and can benefit from the contributions of mathematical professionals. The present volume of AMC consists of 15 papers from this field, many written by mathematicians alone or in collaboration.

Patrick Fowler and Tomaž Pisanski

Guest Editors

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Complete graphs with zero diagonal inverse

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Abstract

If the inverse of a non–singular real symmetric matrix that represents an edge–weighted graph with no loops has zero diagonal, then the inverse itself is the matrix of a loopless graph. Here we show that such graphs having non–zero weight on each edge always exist if their number of vertices is at least 6.

Keywords: NSSD, **G**–*nutful graph, circulant matrix, complete graph.*

Math. Subj. Class.: 05C90, 05B20

1 Introduction

Since the discovery of fullerenes in 1985, an intimate relationship has matured between these carbon molecules and mathematics. The combinatorial, graph theoretical and algebraic properties of fullerenes have been exploited by many researchers (see, for example [1, 3]) to classify the structures of fullerenes and to predict the unique chemical and physical properties of these highly symmetric structures. In "classical" fullerenes, the structure is composed of solely pentagonal and hexagonal regions joined together to form 3–regular polyhedra [3]. However, over the years, non–traditional fullerenes composed of cycles of other sizes, which are general 3–regular polyhedra, have been studied, especially for their regularity properties. This current work is motivated mainly by the beauty of these structures, coupled with the elegance of the interplay between combinatorics, graph theory and algebra. In particular, we consider the algebraic and structural properties of a special family of graphs, termed **G**–nutful graphs, introduced in [8].

The graphs we consider have weighted edges and no loops. If a non–singular real symmetric matrix $\mathbf{G}$ representing such a graph has an inverse $\mathbf{G}^{-1}$ with each entry of its diagonal equal to zero, then the graph is referred to as a NSSD (*Non–Singular graphs with*

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a Singular Deck). This family of graphs has remarkable properties as explored in [2] and [8].

It is the purpose of this work to determine the existence of complete NSSDs. In [8], a characterisation of a graph G which is **G**–nutful is given. The inverse $\mathbf{G}^{-1}$ of a **G**–nutful graph is associated with a complete NSSD. If **G** is the matrix of a complete NSSD graph K_n on n vertices, then the graph of $\mathbf{G}^{-1}$ is said to be $\mathbf{G}^{-1}$–nutful.

As noted in [2, 4, 7], apart from K_2, no other graph was known to be **G**–nutful. Are there any **G**–nutful graphs other than K_2? In this paper, we establish that there exist **G**–nutful graphs of any order at least six. Some of these **G**–nutful graphs turn out to be also complete, in which case both G and the graph of $\mathbf{G}^{-1}$ are nutful.

2 Preliminaries

The *characteristic polynomial* $\phi(\mathbf{M}, \lambda)$ of a square $n \times n$ matrix **M**, over a field F, is the determinant $\det(\lambda\mathbf{I} - \mathbf{M})$, denoted also by $|\lambda\mathbf{I} - \mathbf{M}|$, which is a polynomial of degree n in λ, where **I** denotes the identity matrix. The roots of $\phi(\mathbf{M}, \lambda)$ (in the algebraic closure of F) are the *eigenvalues* of **M**. For a real and symmetric $n \times n$ matrix **M**, the n eigenvalues are real, but not necessarily all distinct. The multiplicity of the eigenvalue 0 of **M** is called the *nullity* $\eta(\mathbf{M})$ of **M**. The matrix **M** is said to be *singular* if $\eta(\mathbf{M}) > 0$ and is said to be *non–singular* otherwise.

A graph G is a collection of points (called *vertices*) and lines (called *edges*) connecting pairs of vertices. If e is an edge connecting two distinct vertices u and v, then we write $e = \{u, v\}$ and say that e is *incident* to u and to v, or, equivalently, that u and v are *adjacent*. The number of edges incident to a vertex is called the *degree* of the vertex. In a ρ–regular graph, each vertex has degree ρ. For each edge e of G, we associate a non–zero real number w, called the *weight* of e. For a real and symmetric matrix **M** whose entries on the leading diagonal are all zero, we can associate a graph $G = \Gamma(\mathbf{M})$ with no loops and with weighted edges, such that $\{i, j\}$ is an edge of G with weight w if and only if the ij^{th} entry of **M** is $w \neq 0$. We say that **M** is an adjacency matrix representing the graph G, or, equivalently, that G is the graph associated with the adjacency matrix **M**. The complete graph K_n on n vertices and having $\binom{n}{2}$ weighted edges is represented by the matrix $\mathbf{K}_n$. Although in the study of molecular structures, graphs usually have a maximum vertex degree of at most three, in this study we place no restriction on the maximum vertex degree. This allows us to consider complete graphs on any number of vertices.

In the sequel, we shall also consider vertex–deleted subgraphs of a graph and their associated adjacency matrices. For any vertex x of a graph G, the subgraph $G - x$ obtained by deleting the vertex x and all the edges of G incident to x is associated with the $(n - 1) \times (n - 1)$ matrix $\mathbf{G} - \mathbf{x}$ obtained by deleting the x^{th} row and column of the adjacency matrix **G** representing G.

An identity due to Jacobi [6] describes the possible changes in the nullity of an adjacency matrix **G** representing the graph G when any two vertices x and y are deleted from G. Denoting the adjugate of **G** by $\operatorname{adj}\mathbf{G}$ and the entry in the x, y position of $\operatorname{adj}\mathbf{G}$ by $(\operatorname{adj}\mathbf{G})_{xy}$, we have the following result.

Lemma 2.1. *Let x and y be two distinct vertices of a graph G with associated adjacency matrix* **G***, and let $j = (\operatorname{adj}(\lambda\mathbf{I} - \mathbf{G}))_{xy}$ be the entry in the x, y position of* $\operatorname{adj}(\lambda\mathbf{I} - \mathbf{G})$*. Then $j^2 = ut - sv$, where s, t, u and v represent the characteristic polynomials of* **G**, $\mathbf{G} - \mathbf{x}$, $\mathbf{G} - \mathbf{y}$ *and* $\mathbf{G} - \mathbf{x} - \mathbf{y}$*, respectively.*

In [2] and [8], the authors introduced a class of graphs termed NSSDs and analysed the properties of these graphs. Formally, NSSDs are defined as follows.

Definition 2.2 ([2])**.** A graph $G = \Gamma(\mathbf{G})$ is a *NSSD* if $\mathbf{G}$ is a non–singular, real and symmetric matrix with each entry of the diagonal equal to zero, and such that all the $(n-1) \times (n-1)$ principal submatrices of $\mathbf{G}$ are singular.

The following is a necessary and sufficient condition for $\Gamma(\mathbf{G})$ to be a NSSD.

Theorem 2.3 ([2])**.** *The matrices* $\mathbf{G}$ *and* $\mathbf{G}^{-1}$ *are real and symmetric with each entry on the respective diagonals equal to zero if and only if* $\Gamma(\mathbf{G})$ *and* $\Gamma(\mathbf{G}^{-1})$ *are both NSSDs.*

Therefore, this class of graphs is closed under taking the inverse of the adjacency matrix, hence giving rise to a duality relationship between $\mathbf{G}$ and its inverse $\mathbf{G}^{-1}$, so that either one of the two can assume the principal role. For simplicity, we may refer to $\Gamma(\mathbf{G}^{-1})$ as the inverse of the graph G.

If the only zero entries in a $n \times n$ symmetric matrix are situated on the leading diagonal, then the graph associated with such a matrix is the complete graph K_n. Of special interest to us for this work are complete graphs which also happen to be NSSDs, referred to in the sequel as *complete NSSDs*. In Section 3 we show that the only complete NSSD on at most five vertices is K_2. In Section 4 we extend the investigation to graphs on at least six vertices, and prove that we can find NSSDs on n vertices for any $n \geq 6$. In particular, the NSSDs we present are complete NSSDs with appropriate edge–weights. In our construction of these complete NSSDs we make use of spectral properties of circulant matrices.

Definition 2.4. A *circulant matrix* is an $n \times n$ matrix $\mathbf{C} = (a_{k,j} : k, j = 1, 2, \ldots, n)$ where $a_{k,j} = a_{j-k(\mathrm{mod}\, n)}$, that is

$$\mathbf{C} = \begin{pmatrix} a_0 & a_1 & \cdots & a_{n-2} & a_{n-1} \\ a_{n-1} & a_0 & a_1 & & a_{n-2} \\ \vdots & a_{n-1} & a_0 & \ddots & \vdots \\ a_2 & & \ddots & \ddots & a_1 \\ a_1 & a_2 & \cdots & a_{n-1} & a_0 \end{pmatrix},$$

denoted by $\mathbf{C} = \langle a_0, a_1, \ldots, a_{n-1} \rangle$.

3 Complete Graphs On Less Than 6 Vertices

We treat the two cases for $n \leq 4$ and $n = 5$ separately.

3.1 Complete Graphs On Less Than 5 Vertices

For a graph **not** to be a NSSD for any associated adjacency matrix, it suffices to show that it has a non–singular vertex–deleted subgraph. This is shown to be the case for $n = 3$ and 4.

Proposition 3.1. *The complete graph* K_n *on* $n \leq 4$ *vertices is a NSSD if and only if* $n = 2$.

Proof. Clearly K_1 is not a NSSD since $\mathbf{K}_1$ is singular. The adjacency matrix representing K_2 is $\begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}$ for some nonzero real number c. Thus K_2 is a NSSD for any edge weight

c by Definition 2.2. The vertex–deleted subgraphs of K_3 are associated with the non–singular matrices $\mathbf{K}_2$, and hence K_3 cannot be a NSSD for any edge weights. Moreover, the adjacency matrix representing K_3 is $\begin{pmatrix} 0 & a_1 & a_2 \\ a_1 & 0 & a_3 \\ a_2 & a_3 & 0 \end{pmatrix}$ for some nonzero real numbers a_1, a_2, a_3, whose determinant is $2a_1a_2a_3 \neq 0$. This means that $\mathbf{K}_3$, which represents every vertex–deleted subgraph of K_4, is always non–singular, implying that K_4 cannot be a NSSD. □

3.2 Complete Graphs On 5 Vertices

Since the weights of K_4 can be assigned such that it can either be singular or non–singular, we cannot utilise the argument used in Proposition 3.1 to prove that K_5 is not a NSSD.

We quote a result from [2] that characterises the nullity of a two–vertex–deleted subgraph of a NSSD depending on whether the two vertices form an edge in its inverse.

Theorem 3.2 ([2])**.** *If $\Gamma(\mathbf{G})$ is a NSSD on at least three vertices, then $\mathbf{G}-\mathbf{x}-\mathbf{y}$ has nullity zero if $\{x, y\}$ is an edge in $\Gamma(\mathbf{G}^{-1})$, and has nullity two if $\{x, y\}$ is not an edge in $\Gamma(\mathbf{G}^{-1})$.*

With the aim to show that K_5 cannot be a NSSD, we seek properties that a NSSD on five vertices could have.

Lemma 3.3. *If a NSSD on five vertices exists, then it must be the complete graph K_5 for appropriate edge weights, and its inverse must also be K_5, possibly with different edge weights.*

Proof. Suppose G is a NSSD on five vertices. Then, for any two vertices x and y, $\mathbf{G}-\mathbf{x}-\mathbf{y}$ has nullity zero or two by Theorem 3.2. But $\mathbf{G}-\mathbf{x}-\mathbf{y}$ has only three vertices. There are only four graphs on three vertices, none of which has nullity two, no matter what weights are assigned to their edges. It follows that $\eta(\mathbf{G}-\mathbf{x}-\mathbf{y}) = 0$, and by Theorem 3.2, $\{x, y\}$ is an edge in $\Gamma(\mathbf{G}^{-1})$ for all vertices x and y. Thus, $\Gamma(\mathbf{G}^{-1})$ is K_5 for some particular edge weights. Since $\mathbf{G}^{-1}$ represents a NSSD on five vertices, we repeat the same argument and obtain that its inverse, which is the original matrix $\mathbf{G}$, also represents a complete graph. □

It follows that if a NSSD on five vertices were to exist, it must be complete. Now we make use of Lemma 3.3 to show that K_5 cannot be a NSSD.

Theorem 3.4. *There are no NSSDs on five vertices.*

Proof. By Lemma 3.3, if a NSSD on 5 vertices exists, it must be the graph K_5 with some edge weights, and its inverse (which is also a NSSD on 5 vertices) must also be K_5, with possibly different edge weights. Let

$$\mathbf{G} = c\mathbf{M} = c\begin{pmatrix} 0 & g_0 & g_1 & g_2 & g_3 \\ g_0 & 0 & g_4 & g_5 & g_6 \\ g_1 & g_4 & 0 & g_7 & g_8 \\ g_2 & g_5 & g_7 & 0 & g_9 \\ g_3 & g_6 & g_8 & g_9 & 0 \end{pmatrix},$$

where $g_i \neq 0$ for all i and $c = \sqrt[5]{|\mathbf{G}|}$, so that $|\mathbf{M}| = 1$. Since $\mathbf{G}$ is a NSSD, so is $\mathbf{M}$. The NSSD

$$\mathbf{G}^{-1} = \frac{1}{c}\mathbf{M}^{-1} = \frac{1}{c}\begin{pmatrix} 0 & h_0 & h_1 & h_2 & h_3 \\ h_0 & 0 & h_4 & h_5 & h_6 \\ h_1 & h_4 & 0 & h_7 & h_8 \\ h_2 & h_5 & h_7 & 0 & h_9 \\ h_3 & h_6 & h_8 & h_9 & 0 \end{pmatrix},$$

where $h_i \neq 0$ for all i. Using Jacobi's Theorem (Lemma 2.1), we have $\left((\operatorname{adj}\mathbf{M})_{xy}\right)^2 = -|\mathbf{M}||\mathbf{M}-\mathbf{x}-\mathbf{y}| = -|\mathbf{M}-\mathbf{x}-\mathbf{y}|$ for any two vertices x and y of G. But $\mathbf{M}-\mathbf{x}-\mathbf{y} = \mathbf{K}_3$ for all vertices x and y, whose determinant is $2g_ig_jg_k$ for distinct values of $i,j,k \in \{0,\ldots,9\}$. Also $\mathbf{M}^{-1}_{xy} = \frac{(\operatorname{adj}\mathbf{M})_{xy}}{|\mathbf{M}|} = (\operatorname{adj}\mathbf{M})_{xy}$, and thus $h_\ell^2 = -2g_ig_jg_k$ for some i,j,k,ℓ. Specifically:

$$\begin{array}{llll} -2g_0g_1g_4 = h_9^2 & -2g_0g_2g_5 = h_8^2 & -2g_0g_3g_6 = h_7^2 & -2g_1g_2g_7 = h_6^2 \\ -2g_1g_3g_8 = h_5^2 & -2g_2g_3g_9 = h_4^2 & -2g_4g_5g_7 = h_3^2 & -2g_4g_6g_8 = h_2^2 \\ & -2g_5g_6g_9 = h_1^2 & -2g_7g_8g_9 = h_0^2 & \end{array}$$

Considering $\mathbf{M}^{-1}$ as the NSSD, we have:

$$\begin{array}{llll} -2h_0h_1h_4 = g_9^2 & -2h_0h_2h_5 = g_8^2 & -2h_0h_3h_6 = g_7^2 & -2h_1h_2h_7 = g_6^2 \\ -2h_1h_3h_8 = g_5^2 & -2h_2h_3h_9 = g_4^2 & -2h_4h_5h_7 = g_3^2 & -2h_4h_6h_8 = g_2^2 \\ & -2h_5h_6h_9 = g_1^2 & -2h_7h_8h_9 = g_0^2 & \end{array}$$

Squaring the last equation, we have $4h_7^2h_8^2h_9^2 = g_0^4$, and multiplying the first three equations together, we obtain $-8g_0^3g_1g_2g_3g_4g_5g_6 = h_7^2h_8^2h_9^2$. Thus $-32g_1g_2g_3g_4g_5g_6 = g_0$. Since $-2g_7g_8g_9 = h_0^2$, we can write

$$16g_0g_1g_2g_3g_4g_5g_6g_7g_8g_9 = g_0^2h_0^2$$

This process can be repeated starting from another group of equations to obtain $16\prod_{j=0}^{9} g_j = g_i^2h_i^2$ for all $i \in \{0,1,\ldots,9\}$. Thus $g_i^2h_i^2 = g_j^2h_j^2 = 16\prod_{k=0}^{9} g_k$ for all $i,j \in \{0,1,\ldots,9\}$.

Since $\mathbf{M}\mathbf{M}^{-1} = \mathbf{I}$, we have, in particular, that $g_0h_0 + g_1h_1 + g_2h_2 + g_3h_3 = 1$. But $g_ih_i = \pm g_jh_j$ for all i,j, and hence $g_0h_0(\pm 1 \pm 1 \pm 1 \pm 1) = 1$. Thus $g_0h_0 = \pm\frac{1}{4}$ or $g_0h_0 = \pm\frac{1}{2}$. Since $g_i^2h_i^2 = g_j^2h_j^2$ for all i,j then either $g_ih_i = \pm\frac{1}{4}$ for all i or $g_ih_i = \pm\frac{1}{2}$ for all i. Additionally, in order for $g_0h_0 + g_1h_1 + g_2h_2 + g_3h_3$ to be equal to 1, none of the g_ih_i's can be equal to $-\frac{1}{4}$, and thus either all g_ih_i are equal to $\frac{1}{4}$ or all g_ih_i are equal to $\pm\frac{1}{2}$.

Suppose $g_ih_i = \pm\frac{1}{2}$ for all i. In the five equations

$$\begin{aligned} g_0h_0 + g_1h_1 + g_2h_2 + g_3h_3 &= 1 \\ g_0h_0 + g_4h_4 + g_5h_5 + g_6h_6 &= 1 \\ g_1h_1 + g_4h_4 + g_7h_7 + g_8h_8 &= 1 \\ g_2h_2 + g_5h_5 + g_7h_7 + g_9h_9 &= 1 \\ g_3h_3 + g_6h_6 + g_8h_8 + g_9h_9 &= 1, \end{aligned}$$

three of the four terms g_ih_i in each equation must have value $\frac{1}{2}$ and the remaining one must be equal to $-\frac{1}{2}$. Combinatorially, this is impossible, for suppose we choose, without loss of generality, $g_0h_0 = -\frac{1}{2}$; then $g_1h_1 = g_2h_2 = g_3h_3 = g_4h_4 = g_5h_5 = g_6h_6 = \frac{1}{2}$.

From the last three equations, we obtain that $g_7h_7 + g_8h_8 = 0$, $g_7h_7 + g_9h_9 = 0$ and $g_8h_8 + g_9h_9 = 0$, implying that $g_7h_7 = g_8h_8 = g_9h_9 = 0$, a contradiction.

The only remaining possibility is that $g_ih_i = \frac{1}{4}$ for all i. Consider $\mathbf{M}\mathbf{M}^{-1} = \mathbf{M}^{-1}\mathbf{M} = \mathbf{I}$. In particular, by multiplying the first row of $\mathbf{M}$ by the second column of $\mathbf{M}^{-1}$, and by multiplying the first row of $\mathbf{M}^{-1}$ by the second column of $\mathbf{M}$, we obtain

$$\begin{aligned} g_1h_4 + g_2h_5 + g_3h_6 &= 0 \\ h_1g_4 + h_2g_5 + h_3g_6 &= 0 \end{aligned}$$

Since $g_ih_i = \frac{1}{4}$, we can write

$$\begin{aligned} \frac{1}{4}\left(\frac{g_1}{g_4} + \frac{g_2}{g_5} + \frac{g_3}{g_6}\right) &= 0 \\ \frac{1}{4}\left(\frac{g_4}{g_1} + \frac{g_5}{g_2} + \frac{g_6}{g_3}\right) &= 0 \end{aligned}$$

Let $p = \dfrac{g_1}{g_4}$, $q = \dfrac{g_2}{g_5}$ and $r = \dfrac{g_3}{g_6}$ so that

$$p + q + r = 0 \tag{3.1}$$

$$\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 0 \tag{3.2}$$

From (3.2) we obtain $pq + pr + qr = 0$. Substituting (3.1) in this equation, we get $(-q - r)q + (-q - r)(r) + qr = 0$, or $q^2 + qr + r^2 = 0$. Fixing r to be any real number, this is a quadratic equation in q with a negative discriminant $-3r^2$, and hence q must be a complex number, which is a contradiction.

Thus $\Gamma(\mathbf{M})$ is not a NSSD, and hence neither is $\Gamma(\mathbf{G})$. □

From Proposition 3.1 and Theorem 3.4, the following result follows immediately.

Corollary 3.5. *The complete graph K_n on $n \leq 5$ vertices is a NSSD if and only if $n = 2$.*

4 Complete Graphs on at Least Six Vertices

In this section, we prove that there indeed exist complete NSSDs on at least six vertices by a direct construction.

Any complete graph on $n \geq 6$ vertices has at least one (Hamiltonian) cycle of length n on all the vertices. If we assign an arbitrary weight $a \neq 0$ to this cycle and a weight of 1 to every other edge of the graph, the matrix obtained is $\mathbf{K}_n^{(a)}$ of the form shown in (4.1):

$$\mathbf{K}_n^{(a)} = \begin{pmatrix} 0 & a & 1 & \cdots & 1 & a \\ a & 0 & a & 1 & \cdots & 1 \\ 1 & a & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & a & 1 \\ 1 & \cdots & 1 & a & 0 & a \\ a & 1 & \cdots & 1 & a & 0 \end{pmatrix} \tag{4.1}$$

4.1 The Characteristic Polynomial of Circulant Matrices

We remark that the real and symmetric matrix shown in (4.1) is the circulant matrix $\langle 0, a, 1, \ldots, 1, a\rangle$. The eigenvalues of such a matrix can thus be obtained by using well–known results on circulant matrices.

Lemma 4.1. *The eigenvalues of the circulant matrix* $\langle 0, a, 1, \ldots, 1, a\rangle$ *are* $\lambda_0 = 2(a-1) - 1 + n$, *and* $\lambda_j = 2(a-1)\cos\left(\frac{2\pi j}{n}\right) - 1$ *for* $j \in \{1, \ldots, n-1\}, a \neq 0$.

Proof. It is well–known (see, for example, [5]) that the eigenvalues of the general circulant matrix $\langle a_0, a_1, \ldots, a_{n-1}\rangle$ are $\lambda_j = \sum_{k=0}^{n-1} a_k \omega_j^k$, for $j \in \{0, \ldots, n-1\}$ and $\omega_0, \ldots, \omega_{n-1}$ are the n^{th} roots of unity given by $\omega_j = e^{2\pi i j/n}$. If we substitute $a_0 = 0$, $a_2 = a_3 = \cdots = a_{n-2} = 1$ and $a_{n-1} = a_1 = a$, then the eigenvalues of $\langle 0, a, 1, \ldots, 1, a\rangle$ are given by $\lambda_j = a(\omega_j + \omega_j^{n-1}) + \sum_{k=2}^{n-2} \omega_j^k$. But

$$\sum_{k=0}^{n-1} \omega_j^k = \begin{cases} \sum_{k=0}^{n-1} 1^k = n & \text{if } j = 0 \\ \sum_{k=0}^{n-1} (-1)^k = 0 & \text{if } n \text{ is even and } j = \frac{n}{2} \\ \dfrac{(\omega_j^k)^n - 1}{\omega_j^k - 1} = \dfrac{(\omega_j^n)^k - 1}{\omega_j^k - 1} = 0 & \text{otherwise} \end{cases}$$

Hence, if $j = 0$, then $\sum_{k=2}^{n-2} \omega_0^k = n - 3$, and thus

$$\lambda_0 = a(1+1) + (n-3) = 2(a-1) - 1 + n.$$

If n is even and $j = \frac{n}{2}$, then $\sum_{k=2}^{n-2} \omega_{n/2}^k = 0 - 1 + 1 + 1 = 1$. Thus

$$\begin{aligned} \lambda_{n/2} = a((-1) + (-1)^{n-1}) + 1 = a((-1)(1 + (-1)^{n-2}) + 1 = 2a(\cos\pi) + 1 \\ = 2(a-1)(\cos\pi) - 1 = 2(a-1)\cos\left(\tfrac{2\pi j}{n}\right) - 1. \end{aligned}$$

For any other case, $\sum_{k=2}^{n-2} \omega_j^k = -1 - \omega_j - \omega_j^{n-1}$, which means that

$$\lambda_j = (a-1)(\omega_j + \omega_j^{n-1}) - 1 = (a-1)(\omega_j + \omega_j^{-1}) - 1 = 2(a-1)\cos\left(\tfrac{2\pi j}{n}\right) - 1,$$

completing the proof. □

The eigenvalues of $\langle 0, a, 1, \ldots, 1, a\rangle$ satisfy several interesting properties. To order the eigenvalues, we use the notation of Lemma 4.1.

Proposition 4.2. *Let $n \geq 6$ and let the complete graph K_n have circulant matrix $\mathbf{K}_n^{(a)}$ given by $\mathbf{K}_n^{(a)} = \langle 0, a, 1, \ldots, 1, a\rangle$, where the parameter a is a non–zero real number. Then the eigenvalues $\lambda_0, \ldots, \lambda_{n-1}$ of $\mathbf{K}_n^{(a)}$ are such that*

(i) $\lambda_0 > \lambda_j$ for all $j = 1, \ldots, n-1$;

(ii) $\lambda_j = \lambda_{n-j}$ for $j = 1, \ldots, \lfloor \frac{n-1}{2} \rfloor$;

(iii) $\lambda_j > \lambda_{j+1}$ $(j = 1, \ldots, \lfloor \frac{n-1}{2} \rfloor)$ when $a > 1$.

For $\mathbf{K}_8^{(2)}$, say, $\lambda_0 = 15$, $\lambda_1 = \lambda_7 = -1 + 4\sqrt{2}$, $\lambda_2 = \lambda_6 = -1$, $\lambda_3 = \lambda_5 = -1 - 4\sqrt{2}$ and $\lambda_4 = -9$.

The characteristic polynomial of $\mathbf{K}_n^{(a)} = \langle 0, a, 1, \ldots, 1, a\rangle$ can be obtained from Lemma 4.1. However, we can actually also determine the characteristic polynomials of all the vertex–deleted subgraphs of $\mathbf{K}_n^{(a)}$. In the sequel, the characteristic polynomial $\phi(\mathbf{K}_n^{(a)}, \lambda)$ will be denoted by $\psi(\mathbf{K}_n^{(a)}, x, c)$ where $x = \lambda$ and $c = 2(a-1), c \neq -2$.

Proposition 4.3. *Let n be any integer greater than 1 and let $\mathbf{K}_n^{(a)}$ be a complete circulant symmetric matrix $\langle 0, a, 1, \ldots, 1, a\rangle$ on n vertices, $a \neq 0$. Then its characteristic polynomial is*

$$\psi(\mathbf{K}_n^{(a)}, x, c) = \begin{cases} (x+1-c-n)\big(p(x,c)\big)^2 & \text{if } n \text{ is odd} \\ (x+1-c-n)(x+1+c)\big(p(x,c)\big)^2 & \text{if } n \text{ is even} \end{cases}$$

and $\psi(\mathbf{K}_n^{(a)} - \mathbf{v}, x, c)$, the characteristic polynomial of each of its vertex–deleted subgraphs, is

$$\begin{cases} \frac{p(x,c)}{n}\big(p(x,c) + 2(x+1-c-n)q(x,c)\big) & \text{if } n \text{ is odd} \\ \frac{p(x,c)}{n}\big((2x+2-n)p(x,c) + 2(x+1-c-n)(x+1+c)q(x,c)\big) & \text{if } n \text{ is even} \end{cases}$$

where $k = \lfloor \frac{n-1}{2} \rfloor$, $c = 2(a-1)$, $p(x,c) = \prod_{j=1}^{k} \left(x + 1 - c\cos\left(\frac{2\pi j}{n}\right)\right)$ and

$$q(x,c) = \frac{\partial p}{\partial x} = \sum_{j=1}^{k} \prod_{q=1, q\neq j}^{k} \left(x + 1 - c\cos\left(\frac{2\pi q}{n}\right)\right).$$

Proof. By Lemma 4.1, the eigenvalues of $\mathbf{K}_n^{(a)}$ are $\lambda_0 = 2(a-1) - 1 + n$ and $\lambda_j = 2(a-1)\cos\left(\frac{2\pi j}{n}\right) - 1$ for $j \in \{1, \ldots, n-1\}$. Furthermore, by Proposition 4.2 (ii), $\lambda_{n-j} = \lambda_j$ for all $j \in \{1, \ldots, k\}$. Also, if n is even, then $\lambda_{n/2} = -2(a-1) - 1$. Hence, for $c = 2(a-1)$, the characteristic polynomial of $\mathbf{K}_n^{(a)}$ is

$$\prod_{j=0}^{n-1}(x - \lambda_j) = (x+1-c-n)\prod_{j=1}^{k}(x-\lambda_j)^2 = (x+1-c-n)\left(\prod_{j=1}^{k}\left(x + 1 - c\cos\left(\frac{2\pi j}{n}\right)\right)\right)^2$$

when n is odd, and

$$\prod_{j=0}^{n-1}(x-\lambda_j) = (x+1-c-n)(x+1+c)\prod_{j=1}^{k}(x-\lambda_j)^2$$
$$= (x+1-c-n)(x+1+c)\left(\prod_{j=1}^{k}\left(x+1-c\cos\left(\tfrac{2\pi j}{n}\right)\right)\right)^2$$

when n is even.

Since every circulant matrix associated with a graph G renders G vertex–transitive, all the vertex–deleted subgraphs of G are isomorphic and hence have the same characteristic polynomial. But the sum of the characteristic polynomials of all the vertex–deleted subgraphs of G is equal to the derivative of the characteristic polynomial of G [9][1]. Thus $\psi(\mathbf{K}_n^{(a)} - \mathbf{v}, x, c) = \frac{1}{n}\frac{\partial}{\partial x}\psi(\mathbf{K}_n^{(a)}, x, c)$, so we now proceed to evaluate this partial derivative.

When n is odd, we have

$$\begin{aligned}
&\psi(\mathbf{K}_n^{(a)} - \mathbf{v}, x, c)\\
&\quad= \frac{1}{n}\frac{\partial}{\partial x}(x+1-c-n)(p(x,c))^2\\
&\quad= \frac{1}{n}\left((p(x,c))^2 + 2(x+1-c-n)p(x,c)\frac{\partial p}{\partial x}\right)\\
&\quad= \frac{p(x,c)}{n}\left(p(x,c) + 2(x+1-c-n)\left(\frac{\partial}{\partial x}\prod_{j=1}^{k}\left(x+1-c\cos\left(\tfrac{2\pi j}{n}\right)\right)\right)\right)\\
&\psi(\mathbf{K}_n^{(a)} - \mathbf{v}, x, c)\\
&\quad= \frac{p(x,c)}{n}\left(p(x,c) + 2(x+1-c-n)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(x+1-c\cos\left(\tfrac{2\pi q}{n}\right)\right)\right)
\end{aligned}$$

When n is even, the result stated in the proposition statement is obtained in a similar manner. □

4.2 The Construction of Complete NSSDs

We have noted in the proof of Proposition 4.3 that the characteristic polynomials of the adjacency matrices of all the vertex–deleted subgraphs of the graph associated with $\mathbf{K}_n^{(a)} = \langle 0, a, 1, \ldots, 1, a\rangle$ are equal. This means that the determinant of the matrix of each of these vertex–deleted subgraphs is the same. Thus, if the determinant of $\mathbf{K}_n^{(a)}$ is non–zero and the determinant of any one of its $(n-1)\times(n-1)$ principal submatrices is zero, then the matrix would represent a NSSD. This is the basis of our construction.

To illustrate the above, let us take the complete graph on seven vertices as an example. By Corollary 3.5 this is the smallest odd number of vertices we can take to possibly find a

[1] This is a well–known result for graphs with 0–1 adjacency matrices. However, this result has been known to hold for any graph with a real and symmetric adjacency matrix from as early as 1968.

NSSD. The matrix $\mathbf{K}_7^{(a)}$ would be of the form

$$\mathbf{K}_7^{(a)} = \begin{pmatrix} 0 & a & 1 & 1 & 1 & 1 & a \\ a & 0 & a & 1 & 1 & 1 & 1 \\ 1 & a & 0 & a & 1 & 1 & 1 \\ 1 & 1 & a & 0 & a & 1 & 1 \\ 1 & 1 & 1 & a & 0 & a & 1 \\ 1 & 1 & 1 & 1 & a & 0 & a \\ a & 1 & 1 & 1 & 1 & a & 0 \end{pmatrix}$$

which has determinant

$$\det(\mathbf{K}_7^{(a)}) = 2(2+a)\big(f(a)\big)^2$$

where

$$f(a) = -1 + 2a + a^2 - a^3$$

The determinant of each $(n-1)\times(n-1)$ principal submatrix of $\mathbf{K}_7^{(a)}$ is

$$\det(\mathbf{K}_7^{(a)} - \mathbf{v}) = f(a)(1 - 6a - a^2 + a^3)$$

We require a value of a such that $\det(\mathbf{K}_7^{(a)}) \neq 0$ and $\det(\mathbf{K}_7^{(a)} - \mathbf{v}) = 0$. We have the conditions:

$$a \neq 0 \tag{4.2}$$
$$2 + a \neq 0 \tag{4.3}$$
$$f(a) \neq 0 \tag{4.4}$$
$$1 - 6a - a^2 + a^3 = 0 \tag{4.5}$$

Thus if we find a value for a that satisfies (4.2), (4.3), (4.4) and (4.5), then a complete NSSD is obtained. We note that the cubic equation (4.5) has the real solutions $a = -2.0938, 0.16296, 2.9308$, which also satisfy (4.2), (4.3) and (4.4). Indeed, if we take $a = 2.9308$, then the inverse of $\mathbf{K}_7^{(a)}$ is

$$\left(\mathbf{K}_7^{(a)}\right)^{-1} = \begin{pmatrix} 0 & 0.2327 & 0.068 & -0.25 & -0.25 & 0.068 & 0.2327 \\ 0.2327 & 0 & 0.2327 & 0.068 & -0.25 & -0.25 & 0.068 \\ 0.068 & 0.2327 & 0 & 0.2327 & 0.068 & -0.25 & -0.25 \\ -0.25 & 0.068 & 0.2327 & 0 & 0.2327 & 0.068 & -0.25 \\ -0.25 & -0.25 & 0.068 & 0.2327 & 0 & 0.2327 & 0.068 \\ 0.068 & -0.25 & -0.25 & 0.068 & 0.2327 & 0 & 0.2327 \\ 0.2327 & 0.068 & -0.25 & -0.25 & 0.068 & 0.2327 & 0 \end{pmatrix}$$

which is the circulant symmetric matrix $\langle 0, 0.2327, 0.068, -0.25, -0.25, 0.068, 0.2327\rangle$. For $a = -2.0938$ or 0.16296, a similar result is obtained.

We remark that the inverse of a non–singular circulant matrix is another circulant matrix; this is evident in $\left(\mathbf{K}_7^{(a)}\right)^{-1}$ above. Furthermore, $\left(\mathbf{K}_7^{(a)}\right)^{-1}$ represents a complete graph on seven vertices such that each one of its three edge–disjoint cycles has edges of weight 0.2327, 0.068 and -0.25, respectively.

Using a similar technique, we can show that if $\mathbf{K}_6^{(a)} = \langle 0, a, 1, 1, 1, a\rangle$, then $a = -1 \pm \sqrt{2}$ for $\mathbf{K}_6^{(a)}$ to be a NSSD. Indeed, if we choose $a = -1 - \sqrt{2} \approx -2.4142$, then

$\left(\mathbf{K}_6^{(a)}\right)^{-1} = \langle 0, -0.6306, 1.5224, -1.5224, 1.5224, -0.6306\rangle$. Furthermore, if $\mathbf{K}_8^{(a)} = \langle 0, a, 1, 1, 1, 1, a\rangle$, then, using the above method, we can show that when $a = 2.1889$, $\left(\mathbf{K}_8^{(a)}\right)^{-1} = \langle 0, -0.2592, 0.3459, 0.1898, -0.3082, 0.1898, 0.3459, -0.2592\rangle$. Hence, we have:

Theorem 4.4. *There exist complete NSSDs on 6, 7 and 8 vertices.*

4.3 Existence of Complete NSSDs on at least Nine Vertices

The method described in the previous subsection may go wrong in the case that a polynomial equation $\xi(a) = 0$ akin to (4.5) having only complex solutions is obtained. Indeed, this scenario happens if we apply our construction to $\mathbf{K}_5^{(a)}$; in this case the quadratic polynomial $\xi(a)$ is $a^2 + a + 1$, which has complex roots. Thus, there is no guarantee that the above construction will always yield a complete NSSD unless we prove that $\xi(a)$ has always at least one real root. This is what we do in the next theorem.

Theorem 4.5. *Let n be any integer greater than 8 and let $\mathbf{K}_n^{(a)}$ be a complete circulant symmetric matrix $\langle 0, a, 1, \ldots, 1, a\rangle$ on n vertices, $a \neq 0$. Then there exists a value of the parameter a strictly between 1 and $1 + \frac{1}{2}\sec\left(\frac{4\pi}{n}\right)$ such that K_n is a NSSD.*

Proof. We can determine the characteristic polynomials of $\mathbf{K}_n$ and $\mathbf{K}_n - \mathbf{v}$ from Proposition 4.3. For K_n to be a NSSD, we need to find a value of c such that $\psi(\mathbf{K}_n^{(a)}, 0, c) \neq 0$ and $\psi(\mathbf{K}_n^{(a)} - \mathbf{v}, 0, c) = 0$, recalling that $c = 2(a-1)$. Considering first the case when n is an odd number greater than 8, we obtain:

$$\begin{aligned} (1-c-n)(p(0,c))^2 &\neq 0 \\ \frac{p(0,c)}{n}\left(p(0,c) + 2(1-c-n)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1 - c\cos\left(\tfrac{2\pi q}{n}\right)\right)\right) &= 0 \end{aligned}$$

where $k = \frac{n-1}{2}$ and $p(0,c)$ is as defined in Proposition 4.3. Hence $c \neq 1-n$, $p(0,c) \neq 0$ and $h(c) = 0$, where

$$h(c) = \prod_{j=1}^{k}\left(1 - c\cos\left(\tfrac{2\pi j}{n}\right)\right) + 2(1-c-n)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1 - c\cos\left(\tfrac{2\pi q}{n}\right)\right) \qquad (4.6)$$

We note that $h(c)$ in (4.6) is a polynomial in c with real coefficients and hence it is continuous. Thus, if we show that there exist two distinct values of c for which $h(c)$ has opposite signs, then (4.6) has a real root by the intermediate value theorem.

Substituting $c = 0$ in (4.6), we obtain $h(0) = \left(\prod_{j=1}^{k} 1\right) + 2(1-n)\sum_{j=1}^{k}\left(\prod_{q=1,q\neq j}^{k} 1\right)$ $= 1 + 2(1-n)\left(\frac{n-1}{2}\right) = 1 - (n-1)^2 < 0$ since $n \geq 9$.

We now substitute an appropriate value of c such that $h(c) > 0$. Note, first of all, that

$\sec\left(\frac{4\pi}{n}\right) > 0$ since $n \geq 9$. Substituting this value for c in (4.6), we obtain

$$h\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = \prod_{j=1}^{k}\left(1-\sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi j}{n}\right)\right) + 2\left(1-\sec\left(\tfrac{4\pi}{n}\right)-n\right)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1-\sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi q}{n}\right)\right).$$

For $j=2$, $\left(1-\sec\left(\frac{4\pi}{n}\right)\cos\left(\frac{2\pi j}{n}\right)\right)=0$. Thus,

$$h\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = 2\left(1-\sec\left(\tfrac{4\pi}{n}\right)-n\right)\prod_{q=1,q\neq 2}^{k}\left(1-\sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi q}{n}\right)\right)$$

implying that

$$h\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = 2\left(1-\sec\left(\tfrac{4\pi}{n}\right)-n\right)\left(1-\frac{\cos\left(\frac{2\pi}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right)\left(\prod_{q=3}^{k}\left(1-\frac{\cos\left(\frac{2\pi q}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right)\right). \quad (4.7)$$

We now check the signs of each bracket in (4.7). Since $1 \leq \sec\left(\frac{4\pi}{n}\right) \leq \sec\left(\frac{4\pi}{9}\right) < 6$, we have that $1-\sec\left(\frac{4\pi}{n}\right)-n < 0$. Thus the first bracket of (4.7) is negative.

The second bracket of (4.7) is

$$1-\frac{\cos\left(\frac{2\pi}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)} = \frac{\cos\left(\frac{4\pi}{n}\right)-\cos\left(\frac{2\pi}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)} = \frac{-2\sin\left(\frac{3\pi}{n}\right)\sin\left(\frac{\pi}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}$$

which is negative since $n \geq 9$ and $\sin\theta > 0$ when $0 < \theta < \pi$.

The third bracket of (4.7) is

$$\begin{aligned}\prod_{q=3}^{k}\left(1-\frac{\cos\left(\frac{2\pi q}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right) &= \prod_{q=3}^{k}\left(\frac{\cos\left(\frac{4\pi}{n}\right)-\cos\left(\frac{2\pi q}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right)\\ &= \prod_{q=3}^{k}\left(\frac{2\sin\left(\frac{\pi(q+2)}{n}\right)\sin\left(\frac{\pi(q-2)}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right) \quad (4.8)\end{aligned}$$

Since the highest value of q is $k=\frac{n-1}{2}$, then the largest angle in (4.8) is $\frac{\pi(\frac{n-1}{2}+2)}{n}$ $= \frac{\pi(n+3)}{2n} < \pi$. Because of this, all the products in (4.8) are positive, and this means that the third bracket of (4.7) is positive. Thus, $h\left(\sec\left(\frac{4\pi}{n}\right)\right)$ in (4.7) is positive.

We now consider the case when n is even. By Proposition 4.3, we obtain

$$\begin{aligned}(1-c-n)(1+c)(p(0,c))^2 &\neq 0\\ \frac{p(0,c)}{n}\left((2-n)p(0,c)+2(1-c-n)(1+c)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1-c\cos\left(\tfrac{2\pi q}{n}\right)\right)\right) &= 0\end{aligned}$$

where $k = \frac{n-2}{2}$. Hence $c \neq 1-n$, $c \neq -1$, $p(0,c) \neq 0$ and $g(c) = 0$, where

$$g(c) = (2-n)\prod_{j=1}^{k}\left(1 - c\cos\left(\tfrac{2\pi j}{n}\right)\right) + \tag{4.9}$$
$$+ 2(1-c-n)(1+c)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1 - c\cos\left(\tfrac{2\pi q}{n}\right)\right)$$

As for the case when n was odd, since $g(c)$ in (4.9) is a polynomial in c, we search for two values of c such that $g(c)$ is positive for one value of c and negative for the other. We show that $c = 0$ and $c = \sec\left(\frac{4\pi}{n}\right)$ are again two such values of c.

Substituting $c = 0$ in (4.9), we obtain

$$g(0) = (2-n)\left(\prod_{j=1}^{k} 1\right) + 2(1-n)(1)\sum_{j=1}^{k}\left(\prod_{q=1,q\neq j}^{k} 1\right) = (2-n) + 2(1-n)\left(\frac{n-2}{2}\right) =$$

$-n(n-2) < 0$ since $n \geq 9$.

Substituting $c = \sec\left(\frac{4\pi}{n}\right)$ in (4.9), we obtain

$$g\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = (2-n)\prod_{j=1}^{k}\left(1 - \sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi j}{n}\right)\right)$$
$$+ 2\left(1 - \sec\left(\tfrac{4\pi}{n}\right) - n\right)\left(1 + \sec\left(\tfrac{4\pi}{n}\right)\right)\sum_{j=1}^{k}\prod_{q=1,q\neq j}^{k}\left(1 - \sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi q}{n}\right)\right)$$

$$g\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = 2\left(1 - \sec\left(\tfrac{4\pi}{n}\right) - n\right)\left(1 + \sec\left(\tfrac{4\pi}{n}\right)\right)\prod_{q=1,q\neq 2}^{k}\left(1 - \sec\left(\tfrac{4\pi}{n}\right)\cos\left(\tfrac{2\pi q}{n}\right)\right)$$

$$g\left(\sec\left(\tfrac{4\pi}{n}\right)\right) = 2\left(1 - \sec\left(\tfrac{4\pi}{n}\right) - n\right)\left(1 + \sec\left(\tfrac{4\pi}{n}\right)\right)\left(1 - \frac{\cos\left(\frac{2\pi}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right)$$
$$\left(\prod_{q=3}^{k}\left(1 - \frac{\cos\left(\frac{2\pi q}{n}\right)}{\cos\left(\frac{4\pi}{n}\right)}\right)\right) \tag{4.10}$$

Since $1 + \sec\left(\frac{4\pi}{n}\right) > 0$ and the product of all the other brackets in (4.10) was shown to be positive in the proof for the case when n is odd, $n \geq 9$, then $g\left(\sec\left(\frac{4\pi}{n}\right)\right)$ in (4.10) is positive.

Consequently, the polynomials (4.6) and (4.9) both have a root between $c = 0$ and $c = \sec\left(\frac{4\pi}{n}\right)$. Since $c = 2(a-1)$, the graph associated with the matrix $\mathbf{K}_n^{(a)}$ represents a NSSD for a value of a between 1 and $1 + \frac{1}{2}\sec\left(\frac{4\pi}{n}\right)$, as required. □

Remark 4.6. Observe that the lower bound for the parameter a in Theorem 4.5 can be improved to $\frac{3}{2}$. Since the upper bound tends to $\frac{3}{2}$ as n increases, we know that the adjacency matrix corresponding to a complete NSSD on a large number of vertices is given by $\langle 0, a, 1, \ldots, 1, a\rangle$ where $a = 1.5 + \varepsilon$ for a sufficiently small positive real value of ε.

We thus have the following existence result from Theorem 4.4 and Theorem 4.5.

Corollary 4.7. *For each $n \geq 6$, there always exists a complete NSSD on n vertices.*

In [8], a subclass of NSSDs referred to as **G**–*nutful graphs* was introduced and defined as follows.

Definition 4.8. A **G**–nutful graph G is either K_2 or a NSSD on at least three vertices having all two vertex–deleted subgraphs of the same nullity.

Recall that a necessary and sufficient condition for G to be a **G**–nutful graph is for its inverse to be a complete NSSD. We have established that besides K_2, there exist other **G**–nutful graphs.

Theorem 4.9. *There exist* **G**–*nutful graphs on any number of vertices greater than five.*

5 Conclusion

The complete graph K_2 has been well–known to be a complete NSSD. In this paper, we have shown that complete NSSDs exist for all positive integers at least six. This disproves a conjecture that appeared in [8] that NSSDs must have an even number of vertices. Indeed, NSSDs on an odd number vertices other than those that are complete graphs have also been found. An example is given by the graph with circulant adjacency matrix $\langle 0, -0.7549, 1, 0, 0, 1, -0.7549\rangle$, whose inverse is given by the circulant matrix $\langle 0, 0.1075, 0.5812, 0.3312, 0.3312, 0.5812, 0.1075\rangle$. However, we have also shown that no complete NSSDs exist on n vertices for $3 \leq n \leq 5$.

In [4, 7] it was conjectured that K_2 is the only *nuciferous graph*, that is a NSSD with 0–1 entries in its adjacency matrix whose inverse is complete. It is still an open problem whether a construction of complete NSSDs similar to that given in Section 4 may lead to an inverse with only 0–1 entries, which would then be nuciferous.

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Modified Wiener index via canonical metric representation, and some fullerene patches*

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Abstract

A variation of the classical Wiener index, the modified Wiener index, that was introduced in 1991 by Graovac and Pisanski, takes into account the symmetries of a given graph. In this paper it is proved that the computation of the modified Wiener index of a graph G can be reduced to the computation of the Wiener indices of the appropriately weighted quotient graphs of the canonical metric representation of G. The computation simplifies in the case when G is a partial cube. The method developed is applied to two infinite families of fullerene patches.

Keywords: Modified Wiener index, canonical metric representation, partial cubes, fullerene patches, nanocones.

Math. Subj. Class.: 05C12, 92E10

1 Introduction

The Wiener index is a central graph invariant in chemical graph theory as well as in metric graph theory, in the latter often being equivalently studied as the average distance. Several variations of the Wiener index were also extensively investigated, including the hyper-Wiener index and the terminal Wiener index. In 1991, Graovac and Pisanski [3]

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introduced the *modified Wiener index* with an idea to design a chemically applicable topological index which adequately takes into account the symmetries of a graph. The index received less attention than it deserves, but was studied recently by Koorepazan-Moftakhar and Ashrafi [13] where bounds on this graph invariant were obtained and exact values for some fullerenes.

Ten years after the seminal paper [3] an additional variation of the Wiener index was proposed in [15] and three years later named in [6] by the same term—the modified Wiener index. In the same paper the so-called variable Wiener index was also introduced; see the recent survey of Liu and Liu [14] on the variable Wiener index and related indices, especially on the related terminology. As it happens, also Graovac (see [16]) used the term modified Wiener index for the variation from [6, 15]. It is thus an unfortunate fact that the term modified Wiener index is nowadays used also for an invariant different from the one of Graovac and Pisanski. Anyhow, in this paper the term modified Wiener index is reserved for the original invariant. If the theory of this index will be more extensively developed in the future (for instance, it would be interesting to see how the invariant performs in the QSAR modelling for predicting physico-chemical properties of molecules), then the research community might wish to find a new name for it (to be honest, the terms "modified" and "variable" are not very descriptive), a possibility would be to call it the *Graovac-Pisanski index*.

We proceed as follows. In the next section concepts needed are formally introduced. The main result and its specialization to partial cubes are presented and proved in Section 3. In the final section we give closed expressions for the modified Wiener index of two infinite families of nanocones. These chemical graphs belong to the family of the so-called fullerene patches [4, 5].

2 Preliminaries

We denote the set $\{1, \ldots, n\}$ with $[n]$. Unless stated otherwise, graphs considered are simple and connected. The distance $d_G(u, v)$ between vertices u and v of G is the usual shortest-path distance. A subgraph of a graph is called *isometric* if the distance between any two vertices of the subgraph is independent of whether it is computed in the subgraph or in the entire graph.

The *Wiener index* $W(G)$ of G is the sum of distances between all pairs of vertices of G. A *weighted graph* (G, w) is a graph $G = (V(G), E(G))$ together with the weight function $w : V(G) \to \mathbb{R}_0^+$. The Wiener index $W(G, w)$ of (G, w), first introduced in [10], is:

$$W(G, w) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} w(u)\, w(v)\, d_G(u, v)\,.$$

Note that if $w \equiv 1$ then $W(G, w) = W(G)$.

The *modified Wiener index* $\widehat{W}(G)$ of G was introduced in [3] as

$$\widehat{W}(G) = \frac{|V(G)|}{2|\mathrm{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \mathrm{Aut}(G)} d_G(u, \alpha(u))\,,$$

where $\mathrm{Aut}(G)$ is the automorphism group of G. Roughly speaking, the modified Wiener index measures how far the vertices of a graph are moved on the average by its automorphisms.

The *Cartesian product* $G \,\square\, H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$, where the vertex (g, h) is adjacent to the vertex (g', h') whenever $gg' \in E(G)$ and $h = h'$, or $g = g'$ and $hh' \in E(H)$.

If G is a graph, then the Djoković-Winkler's relation Θ is defined on $E(G)$ as follows: if $e = xy \in E(G)$ and $f = uv \in E(G)$, then $e\Theta f$ if $d(x,u)+d(y,v) \neq d(x,v)+d(y,u)$. Relation Θ is reflexive and symmetric, hence its transitive closure Θ^* is an equivalence relation. The partition of $E(G)$ induced by Θ^* is called the Θ^**-partition* of $E(G)$. Let G be a graph and let $\{F_1, \ldots, F_k\}$ be the Θ^*-partition of $E(G)$. For any $j \in [k]$, let G/F_j be the graph whose vertex set consists of the connected components of the graph $G - F_j$, two components C and C' being adjacent if there exists an edge $uv \in F_j$ such that $u \in C$ and $v \in C'$. Further, for any $j \in [k]$ let $\alpha_j : G \to G/F_j$ be the mapping that assigns to each vertex of G the component of $G - F_j$ to which it belongs. Now, the *canonical metric representation* of G is the (isometric) mapping $\alpha = (\alpha_1, \ldots, \alpha_k) : G \to G/F_1 \,\square\, \cdots \,\square\, G/F_k$. This mapping is due to Graham and Winkler [2]. The fundamental property of α from [2] that is essential for us is that $\alpha(G)$ is an isometric subgraph of $G/F_1 \,\square\, \cdots \,\square\, G/F_k$.

3 The main result

Our main result (Theorem 3.1) asserts that $\widehat{W}(G)$ can be computed from the weighted Wiener indices of a collection of smaller graphs—the graphs of the canonical metric representation of G. Before stating the result we need to introduce the appropriate weighting functions.

Let G be a connected graph, let $V_1, \ldots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$, and let $F_1, \ldots, F_k$ be the Θ^*-classes of G. For any $i \in [t]$ and any $j \in [k]$ define $w_{ij} : V(G/F_j) \to \mathbb{R}_0^+$ by setting

$$w_{ij}(C) = |V_i \cap C|,\ C \in V(G/F_j)\,.$$

We are now ready for the main result.

Theorem 3.1. *Let G be a connected graph of order n and let $V_1, \ldots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$. If $F_1, \ldots, F_k$ are the Θ^*-classes of G, and G/F_j ($j \in [k]$) and w_{ij} ($i \in [t]$, $j \in [k]$) are as above, then*

$$\widehat{W}(G) = n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{j=1}^{k} W(G/F_j, w_{ij})\,.$$

Proof. We first recall from [3, p. 57] that the modified Wiener index can be equivalently written as $\widehat{W}(G) = n \sum_{i=1}^{t} (W(V_i)/|V_i|)$. Hence we can write

$$\widehat{W}(G) = n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{\{x,y\} \subseteq V_i} d_G(x,y)\,.$$

As already mentioned above, the canonical metric representation α is an isometry. Moreover, it is well-known (cf. for instance [7, Proposition 5.1]) that the distance function is additive on the Cartesian product operation, that is, $d_{G \,\square\, H} = d_G + d_H$. These facts yield

the first equality in the following computation:

$$\begin{aligned}
\widehat{W}(G) &= n\sum_{i=1}^{t}\frac{1}{|V_i|}\sum_{\{x,y\}\subseteq V_i}\sum_{j=1}^{k} d_{G/F_j}(\alpha_j(x),\alpha_j(y)) \\
&= n\sum_{i=1}^{t}\frac{1}{|V_i|}\left(\sum_{j=1}^{k}\sum_{\{x,y\}\subseteq V_i} d_{G/F_j}(\alpha_j(x),\alpha_j(y))\right) \\
&= n\sum_{i=1}^{t}\frac{1}{|V_i|}\sum_{j=1}^{k}\left(\frac{1}{2}\sum_{x\in V_i}\sum_{y\in V_i} d_{G/F_j}(\alpha_j(x),\alpha_j(y))\right) \\
&= n\sum_{i=1}^{t}\frac{1}{|V_i|}\sum_{j=1}^{k} W(G/F_j, w_{ij})\,.
\end{aligned}$$

To see the truth of the last equality, note that a pair of vertices $x \in V_i \cap C$ and $y \in V_i \cap C'$, where C, C' are components of $G-F_j$, contributes $d_{G/F_j}(\alpha_j(x),\alpha_j(y))$ to the summation. For each such pair of vertices the contribution is the same and there are $w_{ij}(C)\cdot w_{ij}(C')$ such pairs. □

We note that a result parallel to Theorem 3.1 was earlier proved in [9] for the Wiener index, see [1, 17] for applications of this result. It was recently further generalized twofold: to vertex-weighted graphs and to partitions coarser that the Θ^*-partition [11].

An important case containing many chemical graphs is the class of graphs isometrically embeddable into hypercubes; these graphs are known as *partial cubes*. It is well known that these graphs are precisely the connected bipartite graphs for which the relation Θ is transitive. Moreover, if F is an arbitrary Θ-class (or, equivalenty, an arbitrary Θ^*-class) of G, then $G - F$ consists of two connected components. It therefore follows that for partial cubes Theorem 3.1 can be simplified as follows:

Corollary 3.2. *Let G be a partial cube of order n and let $V_1, \ldots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$. If $F_1, \ldots, F_k$ are the Θ-classes of G, and $n_{ij} = |V_i \cap C_j|$, $n'_{ij} = |V_i \cap C'_j|$ ($i \in [t]$, $j \in [k]$), where C_j and C'_j are the connected components of $G - F_j$, then*

$$\widehat{W}(G) = n\sum_{i=1}^{t}\frac{1}{|V_i|}\sum_{j=1}^{k} n_{ij}\cdot n'_{ij}\,.$$

4 Modified Wiener index of two families of fullerene patches

To illustrate the applicability of Theorem 3.1 and Corollary 3.2 we determine in this section the modified Wiener index of two families of nanocones.

4.1 $\widehat{W}$ of nanocones NCH(n)

The nanocones NCH(n), $n \geq 1$, are defined as follows. NCH(1) is isomorphic to the 6-cycle ("H" in the name stands for "hexagon"), while for $n \geq 2$, the nanocone NCH(n) is obtained from NCH($n-1$) by adding an additional outer ring of hexagons to it. The construction should be clear from Fig. 1 where NCH(4) is shown. (These nanocones are in chemical graph theory also known as the coronene/circumcoronene series.)

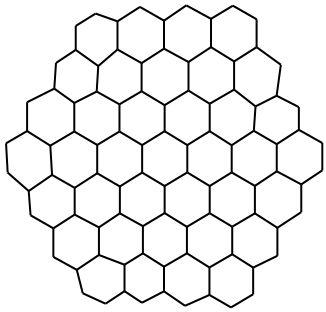

Figure 1: The nanocone NCH(4)

It is well-known that the nanocones NCH(n) are partial cubes (cf. [12]). Using Corollary 3.2 we can thus obtain the next result, a sketch of its proof being given in the rotation of this subsection.

Theorem 4.1. *If* $n \geq 1$, *then* $\widehat{W}(\mathrm{NCH}(n)) = 3n^3(10n^2 - 1)$.

NCH(n) contains n concentric cycles (that is, the cycles iteratively added when the graphs is built from NCH(1)), call them the *layers* of NCH(n) and denote with $L_1, \ldots, L_n$. Clearly, $|L_i| = 12i-6$, $1 \leq i \leq n$. Consequently, $|V(\mathrm{NCH}(n))| = \sum_{i=1}^{n}(12i-6) = 6n^2$.

The Θ-classes of NCH(n) are its orthogonal cuts, in Fig. 2 the horizontal cuts of NCH(4) are shown. In general, the cuts are in three directions and hence NCH(n) contains $3(2n-1)$ Θ-classes.

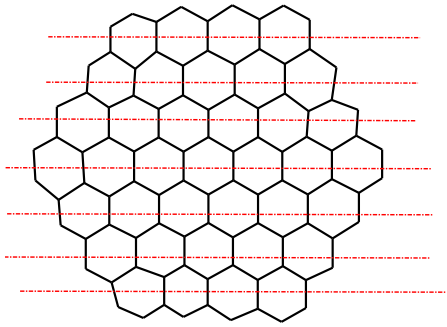

Figure 2: Horizontal Θ-classes of NCH(4)

To apply Corollary 3.2 we also need to know the symmetries of NCH(n); we claim that the automorphism group of NCH(n) is isomorphic to the dihedral group D_{12} of order 12. To simplify the notation set $\Gamma = \mathrm{Aut}(\mathrm{NCH}(n))$. Let α be the rotation of NCH(n) for 60°, and let β be the reflection of NCH(n) over the central vertical line. Clearly, $\Gamma \geq \langle \alpha, \beta \rangle$. On the other hand, if x is any vertex of the middle hexagon of NCH(n), then its orbit x^Γ is formed by the vertices of the middle hexagon and its stabilizer Γ_x consists of the identity and the reflection over the line through x and its antipode on the inner cycle. Hence

$|\Gamma| = |x^\Gamma| \times |\Gamma_x| = 12$. Since $\alpha^6 = \beta^2 = 1$ and $\beta^{-1}\alpha\beta = \alpha^{-1}$, we conclude that Γ is indeed isomorphic to D_{12}. Note furthermore that each orbit of the action of Γ is a subset of some layer L_i, $i \in [n]$. Moreover, the layer L_i contains $i-1$ orbits of size 12 and one orbit of size 6.

For a graph G set

$$\widehat{w}(G) = \widehat{W}(G)/|V(G)|\,,$$

so that $\widehat{W}(\mathrm{NCH}(n)) = 6n^2\widehat{w}(\mathrm{NCH}(n))$. Using the above description of orbits, Corollary 3.2, and considering the contributions of the vertices from L_n, a straightforward (but somehow lengthy) computation yields the recurrence

$$\begin{aligned}\widehat{w}(\mathrm{NCH}(1)) &= \frac{9}{2}\,,\\ \widehat{w}(\mathrm{NCH}(n)) &= \widehat{w}(\mathrm{NCH}(n-1)) + 15n(n-1) + \frac{9}{2}, \quad n \geq 2\,.\end{aligned}$$

The solution of this recurrence is $\widehat{w}(\mathrm{NCH}(n)) = 5n^3 - \frac{n}{2}$ and Theorem 4.1 follows.

4.2 $\widehat{W}$ of nanocones NCP(n)

The nanocones NCP(n), $n \geq 1$, are defined analogously as the nanocones NCH(n), except that now we start with a pentagon (hence the letter "P" in NCP) and then adding rings of hexagons to it. More precisely, NCP(1) is isomorphic to the 5-cycle, while for $n \geq 2$ the nanocone NCP(n) is obtained from NCP($n-1$) by adding an additional outer ring of hexagons to it. See Fig. 3 for NCP(4).

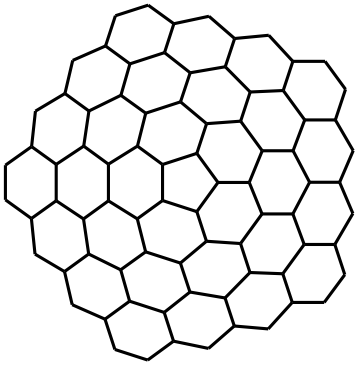

Figure 3: The nanocone NCP(4)

Since nanocones NCP(n) are not partial cubes, we cannot apply Corollary 3.2 for them, hence we need to use the more general Theorem 3.1 to get:

Theorem 4.2. *If $n \geq 1$, then $\widehat{W}(\mathrm{NCP}(n)) = 5n^3(11n^2-2)/3$.*

In the rest of this subsection we give a sketch of the proof of this result.

Just as for NCH(n), let us denote with $L_1, \ldots, L_n$ the *layers* of NCP(n). Since $|L_i| = 10i - 5$, $i \in [n]$, we get that $|V(\mathrm{NCP}(n))| = \sum_{i=1}^{n} 10i - 5 = 5n^2$. The Θ^*-classes of NCP(n) can be described as follows. One class, say F, consists of the edges of the inner

5-cycle together with the edges of the cuts propagating from them, see the left-hand side of Fig. 4. (The right-hand side of the figure shows the graph $\mathrm{NCP}(4) - F$.) All the other Θ^*-classes of NCP(n) are the orthogonal cuts across hexagons. Since each additional layer defines five such cuts, the total number of Θ^*-classes is $1 + 5(n-1) = 5n - 4$.

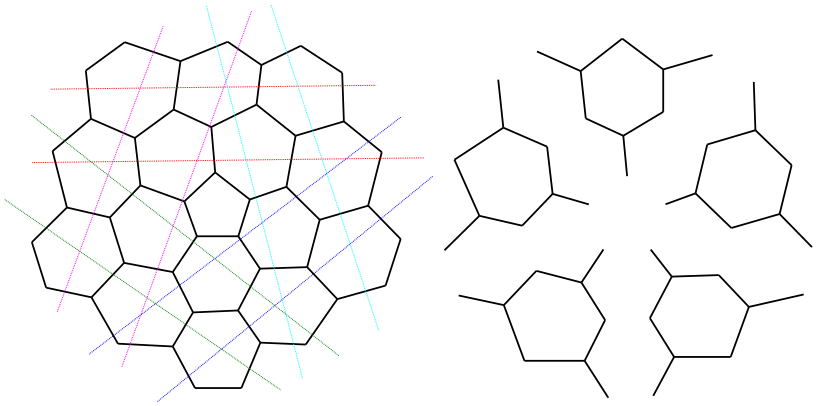

Figure 4: Θ^*-classes of NCP(3)

Similarly as for NCH(n), the automorphism group of NCP(n) is isomorphic to the dihedral group D_{10} of order 10. Set $\Gamma = \mathrm{Aut}(\mathrm{NCP}(n))$, let α be the rotation of NCP(n) for 72°, and let β be the reflection of NCP(n) over the central vertical line. Clearly, $\Gamma \geq \langle \alpha, \beta \rangle$. On the other hand, if x is any vertex of the middle pentagon of NCP(n), then its orbit x^Γ is formed by the vertices of the middle pentagon and its stabilizer Γ_x consists of the identity and the reflection over the line through x and the midpoint of the edge opposite to x. Hence $|\Gamma| = |x^\Gamma| \times |\Gamma_x| = 10$. Since $\alpha^5 = \beta^2 = 1$ and $\beta^{-1}\alpha\beta = \alpha^{-1}$, we conclude that Γ is isomorphic to D_{10}. Furthermore, the layer L_i, $i \in [n]$, contains $i - 1$ orbits of size 10 and one orbit of size 5. Using Theorem 3.1 and considering the contributions of the vertices from L_n, a straightforward computation yields

$$\begin{aligned} \widehat{w}(NCP(1)) &= 3, \\ \widehat{w}(NCP(n)) &= \widehat{w}(NCP(n-1)) + 11n(n-1) + 3, \ \ n \geq 2. \end{aligned}$$

The solution of this recurrence is $\widehat{w}(NCP(n)) = (11n^3 - 2n)/3$ and Theorem 4.2 follows.

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Counting maximal matchings in linear polymers

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Abstract

A matching M in a graph G is maximal if it cannot be extended to a larger matching in G. In this paper we show how several chemical and technical problems can be successfully modeled in terms of maximal matchings. We introduce the maximal matching polynomial and study its basic properties. Then we enumerate maximal matchings in several classes of graphs made by a linear or cyclic concatenation of basic building blocs. We also count maximal matchings in joins and corona products of some classes of graphs.

Keywords: Maximal matching, maximal matching polynomial, cactus graph, cactus chain, Padovan numbers, Perrin numbers, corona product.

Math. Subj. Class.: 05C30, 05C70

1 Introduction

Many problems in natural, technical and social sciences can be successfully formulated in terms of matchings in graphs. Today the matching theory is a well developed branch of graph theory, studying both structural and enumerative aspects of matchings. Its development has been strongly stimulated by chemical applications, in particular by the study of perfect matchings in benzenoid graphs. Additional impetus came with discovery of fullerenes, again mostly dealing with perfect matchings [5, 6, 22, 30], but including also some structural results [1, 7].

For a general background on matching theory and terminology we refer the reader to the classical monograph by Lovász and Plummer [24]. For graph theory terms not defined here we also recommend [29].

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A **matching** M in a graph G is a collection of edges of G such that no two edges from M share a vertex. The cardinality of M is called the **size** of the matching. As the matchings of small size are not interesting (each edge is a matching of size one, and the empty set is the unique matching of size 0), we will be mostly interested in matchings that are, in a sense, "large". Most often, we are interested in matchings that are as large as possible.

A matching M is **maximum** if there is no matching in G with more edges than M. The cardinality of any maximum matching in G is called the **matching number** of G and denoted by $\nu(G)$. Since each vertex can be incident to at most one edge of a matching, it follows that the matching number of a graph on n vertices cannot exceed $\lfloor n/2 \rfloor$. If each vertex of G is incident with an edge of M, the matching M is called **perfect**. Perfect matchings are obviously also maximum matchings. The perfect matchings, also known as **Kekulé structures** in chemical literature, have played a central role in the study of matchings for several decades.

There is, however, an alternative way to quantify the idea of "large" matchings. A matching M in G is **maximal** if no other matching in G contains it as a proper subset. Obviously, every maximum matching is also maximal, but the opposite is generally not true.

Maximal matchings are much less researched that their maximum counterparts. That goes both for their structural and their enumerative aspects. While there is vast literature on perfect and maximum matchings (see, for example, monographs [24] and [4]), the results about maximal matchings are few and scattered through the literature. We mention here two papers that treat, among other topics, maximal matchings in trees [23, 28], one concerned with the structure of equimatchable graphs [17], and a recent paper by the present authors about saturation numbers of benzenoid graphs [11].

Maximal matchings can serve as models of several physical and technical problems such as the block-allocation of a sequential resource or adsorption of dimers on a structured substrate or a molecule. When that process is random, it is clear that the substrate can become saturated by a number of dimers much smaller than the theoretical maximum. The cardinality of any smallest maximal matching in G is the **saturation number** of G. The saturation number of a graph G we denote by $s(G)$. (The same term, saturation number, is also used in the literature with a different meaning; we refer the reader to [14] for more information.)

It is easy to see that the saturation number of a graph G is at least one half of the matching number of G, i.e., $s(G) \geq \nu(G)/2$. Hence, the saturation number provides an information on the worst possible case of clogging; it is a measure of how inefficient the adsorption process can be. However, to fully assess its efficiency, we also need to know how likely it is that the substrate gets saturated by a given number of dimers. In order to answer that question, one must study the enumerative aspects of the problem.

The main goal of this paper is to increase the corpus of knowledge about the enumerative aspects of maximal matchings. Specifically, we compute the efficiency of dimer adsorption for several types of one-dimensional substrates by enumerating maximal matchings of various cardinality in the corresponding graphs. We start with structures of low connectivity and explore how the efficiency depends on the structural properties of their basic building blocks. It turns out that already the structures of the lowest connectivity display interesting patterns of behavior. In some cases we provide explicit formulas for the number of maximal matchings of a given cardinality, while in other cases we establish the recurrences for the enumerating sequences and then use their uni- and bivariate generating

functions to determine their asymptotic behavior. Along the way we make several digressions and consider also some graphs that do not fit the above pattern but are amenable to the same approach. We also explore the connections with other combinatorial structures counted by the same enumerating sequences and provide bijective correspondences when possible.

The paper is organized as follows. In the next section we introduce the maximal matching polynomial and list its basic properties. Section 3 is concerned with enumeration of maximal matchings in the simplest linear polymers, the paths and cycles. Section 4 considers the case when basic building blocs are the cycles of length 3 and 4, enumerating maximal matchings in uniform chain cacti. Section 5 moves on to some linear chains of connectivity 2, such as the ladder graphs. (The graphs of sections 4 and 5 belong to the class of fasciagraphs [21].) In section 6 we use the theory of maximal matching polynomials to obtain general results for some classes of thorny graphs, while in section 7 we consider some composite graphs that arise from simpler components *via* two binary operations, the join and the corona product. Finally, in the concluding section we discuss some open problems and indicate some directions of possible future research.

2 Maximal matching polynomial

Matching polynomials are generating functions for the sequences enumerating matchings in a graph G by their size. There are several forms, the two most common being the matching defect polynomial and the matching generating polynomials. Both forms appear as special cases of general matching polynomials introduced by Farrell in [13]. Fortunately, the two forms are closely related and can be used interchangeably. Throughout this paper we prefer the second form.

Let $\Phi_k(G)$ denote the number of matchings in G of size k. The **matching generating polynomial** (or simply the **matching polynomial**) of G is then defined as

$$g(G;x) = \sum_{k=0}^{\nu(G)} \Phi_k(G) x^k.$$

Clearly, $g(G;1)$ is equal to the total number of matchings in G; this quantity is also known as **Hosoya index** of G and denoted by $Z(G)$. For bipartite graphs, $g(G;x)$ is also known as the **rook polynomial** [25]. We refer the reader to Section 8.5 of [24] for more information on matching polynomials and relationships among them.

The following two properties, together with the fact $g(K_1;x) = 1$, allow us to compute the matching polynomial of any graph by recursively reducing it to trivial components. Here $G - e$ denotes the result of deleting an edge from G but keeping its end-vertices, while $G\backslash e$ denotes the graph obtained from G by deleting both end-vertices of e and all edges incident with them.

Proposition 2.1. *Let G be a graph and e an edge of G. Then*

$$g(G;x) = g(G-e;x) + x \cdot g(G\backslash e;x).$$

□

Proposition 2.2. *Let G be a graph with components $G_1, \ldots, G_k$. Then*

$$g(G;x) = g(G_1;x) \cdot \ldots \cdot g(G_k;x).$$

□

By repeated applications of these results one can obtain a recurrence in terms of vertices and their neighborhoods [24].

Proposition 2.3. *Let $N(u) = \{v_1, \ldots, v_k\}$ be the neighborhood of a vertex u of G. Then*

$$g(G; x) = g(G - u; x) + x \sum_{i=1}^{k} g(G - u - v_i; x).$$

□

Here the first term accounts for the matching that do not cover u, while the sum counts those covering it.

Let P_n and C_n denote the path and the cycle of length n, respectively. Their matching polynomials are given by following formulas:

$$g(P_n; x) = \sum_{k=0}^{\lceil n/2 \rceil} \binom{n+1-k}{k} x^k;$$

$$g(C_n; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n}{n-k} \binom{n-k}{k} x^k.$$

From them it follows that the total numbers of matchings in P_n and C_n are given by the Fibonacci and Lucas numbers F_{n+2} and L_n, respectively. Matching polynomials of paths and cycles are closely related to Fibonacci and Lucas polynomials, respectively. The **Fibonacci polynomials** are defined recursively by $f_0(x) = 0$, $f_1(x) = 1$, $f_2(x) = x$ and

$$f_n(x) = x f_{n-1}(x) + f_{n-2}(x)$$

for $n \geq 3$. The **Lucas polynomials** $\ell_n(x)$ satisfy the same recurrence, but with the initial conditions $\ell_0(x) = 2$, $\ell_1(x) = x$. Evaluated at $x = 1$ they give the Fibonacci and Lucas numbers, respectively. The following result can be easily verified by direct computation.

Proposition 2.4.

$$f_{n+2}(x) = x^{n+1} g(P_n; x^{-2}) \qquad \text{and} \qquad \ell_n(x) = x^n g(C_n; x^{-2}).$$

□

Motivated by wide applicability of matching polynomials, we consider the generating function for the sequence counting maximal matchings in a graph G. Let $\Psi_k(G)$ denote the number of maximal matchings of size k in G. The **maximal matching polynomial** of G is defined as

$$m(G; x) = \sum_{k=s(G)}^{\nu(G)} \Psi_k(G) x^k.$$

For example, $m(P_3; x) = x + x^2$, since P_3 contains one maximal matching of size one (the middle edge) and one of size two (covering the vertices of degree one). From the next two examples, $m(C_3; x) = 3x$ and $m(S_3; x) = 3x$ (where S_3 denotes the star $K_{1,3}$), one can see that graphs are not, in general, determined by their maximal matching polynomials. Some further examples are collected in the following proposition.

Proposition 2.5. $m(\overline{K_n}; x) = 1$;
$m(S_n; x) = nx$;
$m(K_{2n}; x) = \frac{(2n)!}{n!2^n}x^n$;
$m(K_{n,n}; x) = n!x^n$;
$m(K_{m,n}; x) = n^{\underline{m}}x^m$ *for* $m \leq n$.

Proof. The first claim is obvious, since there is only one possible matching (the empty one) in a graph without edges. The second claim is also obvious. The next two follow by noticing that in K_{2n} and $K_{n,n}$ every matching can be extended to a perfect matching [24] and plugging in the expressions for the number of perfect matchings in each case. Finally, the fifth claim follows from the fact that the first edge of any matching in $K_{m,n}$ can be chosen in n ways, the second one in $n-1$ ways and so on. The process ends when there are no more unsaturated vertices in the smaller class of bipartition. (Here $n^{\underline{m}}$ denotes the falling factorial.) □

Let us look at the information encoded in maximal matching polynomials. Its degree is equal to the matching number $\nu(G)$. The lowest degree of x is equal to the saturation number. From there it follows that zero is a root of the maximal matching polynomial of every non-empty graph, and its multiplicity is equal to the saturation number. The set of all powers that appear in $m(G; x)$ is called the **maximal matching spectrum** of G. We denote it by $\sigma_m(G)$. A graph G is **equimatchable** if each maximal matching in G is also a maximum matching [24]. Clearly, a graph G is equimatchable if and only if its maximal matching spectrum is a singleton.

Proposition 2.6. *Maximal matching spectrum of any graph G is a set of consecutive nonnegative integers.*

Proof. If G is an equimatchable graph, the claim is obviously valid. If G is not an equimatchable graph, then $s(G) < \nu(G)$. We show that for each nonnegative integer $s(G) \leq k \leq \nu(G)$ there exist a maximal matching in G of size k. If $k = s(G)$ or $k = \nu(G)$ the claim is trivially valid. Let now $k < \nu(G)$ and let M be a maximal matching in G of size k. (Such a matching surely exists; at least there is a maximal matching whose size is equal to $s(G)$.) As M is not a maximum matching, there is an M-augmenting path P connecting two vertices not covered by M whose terminal edges are not in M (Theorem 1.2.1 of [24]). The edges of P alternate with respect to M. By switching the edges along this path one obtains matching M' of size $k+1$, and M' is also maximal. Hence, for any k between $s(G)$ and $\nu(G)$ there is a maximal matching in G of size k. □

Corollary 2.7. *Let G be a nontrivial graph. Then*

$$\sigma_m(G) = \mathbb{N} \cap [s(G), \nu(G)].$$

□

Corollary 2.8. *The sequence of coefficients of the maximal matching polynomial of a graph G contains no internal zeros.* □

The maximal matching polynomials share a number of properties with the matching polynomials. For example, Proposition 2.2 is valid also for maximal matching polynomials. However, there is a crucial difference. While the recurrences for matching polynomials are

local, those for the maximal matching polynomials are not. The non-locality means that there is no result for maximal matching polynomials analogous to Proposition 2.1, since we cannot split the set of all maximal matchings into those containing an edge e and those not containing it, without taking into account the edge-neighborhood of e. Similarly, no result analogous to Proposition 2.3 can be stated for maximal matching polynomials of general graphs. This non-locality is the main source of the difficulties while trying to count maximal matchings.

There are, however, classes of graphs in which the edge- and vertex-neighborhoods lead to recurrent relations only a bit more complicated than those for ordinary matching polynomials. As a rule, such graphs are of low connectivity and/or contain vertices of degree one. The fact that (the unique) neighbor of a pendent vertex must be covered by an edge of every maximal matching gives us an analogue of Proposition 2.3. For a given vertex $u \in V(G)$ we denote by $N_1(u)$ the set of all its neighbors of degree one.

Proposition 2.9. *Let G be a simple connected graph and $u \in V(G)$ its vertex such that $|N_1(u)| = t > 0$. Then*

$$m(G;x) = tx \cdot m(G-u;x) + x \sum_{v \in N(u) \setminus N_1(u)} m(G-u-v;x).$$

Proof. Vertex u must be covered by an edge in each maximal matching of G. It can be one of t pendent edges, in which case the remaining edges must form a valid maximal matching in $G-u$, or it can be one of the remaining edges incident to u, say uv, in which case the remaining edges must form a maximal matching in $G-u-v$. In both cases, the size of the maximal matching formed by the remaining edges is one less than the size of matching that covers u, hence the factor x in both terms. □

We know that the generating matching polynomials are log-concave [18, 19]. It would be interesting to know if this property is also valid for maximal matching polynomials.

We will make frequent use of the above results in the following sections.

3 Paths and cycles

We remind the reader that throughout this paper P_n denotes the path of length n, hence on $n+1$ vertices. As a motivating example, we consider a parking lot made of $n+1$ parallel concrete strips such that a car can be parked on any two neighboring strips, as shown in Fig. 1. In ideal situation, when all drivers park responsibly, the lot can accommodate

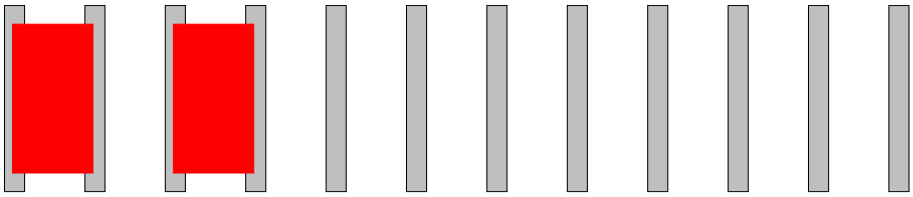

Figure 1: A parking lot with two parked cars.

$\lceil n/2 \rceil$ cars. However, if the drivers are careless and park randomly, the lot can become

saturated by a smaller number of cars, as shown in Fig. 2. In the worst possible case, it can become saturated by $\lceil n/3 \rceil$ cars. The problem can be naturally interpreted as a problem of

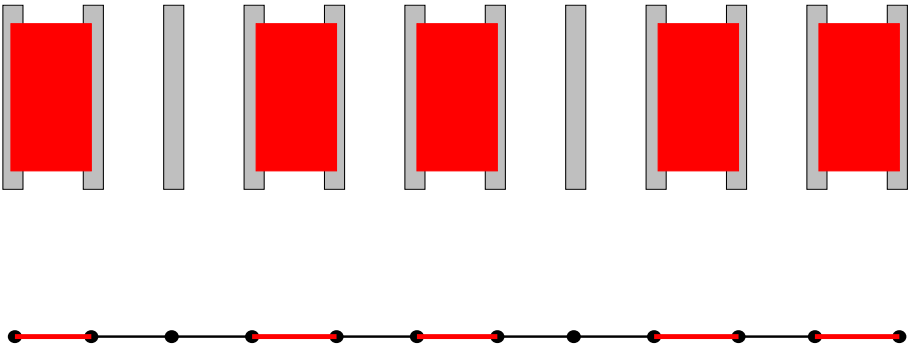

Figure 2: A saturated parking lot and the corresponding maximal matching.

maximal matching in P_n, as shown in Fig 2. In order to determine the expected number of cars under the random regime of parking, we need to count the number of maximal matching of different sizes in P_n.

We start by counting all maximal matchings in P_n. Let ψ_n denote the total number of maximal matchings in P_n.

Proposition 3.1. *The sequence ψ_n is given by the recurrence*

$$\psi_n = \psi_{n-2} + \psi_{n-3}$$

for $n \geq 3$. The initial conditions are $\psi_0 = \psi_1 = 1, \psi_2 = 2$.

Proof. Let us label the vertices of P_n by $v_0, v_1, \ldots, v_n$. Then any maximal matching in P_n must cover v_{n-1}. Those covering it by the edge $v_{n-1}v_n$ are counted by ψ_{n-2}; those covering it by $v_{n-2}v_{n-1}$ are counted by ψ_{n-3}. The initial conditions are verified by direct computation. □

The sequence (ψ_n) is known as the **Padovan sequence**. It appears (shifted by 6) as A000931 in the On-line Encyclopedia of Integer Sequences [26] (in the rest of this paper simply the OEIS). The number of maximal matchings in paths is not mentioned among some seventeen combinatorial interpretations listed there. Hence, we have provided a new combinatorial representation of the Padovan sequence. It would be interesting to provide explicit bijections between maximal matchings in paths and some combinatorial structures listed in the OEIS entry.

Let $\psi_{n,k}$ denote the number of maximal matchings in P_n of size k. It is clear that $\psi_{n,k} = 0$ for too small or too large k. By the same reasoning as in Proposition 3.1 we can prove the recurrence for $\psi_{n,k}$.

Proposition 3.2.

$$\psi_{n,k} = \psi_{n-2,k-1} + \psi_{n-3,k-1}$$

for $n \geq 3$, with the initial conditions $\psi_{0,0} = 1$, $\psi_{1,0} = 0$, $\psi_{1,1} = 1$, $\psi_{2,0} = 0$, $\psi_{2,1} = 2$. □

Now we can proceed and obtain the bivariate generating function $\Psi(x,y)$ for $\psi_{n,k}$. We omit the computational details.

Proposition 3.3.

$$\Psi(x,y) = \sum_{n\geq 0}\sum_{k\geq 0} \psi_{n,k} x^n y^k = \frac{1+xy+x^2y}{1-x^2y-x^3y}.$$

□

The ordinary generating function $\Psi(x) = \sum_{n\geq 0} \psi_n x^n$ is now obtained as

$$\Psi(x) = \Psi(x,1) = \frac{1+x+x^2}{1-x^2-x^3}.$$

Now we employ a variant of Darboux theorem to extract the information about the asymptotic behavior of ψ_n [2]: If the generating function $f(x) = \sum_{n\geq 0} a_n x^n$ of a sequence (a_n) can be written in the form $f(x) = \left(1-\frac{x}{w}\right)^{\alpha} h(x)$, where w is the smallest modulus singularity of f and h is analytic in w, then $a_n \sim \frac{h(w)n^{-\alpha-1}}{\Gamma(-\alpha)w^n}$, where Γ denotes the gamma function.

By a straightforward computation we find the smallest modulus singularity of $\Psi(x)$ as the only real solution of $1-x^2-x^3=0$:

$$w = \frac{1}{6}\left(-2 + (100-12\sqrt{69})^{1/3} + (100+12\sqrt{69})^{1/3}\right) \approx 0.754878.$$

Its reciprocal value, $1/w \approx 1.324718$, is known as the **plastic constant** [15]. From there we obtain the asymptotics for ψ_n.

Proposition 3.4.

$$\psi_n \sim g(w)w^{-n} = 0.956611 \cdot 1.324718^n.$$

□

Using the same apparatus we can also compute the expected size of a maximal matching in P_n. Let us denote it by $\pi(P_n)$. It can be computed as

$$\pi(P_n) = \frac{[x^n]\frac{\partial \Psi(x,y)}{\partial y}\,|_{y=1}}{[x^n]\Psi(x,y)\,|_{y=1}},$$

where $[x^n]F(x)$ denotes the coefficient of x^n in the expansion of $F(x)$. We omit the computational details and present only the final result.

Proposition 3.5. *The expected size of a maximal matching in P_n is given by $\pi(P_n) \approx 0.41149559n$.* □

Now we define the **efficiency** $\varepsilon(G)$ of random parking on a graph G as the ratio of the expected size of a maximal matching in G and its matching number (the ideal case). Hence, $\varepsilon(G) = \frac{\pi(G)}{\nu(G)}$. In our case,

$$\varepsilon(P_n) = \frac{\pi(P_n)}{\left\lceil \frac{n}{2} \right\rceil}.$$

For large values of n this quantity behaves as $2\pi(P_n) \approx 0.823$. Hence, one can expect that random (or careless) parking will result in using about 82.3% of the full capacity of a linear parking lot.

We could now use the bivariate generating function $\Psi(x, y)$ to obtain closed formulas for the numbers $\psi_{n,k}$. Instead, we provide a combinatorial proof.

Proposition 3.6.

$$\psi_{n,k} = \binom{k+1}{3k-n}.$$

Proof. We use the formula for balls and boxes in the table of the Twelvefold Way at p. 33 in [27]. The balls are the edges participating in a maximal matching, the boxes are defined by the unmatched vertices. There are k edges and $n+1-2k$ unmatched vertices. They define $n-2k+2$ boxes, $n-2k$ between two vertices and additional 2, one to the left of the leftmost unmatched vertex, the other one to the right of the rightmost one. Into each of $n-2k$ internal boxes we place one ball (since the unmatched vertices cannot be adjacent). The remaining $3k-n$ balls can be distributed at will among all $n-2k+2$ boxes. As the number of ways to place a identical balls into b distinct boxes is equal to $\binom{a+b-1}{a}$, the claim follows by using the symmetry property of binomial coefficients. □

As usual, we assume that a binomial coefficient is equal to zero if its lower index exceeds the upper one or becomes negative.

Corollary 3.7. *The maximal matching polynomial of P_n is given by*

$$m(P_n; x) = \sum_{\lceil n/3 \rceil}^{\lceil n/2 \rceil} \binom{k+1}{3k-n} x^n.$$

□

Corollary 3.8.

$$\psi_n = \sum_{\lceil n/3 \rceil}^{\lceil n/2 \rceil} \binom{k+1}{3k-n}.$$

□

The last result gives us the decomposition of Padovan numbers similar to the familiar expression for the Fibonacci numbers, $F_n = \sum_{k \geq 0} \binom{n-k}{k}$. The maximal matching polynomials of P_n satisfy the recurrence $m(P_n; x) = x(m(P_{n-2}; x) + m(P_{n-3}; x))$. Evaluated at $x = 1$, they give the Padovan numbers. Hence, one could be tempted to call them **Padovan polynomials**. However, the name is already used for another family of polynomials satisfying the recurrence $p_n(x) = xp_{n-2}(x) + p_{n-3}(x)$ with initial conditions $p_1(x) = 1$, $p_2(x) = 0$ and $p_3(x) = x$. It would be interesting to explore our version of Padovan polynomials in more detail and develop a theory analogous to the theory of Fibonacci polynomials. We do not know if the expression of Corollary 3.8 is new, but it does not appear in the OEIS.

Before we move to the cycles, we mention that a similar problem was considered in the context of polymerization of organic molecules. Jackson and Montroll [20] used probabilistic reasoning and obtained the value of 0.177 for the average fraction of free radicals

in a polymer chain, the same value as the expected fraction of wasted space in our parking lot model. The dynamic aspect of the process was studied by Flory [16], who obtained a slightly larger value of 86.47% (the exact value is $1 - e^{-2}$) for a quantity that we call the efficiency. The difference indicates that some of the most unfavorable configurations are quite unlikely to arise during the process. More information on various models of random and cooperative sequential adsorption can be found in a survey by Evans [12].

Let us now consider the number of maximal matchings in a cycle C_n of length $n \geq 3$. We denote it by φ_n, and the number of maximal matchings in C_n of size k by $\varphi_{n,k}$.

Proposition 3.9. *The numbers $\varphi_{n,k}$ are given by the recurrence*

$$\varphi_{n,k} = \varphi_{n-2,k-1} + \varphi_{n-3,k-1}$$

for $n \geq 3$, $k \geq 2$, with the initial conditions $\varphi_{0,0} = 3$, $\varphi_{1,0} = \varphi_{1,1} = \varphi_{2,0} = 0$, $\varphi_{2,1} = 2$. The closed form expression is

$$\varphi_{n,k} = \frac{n}{k}\binom{k}{n-2k}.$$

Proof. Let us first consider a cycle C_n for $n \geq 6$. A vertex, say n, can be covered by an edge of a maximal matching of size k in two ways; in each case, the rest of the considered maximal matching must be a maximal matching of size $k-1$ in P_{n-3}. If a vertex is not covered by an edge, then both of its neighbors must be covered, and the rest must be a maximal matching of size $k-2$ in P_{n-6}. Hence, $\varphi_{n,k} = 2\psi_{n-3,k-1} + \psi_{n-6,k-2}$. The recurrence now follows by plugging in expressions for $\psi_{n,k}$. It can be checked by direct computation that the recurrence remains valid also for $n = 3, 4, 5$, and the initial conditions are then computed by extending the recurrence backwards to $n = 0$. The formula follows by taking into account the formula for $\psi_{n,k}$. □

The sequence $\varphi_n = \sum_k \varphi_{n,k}$ satisfies the same recurrence as ψ_n, but with different initial conditions, $\varphi_0 = 3$, $\varphi_1 = 0$ and $\varphi_2 = 2$. It is known as the sequence of **Perrin numbers**, and it appears as A001608 in the OEIS. It has the same asymptotics as the Padovan sequence and it can be shown by the same methods we used for paths that the expected size of a maximal matching (and hence the efficiency) in C_n is the same as for the path of the same length. We omit the details.

From Proposition 3.9 we can derive an expression for Perrin numbers in terms of binomial coefficients similar to the expression for Lucas numbers. Again, it is not listed in the OEIS entry.

Corollary 3.10.

$$\varphi_n = \sum_{k \geq 0} \frac{n}{k}\binom{k}{n-2k}.$$

□

4 3- and 4- uniform chain cacti

A **cactus** is a connected graph in which any block is an edge or a cycle. If all blocks of a cactus G are cycles of the same size, say k, we say that G is a **k-uniform cactus**. In

this section we consider 3- and 4-uniform cacti in which each block has at most two cut-vertices, and each cut-vertex is shared by exactly two blocks. Such cacti are called **cactus chains** or **chain cacti**. The number of blocks is the **length** of the chain. Obviously, trees are uniform cacti, all their blocks being copies of K_2, and paths fit our definitions as the simplest possible cactus chains. This fact lies behind our decision to denote by n the length of P_n and not the number of vertices.

All cactus chains of length n have $n-1$ cut-vertices. Also, every cactus chain of length n has exactly two blocks with only one cut-vertex. Such blocks are called **terminal**; the remaining (if any) blocks are **internal**. We consider here the cactus chains whose blocks are either triangles or squares. Our goal is to investigate how the richer block structure imposed on the same connectivity pattern affects the number of maximal matchings in such graphs. For both classes we determine the recurrences satisfied by the sequences enumerating maximal matchings of a given size and by the sequence enumerating the total number of maximal matchings. From there we proceed to determine the asymptotics, the expected size and the efficiency using the generating functions in much the same way as in the previous section. We omit most computational details.

4.1 3-uniform cactus chains

It is easy to see that all 3-uniform cactus chains of the same length are isomorphic. Hence we denote such a chain of length n by T_n; an example is shown in Fig. 3. We will also need auxiliary graphs T'_n such as shown in Fig. 4. The number of maximal matchings in them

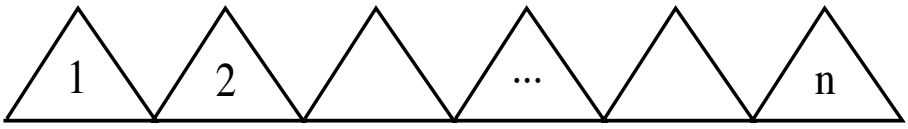

Figure 3: A 3-uniform cactus chain.

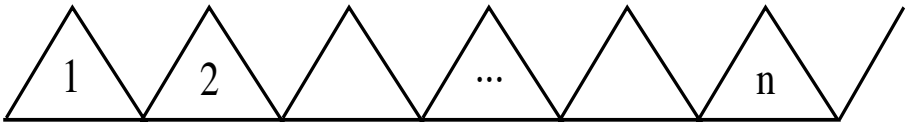

Figure 4: Auxiliary chain for 3-uniform cactus chains.

we denote by t_n and t'_n, respectively; where $t_{n,k}$ and $t'_{n,k}$ appear, they denote the number of maximal matchings of size k in T_n and T'_n, respectively.

Graph T_n has an odd number of vertices. Hence, it cannot have a perfect matching. It has, however, near-perfect matchings, i.e., matchings that saturate all vertices except one. In fact, $T_n - v$ has a perfect matching for each $v \in V(T_n)$. Graphs with this property are called **factor-critical** graphs. Hence, $\nu(T_n) = n$. The saturation number of T_n is given by $s(T_n) = \left\lceil \frac{n+1}{2} \right\rceil$. The claim follows by noticing that any matching of smaller size leaves at least $n+1$ vertices uncovered, and at least two of them must belong to the same triangle.

Let us look at the rightmost downward edge in T_n. Each maximal matching of size k must cover at least one of its end-vertices. Those that cover both its end-vertices are counted by $t_{n-1,k-1}$; those that cover only one are counted by $2t'_{n-2,k-1}$. Hence, $t_{n,k} = t_{n-1,k-1} + 2t'_{n-2,k-1}$. Now look at the pending edge of T'_n. Every maximal matching of size k must cover at least one if its end-vertices. Those that cover both are counted by $t'_{n-1,k-1}$; those that cover the cut-vertex by the horizontal edge are counted by $t'_{n-2,k-1}$, and those that cover the cut-vertex by the downward edge are counted by $t_{n-1,k-1}$. Hence, $t'_{n,k} = t'_{n-1,k-1} + t'_{n-2,k-1} + t_{n-1,k-1}$. From there, we can express $t_{n,k}$ as $t_{n,k} = t'_{n+1,k+1} - t'_{n,k} - t'_{n-1,k}$ and obtain a recurrence for $t'_{n,k}$. Once we have the recurrence, we compute the bivariate generating function for $t'_{n,k}$, and then finally the recurrence and the bivariate generating function $T(x,y)$ for $t_{n,k}$. We leave out the details and state only the final result.

Proposition 4.1.

$$T(x,y) = \sum_{n\geq 0}\sum_{k\geq 0} t_{n,k}x^n y^k = \frac{1+xy-x^2y}{1-2xy+x^2y(y-1)-x^3y^2}.$$

□

Corollary 4.2.

$$T(x) = \sum_{x\geq 0} t_n x^n = \frac{1+x-x^2}{1-2x-x^3}.$$

□

Corollary 4.3. *The sequence t_n satisfies the recurrence*

$$t_n = 2t_{n-1} + t_{n-3}$$

with the initial conditions $t_0 = 1$, $t_1 = 3$ and $t_2 = 5$. □

Corollary 4.4. *The asymptotic behavior of t_n is given by $t_n \sim 2.205569^n$.* □

Sequence t_n does not appear in the OEIS. However, the closely related sequence t'_n that satisfies the same recurrence and initial conditions except for $t'_2 = 7$ instead of $t_2 = 5$, is there as the entry A193641. It counts the words of length n over the alphabet $\{0, 1, -1\}$ such that each letter appears in a subsequence of length 2 with the sum zero. We were unable to find a neat bijective correspondence between such words and maximal matchings in T'_n.

When one tabulates $t_{n,k}$ as a triangular array, on its main diagonal appear the numbers of **maximum matchings** in T_n. The following result can be derived from the fact that T_n is factor-critical and that all its blocks are odd cycles. It has been established in a recent paper [9] that such graphs have the minimum possible number of maximum matchings and that this number is equal to the number of vertices.

Proposition 4.5.

$$t_{n,n} = 2n + 1.$$

□

We close the subsection by stating the result about the efficiency on 3-uniform cactus chains.

Corollary 4.6.

$$\varepsilon(T_n) \approx 0.74817n.$$

□

From the above results we can conclude that the additional structure present in the blocks of T_n does not complicate the recurrences - they remain of length 3. The structural enrichment is reflected, though, in the asymptotic behavior of the number of maximal matchings, a consequence of the increased difference between the matching number and the saturation number. Even when the asymptotic behavior is adjusted and expressed in terms of the number of vertices p, $t_n = t_{(p-1)/2} \sim 2.20557^{(p-1)/2} \sim 1.48512^p$, the resulting constant 1.48512 is larger than for P_n. Another consequence is a smaller efficiency, reflecting the fact that in a graph with richer structure of blocks and the same connectivity pattern there are more ways for things to go wrong, i.e., to achieve saturation by a smaller number of dimers.

4.2 4-uniform cactus chains

Unlike their 3-uniform counterparts, the 4-uniform chains of a given length are not all isomorphic. In order to distinguish between various cases, we introduce some terminology borrowed from the benzenoid graphs and 6-uniform cactus chains [8].

Let us look at an internal cycle of a 4-uniform chain. If its two cut-vertices are adjacent, we say that this cycle is an **ortho-cycle**; if the cut-vertices are not adjacent, the cycle is a **para-cycle**. If all internal cycles are of the same type, say, ortho, we call such chain an **ortho-chain** and denote it by O_n; if all internal cycles are para-cycles, we call the chain a **para-chain** and denote it by Q_n. As in the previous subsection, we leave out routine computations and present only the results. The case of para-chains is simpler and we consider it first.

4.2.1 Para-chains

Let $q_{n,k}$ denote the number of all maximal matchings of size k in Q_n, and q_n the total number of maximal matchings in Q_n. An example is shown in Fig 5. It turns out that those

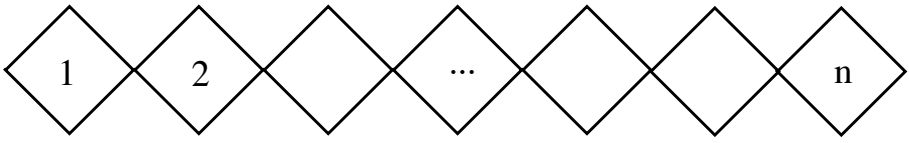

Figure 5: A para chain of length n.

sequences satisfy simpler, i.e., shorter recurrences than sequences t_n and ψ_n. In order to find the recurrences one needs to consider also the auxiliary chains shown in Fig. 6. As before, we omit the details.

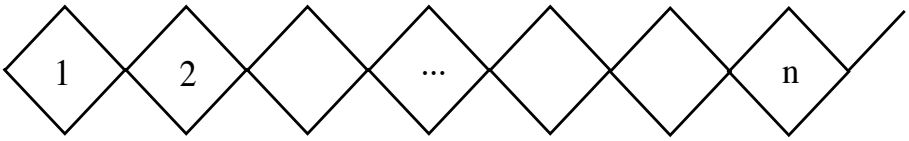

Figure 6: Auxiliary graph for para chains.

Proposition 4.7. *The bivariate generating function $Q(x, y)$ for the sequence $q_{n,k}$ is given by*

$$Q(x, y) = \frac{2xy^2}{1 - 4xy + 2(xy)^2}.$$

□

Several results now follow as corollaries.

Corollary 4.8. *The sequence q_n satisfies the recurrence $q_n = 4q_{n-1} - 2q_{n-2}$ with the initial conditions $q_0 = 0, q_1 = 2$. Its generating function $Q(x)$ is given by $Q(x) = \frac{2x}{1-4x+2x^2}$.* □

Corollary 4.9.

$$q_n = \frac{\left(2 + \sqrt{2}\right)^n}{\sqrt{2}} - \frac{\left(2 - \sqrt{2}\right)^n}{\sqrt{2}}.$$

□

The sequence q_n provides a new combinatorial interpretation of sequence A060995 from the OEIS. It counts, among other things, a number of routes of length $2n$ on the sides of an octagon from a point to opposite point. It would be interesting to provide explicit bijection between such routes and our maximal matchings. It could be also worthwhile to explore its connections with the closely related sequence A007070.

Corollary 4.10. *Graph Q_n is equimatchable. Its matching number is equal to $n + 1$, and its maximal matching polynomial is given by $m(Q_n; x) = q_n x^{n+1}$.* □

The above result follows from the bivariate generating function,

$$Q(x, y) = 2xy^2 \left(1 + 4(xy) + 14(xy)^2 + 48(xy)^3 + \ldots\right).$$

Another way to derive it is to observe that each cut-vertex must be saturated by an edge of a maximal matching, and that no edge can saturate more that one cut-vertex. That gives us $n - 1$ edges in a maximal matching and the remaining two can be chosen one from each of the two terminal cycles. This fact is also responsible for the small length of the recurrence.

4.2.2 Ortho-chains

An example of an ortho-chain is shown in Fig. 7. A moments reflection should suffice to convince the reader that the property of para-chains regarding the saturation of all cut-vertices by all maximal matchings is not preserved for ortho-chains. Hence, it is no wonder that the numbers of maximal matchings in them satisfy again a recurrence of length 3. We state here without proof the basic results for the sequence o_n counting all maximal matchings in O_n

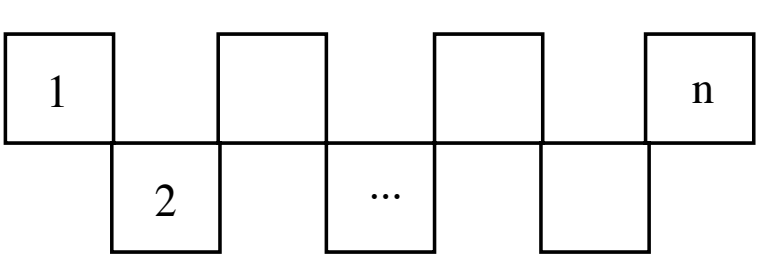

Figure 7: An ortho-chain of length n.

Proposition 4.11. *The sequence o_n satisfies the recurrence $o_n = 2o_{n-1} + 2o_{n-2} - 2o_{n-3}$ for $n \geq 3$ with the initial conditions $o_0 = 0$, $o_1 = 2$ and $o_2 = 8$. Its generating function is given by $O(x) = \frac{2x+4x^2}{1-2x-2x^2+2x^3}$. Asymptotically, $o_n \sim 0.36779 \cdot 2.48119^n$.* □

The sequence does not seem to be in the OEIS.

It would be interesting to examine whether the two considered types of chains are extremal among all chains of a given length. Such behavior is confirmed for matchings and independent sets in hexagonal chains [8].

The methods of this section could be successfully applied also to other types of cactus chains, such as the spiro-chains made of hexagons.

5 Linear polymers of connectivity 2

In this section we move to linear polymers of larger connectivity. As expected, the increase in connectivity will result in longer recurrences; in the two considered cases the lengths will be 8 and 5, respectively. Less clear, however, is the connection between the connectivity and efficiency.

The two polymers considered in this section are shown in Fig. 8 and 9, respectively. The first one, R_n, could be also interpreted as the second power of P_{2n+1}. (The second power,

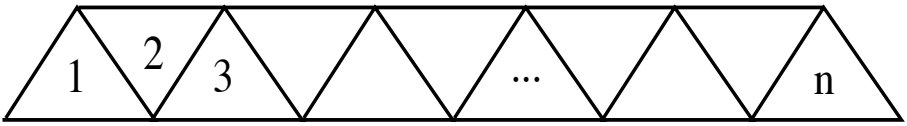

Figure 8: A 2-connected linear polymer with triangular faces.

Figure 9: The ladder graph.

G^2, of a graph G is obtained by connecting by an edge each pair of vertices at distance 2 in G.) The second one is the ladder graph L_n, also known as the linear polyomino.

The results of this section were obtained by the same methods as in the previous cases. We state them in the most condensed form, giving only the generating functions and asymptotic behavior. As before, we omit the computational details.

We denote by r_n and l_n the number of maximal matchings in R_n and L_n, respectively.

Proposition 5.1. *The generating function $R(x)$ for the sequence r_n is given by*

$$R(x) = \frac{1 + 3x + 2x^2 + 2x^3 - x^5 - x^6 - x^7}{1 - x^2 - 2x^3 - x^4 - x^5 + x^6 + x^8}.$$

Asymptotically, $r_n \sim 1.454145 \cdot 1.625957^n$. The efficiency of R_n is given by $\varepsilon(R_n) \approx 0.849$. □

Proposition 5.2. *The generating function $L(x)$ for the number of maximal matchings in the ladder graph L_n is given by*

$$L(x) = \frac{1 + x^2 + x^3 + x^4}{1 - 2x - x^4 - x^5}.$$

Its asymptotic behavior is given by $l_n \sim 1.110879 \cdot 2.147899^n$. The efficiency of L_n is $\varepsilon(L_n) \approx 0.861799$. □

One can see that the recurrence length seems to be influenced more by the highest degree than by the cycle length. This is in line with the intuitive feeling that the recurrence length is mostly dependent on the local complexity. It would be interesting to test this assumption by computing the number of maximal matchings in other chains of connectivity two. According to results reported in [10], the number of maximal matchings in linear polyacenes satisfies a recurrence of legth 5, while for fibonacenes and helicenes the length of recurrence is 7.

Results of the above type could be also obtained by using the method of transfer matrices.

6 Thorny graphs

Let G be a graph on n vertices and m edges. For an ordered n-tuple $(p_1, \ldots, p_n)$ of non-negative integers we construct a **thorny graph** $T^*(G)$ by attaching p_i pendent vertices to vertex v_i of G. When $p_i = p$ for all i we call such graph a p**-bristle graph** and denote it by $T_p(G)$. When $p_i = p - deg(v_i)$, the resulting graph is called p**-thorny graph**. If G is imagined to be the H-deleted graph of an alkane, then the 4-thorny graph $T^*(G)$ is the H-included graph. Thorny graphs were defined by Cayley [3] and later appeared in the chemical literature as plerographs.

One of the simplest cases arises when $G = P_n$. In that case its p-bristle graph $T_p(P_n)$ is called a p-caterpillar. An example is shown in Fig 10 below.

Proposition 6.1. *The number of maximal matchings in $T_p(P_n)$ is equal to the value of the $(n+2)$-nd Fibonacci polynomial evaluated at p, i.e., $\Psi(T_p(P_n)) = F_{n+2}(p)$.*

Proof. For $p > 0$ it is clear that every vertex of the original P_n must be covered by an edge of a maximal matching. If the vertex n is covered by the edge $v_{n-1}v_n$, the remaining edges of a maximal matching must form a valid maximal matching in $T_p(P_{n-2})$, and hence are

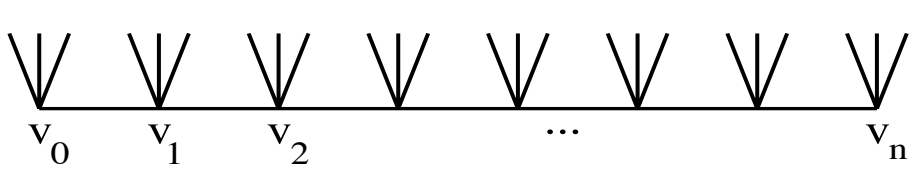

Figure 10: A 3-caterpillar of length n.

counted by $\Psi(T_p(P_{n-2}))$. If v_n is covered by one of p pending edges, the remaining maximal matchings are counted by $p\Psi(T_p(P_{n-1}))$. Hence the number of maximal matchings in $T_p(P_n)$ satisfies the recurrence

$$\Psi(T_p(P_n)) = p\Psi(T_p(P_{n-1})) + \Psi(T_p(P_{n-2}))$$

with initial conditions $\Psi(T_p(P_0)) = p$, $\Psi(T_p(P_1)) = p^2 + 1$. This is the same recurrence with the same initial conditions as the one satisfied by the Fibonacci polynomials, and the claim follows. □

We remind the reader that the Fibonacci polynomials are related to matching polynomials of paths. It can be shown that their appearance here as maximal matching polynomials of caterpillars is not a coincidence. Our next result establishes the relationship between maximal matching polynomials of p-bristle graphs and matching polynomials of their underlying graphs.

Theorem 6.2. *Let $p > 0$. Then the maximal matching polynomial of a p-bristle graph $T_p(G)$ is given as*

$$m(T_p(G); x) = (px)^n g(G; (p^2x)^{-1}),$$

where $g(G; x)$ is the matching (generating) polynomial of G.

Proof. Each vertex of G must be covered by an edge of a maximal matching in $T_p(G)$, either by an edge of G, or by any of p new edges. Obviously, $\nu(T_p(G)) = n$, and it is achieved when no edge of G participates in a matching of $T_p(G)$. Let M be a maximal matching in $T_p(G)$ of size l, and let k out of those l edges belong to $E(G)$. These k edges form a matching of size k in G, and each such matching can be extended to a maximal matching in $T_p(G)$ in p^{n-2k} different ways. Then $l = k + n - 2k = n - k$ and $\Psi_{n-k}(T_p(G)) = p^{n-2k}\Phi_k(G)$. The maximal matching polynomial of $T_p(G)$ is now given as $m(T_p(G); x) = \sum_{l=s(T_p(G))}^{n} \Psi_l(T_p(G))x^l$. By switching to summation over k (the number of edges belonging to $E(G)$) we obtain

$$\begin{aligned} m(T_p(G); x) &= \sum_{k=0}^{\nu(G)} \Psi_{n-k}(T_p(G))x^{n-k} = \sum_{k=0}^{\nu(G)} p^{n-2k}\Phi_k(G)x^{n-k} \\ &= (px)^n \sum_{k=0}^{\nu(G)} \Phi_k(G)(xp^2)^{-k} = (px)^n g(G; (p^2x)^{-1}). \end{aligned}$$

□

Now the results on the number of maximal matchings in p-thorny graphs of cycles and stars follow as corollaries of the above theorem.

Corollary 6.3. *Let $p > 0$. Then the number of maximal matchings in $T_p(C_n)$ is given as the value of the n-th Lucas polynomial evaluated at $x = p$. Hence, $\Psi(T_p(C_n)) = \ell_n(p)$.* □

Corollary 6.4. *Let S_n denote the star $K_{1,n}$ and $p > 0$. Then $\Psi(T_p(S_n)) = (n+p^2)p^{n-1}$.* □

We close the section by another direct consequence of Theorem 6.2.

Corollary 6.5. *Let $p > 0$. Then $T_p(G)$ is equimatchable if and only if G contains no edges.* □

7 Composite graphs

Many interesting graphs arise from simpler building blocks *via* some binary operations known as graph products. We consider here two such operations, the sum (also known as join) and the corona product, and apply some of the results obtained in previous sections to enumerate maximal matchings in resulting graphs.

7.1 Sum

Let G_1 and G_2 be two graphs with vertex sets $V(G_i)$ and edge sets $E(G_i)$ for $i = 1, 2$. Their **sum** is the graph $G_1 + G_2$ on the vertex set $V(G_1) \cup V(G_2)$ and the edge set $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{\{u, v\}; u \in V(G_1), v \in V(G_2)\}$. In other words, we retain all edges of the component graphs and also join every vertex of G_1 to every vertex of G_2. The sum of two graphs is sometimes called their **join**. We consider here two special cases when one of the graphs is a single vertex and the other one is a path or a cycle. In the first case we obtain the **fan graph** $J_n = K_1 + P_n$, in the second case the well known **wheel graph** on n spokes $W_n = K_1 + C_n$. Examples are shown in Fig. 11.

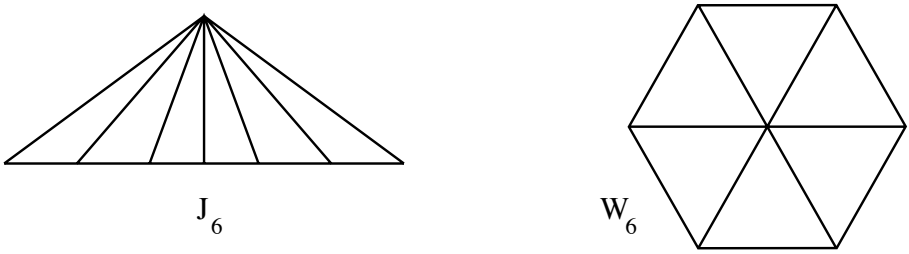

Figure 11: A fan and a wheel of length 6.

Proposition 7.1.

$$\Psi(J_n) = \sum_{k=0}^{n} \psi_{k-1}\psi_{n-k-1} + \frac{1-(-1)^n}{2},$$

where ψ_k is the number of maximal matchings in a path of length k for $k \geq 0$ and $\psi_{-1} = 1$.

Proof. Let $n \geq 1$ be odd. Then a maximal matching in J_n is either a perfect matching in P_n, or it contains an edge covering the vertex of K_1. The first case is counted by the term $\frac{1-(-1)^n}{2}$. In the second case, if the edge connects K_1 to vertex k in P_n, it splits the base path into two paths of lengths $k-1$ and $n-k-1$. The result follows by summing over k and taking care of border cases. The case of even n follows in the same way. □

The above result provides a combinatorial interpretation for the convolution of the Padovan sequence with itself.

Proposition 7.2.

$$\Psi(W_n) = n\psi_{n-2} + (1 + (-1)^n),$$

where ψ_k is the number of maximal matchings in a path of length k.

Proof. As in the previous proposition, for even n a maximal matching in W_n is either one of the two perfect matchings in C_n (counted by the term $(1 + (-1)^n)$, or it contains a spoke. In the second case, the rest must be a valid maximal matching in P_{n-2}, counted by ψ_{n-2}. The case of odd n is simpler, as any of n spokes can cover the central vertex leaving a maximal matching in P_{n-2}. □

Neither of the above sequences appears in the OEIS.

It would be interesting to count maximal matchings in sums of two identical graphs, $G + G$.

7.2 Corona product

For two graphs G_1 and G_2 we define their **corona product** $G_1 \circ G_2$ as the graph obtained by taking $|V(G_1)|$ copies of G_2 and joining each vertex of the i-th copy with vertex $v_i \in V(G_1)$. Unlike in the sum, the components enter the corona product in an asymmetric way. For our purpose it is important that no matter what are connectivities of the components, the corona product has the connectivity one. That will allow us to apply the decompositions that worked in previous sections and count maximal matchings in some simple cases. The p-bristle graph of the previous section is a corona product of G and $\overline{K_p}$, while $J_n = K_1 \circ P_n$ and $W_n = K_1 \circ C_n$. We consider first the case $P_n \circ P_1 = P_n \circ K_2$.

Proposition 7.3. *The sequence $p_n = \Psi(P_n \circ P_1)$ satisfies the recurrence $p_n = 2p_{n-1} + 3p_{n-2} + p_{n-3}$ with the initial conditions $p_0 = 3$, $p_1 = 9$, $p_2 = 28$.*

Proof. An example of $P_n \circ P_1$ is shown in Fig. 12 below. Each maximal matching in $P_n \circ P_1$ either covers vertex labeled v_n in P_n or does not cover it. In the first case, the remaining edges must form either a valid matching in $P_{n-1} \circ P_1$ (if v_n is covered by one

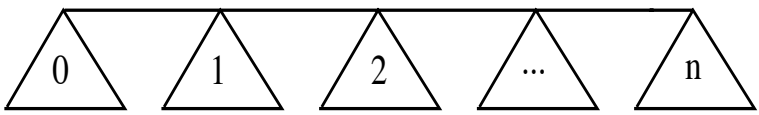

Figure 12: $P_n \circ P_1$.

of two edges toward its copy of P_1) or a valid maximal matching in $P_{n-2} \circ P_1$ (if v_n is covered by $v_{n-1}v_n$). There are altogether $2p_{n-1} + p_{n-2}$ maximal matchings covering v_n. Maximal matchings that do not cover v_n must cover v_{n-1} and are counted by the expression of the same type, with indices decreased by one. The claim now follows by adding the two contributions. □

The sequence (p_n) appears as A084084 in the OEIS without combinatorial interpretations.

Our last example in this section demonstrates interesting connections between maximal matchings and tilings.

Proposition 7.4.

$$\Psi(P_n \circ K_3) = 3^{n+1}F_{n+2}.$$

Proof. The result follows by the same reasoning as in the previous proposition, but the resulting recurrence is shorter, since each vertex of the backbone P_n must be covered by an edge of any maximal matching. The situation is shown in Fig. 13. Taking into account

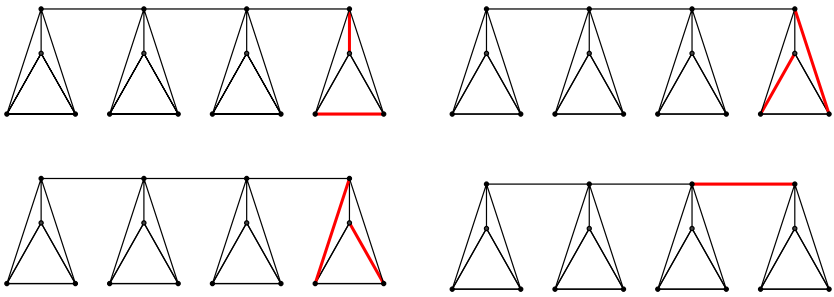

Figure 13: Maximal matchings covering v_n in $P_n \circ K_3$.

that there are 3 (maximal) matchings in K_3 we obtain a recurrence of length 2,

$$\Psi(P_n \circ K_3) = 3\Psi(P_{n-1} \circ K_3) + 9\Psi(P_{n-2} \circ K_3).$$

The same recurrence with the same initial conditions is satisfied by the sequence $3^{n+1}F_{n+2}$, hence the claim. □

We leave to the reader to show that the sequence $3^{n+1}F_{n+2}$ also counts tilings of a row of n unit squares by unit squares and dominoes such that the squares come in any of 3 colors and the dominoes in any of 9 colors.

The recurrence for the number of maximal matchings in $P_n \circ K_3$ is shorter than the recurrence for a simpler graph $P_n \circ K_2$. That is a consequence of factor-criticality of K_3. It could be shown that the number of maximal matchings of $P_n \circ G$ satisfies a recurrence of length 2 whenever G is factor-critical.

8 Concluding remarks

The present manuscript is, to the best of our knowledge, the first systematic attempt to address enumerative aspects of maximal matchings. We have counted maximal matchings in several classes of graphs of low connectivity. In most cases, we have obtained complete information, including the generating functions and asymptotic behavior of the enumerating sequences; in some particular cases we were even able to obtain closed formulas. The obtained results are, however, far from comprehensive. In this section we list some open problems and possible directions for future research.

One obvious direction is to continue our work on cactus chains. It could be done by considering uniform cacti whose blocks are larger cycles, such as hexagons. With larger cycles comes also greater variability in the connectivity patterns, leading to the problem of finding the extremal chains among all uniform chains of the same length. We left the problem open even for 4-uniform chains.

Another possibility is to look at non-uniform chains. Examples of such chains can be obtained from uniform chains by expanding each cut-vertex into an edge. We have done some preliminary work on this type of chains and noticed that the enumerating sequences also appear in some other combinatorial contexts. Providing explicit bijections among the corresponding families is the goal of our paper currently under preparation.

Among the linear polymers of connectivity 2 the most interesting ones are, without doubt, the benzenoid chains. Some recent findings are reported in [10]. There are indications that the extremality patterns valid for perfect matchings and all matchings do not persist for maximal matchings.

We have addressed here only the composite graphs of low connectivity. However, many interesting operations such as, e.g., the Cartesian product, actually increase the connectivity. It would be probably too ambitious to hope for general enumerative results for Cartesian products, but the cases when one factor is a path or a cycle should not be out of reach. Another interesting thing in such graphs would be their saturation number; at the present, there are only few known results of this type.

Finally, it would be worthwhile to try to develop a general theory of maximal matching polynomials and to see if they could play as important role in the study of maximal matchings as the matching polynomials have played so far in the general context of matchings. In particular, it would be interesting to see if their coefficients form log-concave or unimodal sequences for all graphs.

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The modified Wiener index of some graph operations

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Abstract

Graovac and Pisanski [On the Wiener index of a graph, J. Math. Chem. **8** (1991) 53 – 62] applied an algebraic approach to generalize the Wiener index by symmetry group of the molecular graph under consideration. In this paper, exact formulas for this graph invariant under some graph operations are presented.

Keywords: Modified Wiener index, graph operation, automorphism group.

Math. Subj. Class.: 20C15, 20D15

1 Introduction

Throughout this paper graph means simple connected graphs. The distance between the vertices u, v of a graph G, $d_G(u, v)$ (or $d(u, v)$ for short), is defined as the number of edges in a shortest path connecting them. The sum of all distances between vertices in G is called the *Wiener index* of G [9]. The first study of this number were made by Harold Wiener in 1947 who realized that there are correlations between this graph invariant and the boiling points of paraffin. We encourage the reader to consult [1, 2] and references therein for information about the effect of this graph invariant on trees and hexagonal systems and [4] for some applications in chemistry.

Let $G = (V, E)$ be a simple graph with the vertex set V and the edge set E. Graovac and Pisanski [3] in a seminal paper applied the symmetry group of the graph under consideration to generalize the Wiener index. To explain, we assume that Γ is the automorphism group of G. Then the *distance number* of an automorphism g, $\delta(g)$, is defined as the average of $d(u, g(u))$ over all vertices $u \in V(G)$ and

$$\delta(G) = \frac{1}{|\Gamma|}\sum_{g\in\Gamma}\delta(g) = \frac{1}{|\Gamma||V(G)|}\sum_{u\in V(G)}\sum_{g\in\Gamma} d(u, g(u)).$$

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Define:

$$\widehat{W}(G) = \frac{|V(G)|}{2|\Gamma|} \sum_{u \in V(G)} \sum_{g \in \Gamma} d(u, g(u)).$$

It can be easily shown that

$$\widehat{W}(G) = \frac{1}{2}|V(G)|^2 \delta(G).$$

The authors of [3], in their pioneering work used the name "*modified Wiener index*" for this graph invariant. Suppose $e = uv \in E(G)$ and $V(e) = \{u, v\}$. The line graph $L(G)$ is a graph with $E(G)$ as vertex set. Two different vertices of $V(L(G))$ are adjacent if and only if they have a common vertex in G. The subdivision graph $S(G)$ is the graph obtained by inserting an additional vertex in each edge of G. In other words, each edge of the subdivision graph is replaced by a path of length 2.

Suppose G is a graph. Following Yan et al. [8], we set $EE(G) = \{\{e, f\} \mid e, f \in E(G) \ \& \ |V(e) \cap V(f)| = 1\}$ and $EV(G) = \{\{e, v\} \mid v \in V(G) \ \& \ v \in V(e) \ \& \ e \in E(G)\}$, where $V(e)$ is the set of all end vertices of the edge e. Define the line graph $L(G)$, the subdivision graph $S(G)$, the total graph $T(G)$ and the graphs $R(G)$ and $Q(G)$ as follows:

$$\begin{aligned}
&V(L(G)) = E(G), && E(L(G)) = EE(G),\\
&V(S(G)) = V(G) \cup E(G), && E(S(G)) = EV(G),\\
&V(T(G)) = V(G) \cup E(G), && E(T(G)) = E(G) \cup EV(G) \cup EE(G),\\
&V(R(G)) = V(G) \cup E(G), && E(R(G)) = E(G) \cup EV(G),\\
&V(Q(G)) = V(G) \cup E(G), && E(Q(G)) = EV(G) \cup EE(G).
\end{aligned}$$

Throughout this paper we use the standard notations of group theory and graph theory. We refer to [5], for the main properties of product graphs. If G is a connected graph then the diameter $d = \mathrm{diam}(G)$ is defied as the length of the largest distance between two vertices in G. Moreover, define

$$\overline{D}(g, i) = |\{\{u, g(u)\} \mid u \in V(G) \ \& \ d_G(u, g(u)) = i\}|; 1 \leq i \leq d,$$

and $\overline{D}(\Gamma, i) = \sum_{g \in \Gamma} \overline{D}(g, i);\ 1 \leq i \leq d$. The number of $\{u, v\}$ such that $d(u, v) = i$ in $\widehat{W}(G)$ is equal to $\overline{D}(G, i) = \overline{D}(\Gamma, i)$. Suppose x and y are vertices of G. We write $x \sim_G y$ to show that x, y are adjacent in G. They are called equivalent, $x \approx_G y$, if there exists an automorphism α such that $\alpha(x) = y$. The path, cycle and complete graphs with n vertices are denoted by P_n, C_n and K_n, respectively. The number of edges in a path P is denoted by $l(P)$ and named the length of P. Our other notations are standard and taken mainly from the standard books on these topics.

Main Theorem. *Suppose G is a tree of diameter d. Then the following relations hold:*

1. $\widehat{W}(L(G)) = \frac{n-1}{n}\widehat{W}(G) - \frac{n-1}{2|\Gamma|}\sum_{i=1}^{d} \overline{D}(G, i)$,
2. $\widehat{W}(S(G)) = \frac{4n-2}{n}\widehat{W}(G) + \frac{4n-2}{n-1}\widehat{W}(L(G))$,
3. $\widehat{W}(T(G)) = \frac{2n-1}{n}\widehat{W}(G) + \frac{2n-1}{n-1}\widehat{W}(L(G))$,

4. $\widehat{W}(Q(G)) = \frac{4n-2}{n}\widehat{W}(G)$,
5. $\widehat{W}(R(G)) > \frac{4n-2}{n}\frac{|\Gamma|}{|\mathrm{Aut}(R(G))|}\widehat{W}(G)$.

2 Proof of the Main Theorem

In [6], a character theoretical method for computing the modified Wiener index of graphs is presented and in [8], the authors computed exact formulas for the Wiener index under five graph operations. The aim of this paper is to continue these papers by computing the modified Wiener index of trees under the graph operations $L(-), S(-), T(-), Q(-)$ and $R(-)$. For simplicity of our argument, we assume that $\Gamma = \mathrm{Aut}(G)$ and $\overline{W}(G) = \frac{2|\Gamma|}{|G|}\widehat{W}(G)$ then $\overline{W}(G) = \sum_{i=1}^{d} i.\overline{D}(G,i)$. We will start by stating a well-known result in algebraic graph theory.

Lemma 2.1. *Suppose G is a tree with at least three vertices. Then* $\mathrm{Aut}(L(G)) \cong \mathrm{Aut}(G)$.

Proof. It is an immediate consequence of [7, Corollary 1.4]. □

Theorem 2.2. *Let G be a tree with $n \geq 3$ vertices and $\Gamma = \mathrm{Aut}(G)$. Then,* $\widehat{W}(L(G)) = \frac{n-1}{n}\widehat{W}(G) - \frac{n-1}{2|\Gamma|}\sum_{i=1}^{d}\overline{D}(G,i)$.

Proof. Suppose $e = uv$ and $f = xy$ are vertices of $L(G)$ such that $e \approx_{L(G)} f$ and $d_{L(G)}(e,f) = i$. So, there are $\sigma \in \mathrm{Aut}(G)$ and $\bar{\sigma} \in \mathrm{Aut}(L(G))$ such that $\bar{\sigma}(e) = f$, $\sigma(u) = x$ and $\sigma(v) = y$. Choose a shortest path $e = e_0, e_1, \ldots, e_i = f$ in $L(G)$. Set $e = e_0 = u_0u_1, e_1 = u_1u_2, \ldots, e_{i-1} = u_{i-1}u_i$, $f = e_i = u_iu_{i+1}$, $u = u_0$, $v = u_1$, $y = u_i$ and $x = u_{i+1}$. Since G is a tree, $u = u_0, u_1, \ldots, u_i, u_{i+1} = x$ is a shortest path in G connecting $u = u_0$ and $x = u_{i+1}$. Thus $d_G(u,x) = i+1$. Therefore, for any vertices e and f of $L(G)$ at distance i, we fined two vertices u_e and u_f of G at distance $i+1$, corresponding to e and f, respectively.

We now assume that r and s are vertices in G at distance i and $r = v_0, v_1, \ldots, v_{i-1}$, $v_i = s$ is the unique shortest path connecting r and s. Then the edges v_0v_1 and $v_{i-1}v_i$ are at distance $i-1$ in $L(G)$. Hence, $\overline{D}(L(G),i) = \overline{D}(G,i+1)$. Therefore,

$$\begin{aligned}\overline{W}(L(G)) &= \sum_i i\overline{D}(L(G),i)\\ &= \sum_i (i-1)\overline{D}(G,i)\\ &= \sum_i i\overline{D}(G,i) - \sum_i \overline{D}(G,i)\\ &= \overline{W}(G) - \sum_i \overline{D}(G,i).\end{aligned}$$

Therefore, $\frac{2|\mathrm{Aut}(L(G))|}{|V(L(G))|}\widehat{W}(L(G)) = \frac{2|\Gamma|}{|V(G)|}\widehat{W}(G) - \sum_i \overline{D}(G,i)$, which completes our argument. □

Lemma 2.3. *Suppose G is a tree. Then* $\mathrm{Aut}(S(G)) \cong \mathrm{Aut}(G)$.

Proof. Define $\Phi : \mathrm{Aut}(G) \longrightarrow \mathrm{Aut}(S(G))$ given by $\Phi(\alpha)|_{V(G)} = \alpha$ and if $e = xy \in E(G)$ then $\Phi(\alpha)(e) = \alpha(x)\alpha(y) \in E(G)$. Notice that if $x \sim_G y$ and t, t' are vertices

in $S(G)$ such that $x \sim_{S(G)} t \sim_{S(G)} y$ and $\Phi(\alpha)(x) \sim_{S(G)} t' \sim_{S(G)} \Phi(\alpha)(y)$ then $\Phi(\alpha)(t) = \Phi(\alpha)(t')$. It can easily be proved that $\Phi(\alpha)$ is a permutation of $S(G)$. We show that $ab \in E(S(G))$ if and only if $\Phi(\alpha)(a)\Phi(\alpha)(b) \in E(S(G))$. Suppose $a \sim_{S(G)} b$ and $a \in G$. Then there exists $c \in G$ such that $a \sim_G c$ and $a \sim_{S(G)} b \sim_{S(G)} c$. Since $\alpha \in \mathrm{Aut}(G)$, $ac \in E(G)$ if and only if $\alpha(a)\alpha(c) \in E(G)$. Hence, there exists $l \in S(G)$ such that $\Phi(\alpha)(a) \sim_{S(G)} l \sim_{S(G)} \Phi(\alpha)(c)$. This implies that $\Phi(\alpha)(b) = l$. So, $ab \in E(S(G))$ if and only if $\Phi(\alpha)(a)\Phi(\alpha)(b) \in E(S(G))$. Similarly, if $\overline{\sigma} \in \mathrm{Aut}(S(G))$ then $\sigma = \overline{\sigma}|_G \in \mathrm{Aut}(G)$. Thus, Φ is invertible. □

Theorem 2.4. *Let G be a tree with $n \geq 3$ vertices. Then*

$$\widehat{W}(S(G)) = \frac{4n-2}{n}\widehat{W}(G) + \frac{4n-2}{n-1}\widehat{W}(L(G)).$$

Proof. Suppose $x, y \in V(S(G))$ are in the same orbit of $\mathrm{Aut}(S(G))$, $d_{S(G)}(x,y) = k$ and $\tau(x) = y$, where $\tau \in \mathrm{Aut}(S(G))$. It is obvious that both of x and y must be together in $V(G)$ or $E(G)$. We first assume that $x, y \in V(G)$. Choose the shortest path $P_1 : x = u_0, u_1, \ldots, u_k = y$ in $S(G)$. Obviously, if i is even then $u_i \in G$ and so $k = 2k'$. Since G is tree, $P_2 : x = u_0, u_2, \ldots, u_{k'} = y$ is the unique path connecting x and y in G. Hence, $d_{S(G)}(x,y) = 2d_G(x,y)$.

Next we assume that $x, y \notin V(G)$, $P_3 : x = u_0, u_1, \ldots, u_k = y$ is a shortest path in $S(G)$. Choose edges $ab, cd \in E(G)$ such that $a \sim_{S(G)} x \sim_{S(G)} b$ and $c \sim_{S(G)} y \sim_{S(G)} d$. Suppose that $\tilde{x}$ and $\tilde{y}$ are corresponding vertices of x and y in $L(G)$, respectively. Since $S(G)$ is tree, the path P_3 is unique and so the vertices u_i, i is even, are corresponding to vertices $\tilde{u}_i$ in $L(G)$. This proves that k is even, say $k = 2k'$. In a similar way, there exists a path $P_2 : \tilde{x} = \tilde{u}_0, \tilde{u}_1, \ldots, \tilde{u}_{k'} = \tilde{y}$ in $L(G)$. So, we have again $d_{S(G)}(x,y) = 2d_{L(G)}(\tilde{x}, \tilde{y})$. Thus,

$$\begin{aligned}
\overline{W}(S(G)) &= \frac{1}{2}\sum_i i\overline{D}(S(G), i) \\
&= \frac{1}{2}\sum_i 2i\overline{D}(G, i) + \frac{1}{2}\sum_i 2i\overline{D}(L(G), i) \\
&= 2\overline{W}(G) + 2\overline{W}(L(G)).
\end{aligned}$$

Therefore, $\frac{|\mathrm{Aut}(S(G))|}{|V(S(G))|}\widehat{W}(S(G)) = \frac{2|\mathrm{Aut}(G)|}{|V(G)|}\widehat{W}(G) + \frac{2|\mathrm{Aut}(L(G))|}{|V(L(G))|}\widehat{W}(L(G))$, which completes our proof. □

Lemma 2.5. *Suppose G is a tree with at least three vertices. Then* $\mathrm{Aut}(T(G)) \cong \mathrm{Aut}(G)$.

Proof. The map $\Phi : \mathrm{Aut}(G) \longrightarrow \mathrm{Aut}(T(G))$ defined in a similar way as Lemma 2.3, is an isomorphism. Since if $\alpha \in \mathrm{Aut}(G)$ then $\Phi(\alpha) \in \mathrm{Aut}(T(G))$ and for $\beta \in \mathrm{Aut}(T(G))$ we have $\alpha = \beta|_G \in \mathrm{Aut}(G)$, as desired. □

Theorem 2.6. *With hypothesis of Lemma 2.5,* $\widehat{W}(T(G)) = \frac{2n-1}{n}\widehat{W}(G) + \frac{2n-1}{n-1}\widehat{W}(L(G))$.

Proof. Suppose x and y are vertices of $T(G)$ such that $x \approx_{T(G)} y$ and $d_{T(G)}(x,y) = k$. If $x, y \in G$ then we claim that $d_G(x,y) = k$. To prove, we first notice that G is a subgraph of $T(G)$. Next we assume that $P : x = u_0, u_1, \ldots, u_h = y$ is the unique path in G

and $P' : x = v_0, v_1, \ldots, v_k = y$ is a shortest path in $L(G)$ connecting x and y. If v_1 is a vertex in $L(G)$ and v_2 is a vertex in G then by interchanging v_0, v_1, v_2 by v_0, v_2 we obtain another path P'' in $L(G)$ such that $l(P'') < l(P')$, a contradiction. Thus, if $v_1 \in V(L(G)))$ then $v_2, v_3, \ldots, v_{k-1} \in V(L(G))$ and $l(P) < l(P')$. This shows that $v_1 \notin V(L(G))$. By continuing this method, one can see that all vertices of P' are in vertices of G. Therefore, $P = P'$. A similar argument shows that in other case that x and y are corresponding to vertices in $L(G)$, a shortest path in $L(G)$ and $T(G)$ will be the same and so $\overline{W}(T(G)) = \overline{W}(G) + \overline{W}(L(G))$. Therefore, $\frac{|\mathrm{Aut}(T(G))|}{|V(T(G))|}\widehat{W}(T(G)) = \frac{|\Gamma|}{|V(G)|}\widehat{W}(G) + \frac{|\mathrm{Aut}(L(G))|}{|V(L(G))|}\widehat{W}(L(G))$, which completes the proof. □

Lemma 2.7. *Suppose G is a tree with at least three vertices. Then* $\mathrm{Aut}(Q(G)) \cong \mathrm{Aut}(G)$.

Proof. Since $Q(G) = L(G) \cup S(G)$, Lemmas 2.1, 2.3 and a similar argument as Lemma 2.3 completes the proof. □

Theorem 2.8. *With hypothesis of Lemma 2.7,* $\widehat{W}(Q(G)) = \frac{4n-2}{n}\widehat{W}(G)$.

Proof. Suppose x and y are vertices of $Q(G)$ such that $x \approx_{Q(G)} y$. If x, y are corresponding to the vertices of $L(G)$ then $d_{Q(G)}(x, y) = d_{L(G)}(x, y)$. Suppose x, y are vertices of G with distance k and $P : x = u_0, u_1, \ldots, u_{k-1}, u_k = y$ is a shortest path in G connecting x and y. If x and y are adjacent in G then distance between them in $Q(G)$ will be 2. In other case, the path $P' : x = u_0, e_1, \ldots, e_k, u_k = y$ has length $k + 1$, where $e_i = u_{i-1}u_i$, $1 \leq i \leq k$. In the case that $x, y \in L(G)$, the sum of distances is $\sum_i i\overline{D}(L(G), i)$ and in the second case the summation will be $\sum_i \overline{D}(G, i) + \sum_i \widehat{D}(G, i)$. Then we have $\overline{W}(Q(G)) = \overline{W}(G) + \frac{1}{2}\sum_i \widehat{D}(G, i) + \overline{W}(L(G))$. By applying Theorem 1, the result is obtained. □

Lemma 2.9. *Suppose G is a tree with at least three vertices. Then* $\mathrm{Aut}(G)$ *is isomorphic to a proper subgroup of* $\mathrm{Aut}(R(G))$.

Proof. It is easy to see that the mapping $\Phi : \mathrm{Aut}(G) \longrightarrow \mathrm{Aut}(R(G))$ given by the same definition as Lemma 2.3 is a one-to-one homomorphism, as desired. Since G is a tree, it has at least a pendant vertex and so $R(G)$ has an automorphism of order 2 in $\mathrm{Aut}(R(G)) \setminus \Phi(\mathrm{Aut}(G))$, proving the lemma. □

Theorem 2.10. *With hypothesis of Lemma 2.9,* $\widehat{W}(R(G)) > \frac{4n-2}{n}\frac{|\mathrm{Aut}(G)|}{|\mathrm{Aut}(R(G))|}\widehat{W}(G)$.

Proof. Suppose x and y are vertices in $R(G)$. Similar to Theorem 2.8, if $x, y \in G$ then $d_{R(G)}(x, y) = d_G(x, y)$. In this case, the sum of distances is at least $\sum_i i\overline{D}(G, i)$. If x and y are corresponding to vertices w and z of $L(G)$ such that $d_{L(G)}(w, z) = k$ then $d_{R(G)}(x, y) = k + 1$ and so the sum of distances is at least $\sum_i i\overline{D}(L(G), i) + \sum_i \widehat{D}(G, i)$.

Now, we assume that u and v are two pendants in G and in the same orbits under the action of $\mathrm{Aut}(G)$ on vertices and e and f are edges such that u is incident to e and f is incident to v. Then e and f are in the same orbits under the action of $\mathrm{Aut}(G)$ on edges. Hence, in $R(G)$, all elements of $\{u, v, e, f\}$ are in the same orbits under the action of $\mathrm{Aut}(R(G))$. Since, corresponding to $d_G(u, v)$ in $\overline{W}(G)$ there exists at least a quantity in the form of $d_{R(G)}(u, v) + d_{R(G)}(e, f) + d_{R(G)}(u, f) + d_{R(G)}(v, e) + d_{R(G)}(u, e) +$

$d_{R(G)}(v,f)$ in $\overline{W}(R(G))$, by Theorem 1, $\overline{W}(R(G)) > 2\overline{W}(G)$, which completes our argument. □

3 Examples

In this section, we apply our results in the pervious section. We denote the cyclic group of order n by $\mathbb{Z}_n$ and the symmetric group on n symbols by $\mathrm{Sym}(n)$. We notice that by Lemmas 2.1–2.7, if G is a tree with at least three vertices then

$$\mathrm{Aut}(G) \cong \mathrm{Aut}(L(G)) \cong \mathrm{Aut}(S(G)) \cong \mathrm{Aut}(T(G)) \cong \mathrm{Aut}(Q(G)),$$

and also by Lemma 2.9, $\mathrm{Aut}(G) \leq \mathrm{Aut}(R(G))$.

Example 3.1. In this example, $\widehat{W}(P_n)$, $\widehat{W}(L(P_n))$, $\widehat{W}(S(P_n))$, $\widehat{W}(T(P_n))$, $\widehat{W}(Q(P_n))$ and $\widehat{W}(R(P_n))$ are calculated where P_n is a path with n vertices. To do this, we assume that $V(P_n) = \{v_i\}_{i=1}^{n}$ and $E(P_n) = \{e_i = v_iv_{i+1}\}_{i=1}^{n-1}$. We first notice that the automorphism group of P_n is generated by an element α of order 2, where

$$\alpha = \begin{cases} (v_1,v_n)(v_2,v_{n-1})\dots(v_{\frac{n}{2}},v_{\frac{n+2}{2}}) & n \text{ is even} \\ (v_1,v_n)(v_2,v_{n-1})\dots(v_{\frac{n-1}{2}},v_{\frac{n+1}{2}}) & n \text{ is odd.} \end{cases}$$

Therefore, $\mathrm{Aut}(P_n) \cong \mathbb{Z}_2$. The modified Wiener index of P_n was computed in [3, Example 5.6] as

$$\widehat{W}(P_n) = \begin{cases} \frac{n^3}{8} & n \text{ is even} \\ \frac{n^3-n}{8} & n \text{ is odd.} \end{cases}$$

On the other hand, if n is even, then

$$\overline{D}(P_n,i) = \begin{cases} 0 & i \text{ is even} \\ 2 & i \text{ is odd,} \end{cases}$$

and if n is odd, then

$$\overline{D}(P_n,i) = \begin{cases} 2 & i \text{ is even} \\ 0 & i \text{ is odd.} \end{cases}$$

Therefore,

$$\sum_{i=1}^{n-1} \overline{D}(P_n,i) = \begin{cases} n & n \text{ is even} \\ n-1 & n \text{ is odd.} \end{cases}$$

By applying Theorems 2.2–2.10, we obtained the following equations,

$$\widehat{W}(L(P_n)) = \begin{cases} \frac{n^3-3n^2+2n}{8} & n \text{ is even} \\ \frac{(n-1)^3}{8} & n \text{ is odd,} \end{cases}$$

$$\widehat{W}(S(P_n)) = \frac{2n^3-3n^2+n}{4},$$

$$\widehat{W}(T(P_n)) = \frac{2n^3-3n^2+n}{4},$$

$$\widehat{W}(Q(P_n)) = \begin{cases} \frac{2n^3-n^2}{4} & n \text{ is even} \\ \frac{2n^3-n^2-2n+1}{4} & n \text{ is odd,} \end{cases}$$

$$\widehat{W}(R(P_n)) = \begin{cases} \frac{2n^3-n^2}{4} & n \text{ is even} \\ \frac{2n^3-n^2+2n-1}{4} & n \text{ is odd.} \end{cases}$$

For the last equality, we notice that the automorphism group of $R(P_n)$ can be generated by three elements α, β and γ as follows:

$$\alpha = (v_1, e_1),$$
$$\beta = (v_n, e_n),$$
$$\gamma = \begin{cases} (v_1,v_n)(v_2,v_{n-1})\dots\left(v_{\frac{n}{2}}, v_{\frac{n}{2}+1}\right)(e_1,e_{n-1})(e_2,e_{n-2})\dots\left(e_{\frac{n}{2}-1}, e_{\frac{n}{2}+1}\right) & n \text{ is even} \\ (v_1,v_n)(v_2,v_{n-1})\dots\left(v_{\frac{n-1}{2}}, v_{\frac{n+3}{2}}\right)(e_1,e_{n-1})(e_2,e_{n-2})\dots\left(e_{\frac{n+1}{2}}, e_{\frac{n+3}{2}}\right) & n \text{ is odd.} \end{cases}$$

It is easy to see that this group is isomorphic to the dihedral group D_8.

In the following example to compute the modified Wiener index, we apply the concept of semidirect product and wreath product of groups together with our results in last section. Let G be a group with a subgroup H and a normal subgroup N such that $G = HN$ and $H \cap N = 1$. Then G is called the semidirect product of N by H. To define the notion of wreath product, we assume that A and H are groups, X is a set and H acts on X. Define $K = \prod_{w\in X} A_w$, where $A_w \cong A$. If we consider the elements of K as arbitrary sequences of elements of A with componentwise multiplication then the action of H on X can be extended in a natural way to an action of H on the group K by $h(a_\omega) = (a_{h^{-1}\omega})$. Then the wreath product $A \wr H$ of A by H is the semidirect product H by K.

Example 3.2. Suppose S_n is an star with a vertex of degree n and n pendant vertices. Since S_n has exactly one vertex of degree n, this vertex will be fixed under each automorphism of S_n. On the other hand, all pendants can be imaged under permutations to each other. Thus $\mathrm{Aut}(S_n) \cong \mathrm{Sym}(n)$. According to [3, Example 5.8], the modified Wiener index of S_n with $n+1$ vertices is equal to

$$\widehat{W}(S_n) = n^2 - 1.$$

Also,

$$\overline{D}(S_n, i) = \begin{cases} 0 & i = 1 \\ (n-1)n! & i = 2. \end{cases}$$

Therefore, by applying Theorems 2.2–2.10,

$$\widehat{W}(L(S_n)) = \frac{n^2-n}{2},$$
$$\widehat{W}(S(S_n)) = 5n^2-3n-3,$$
$$\widehat{W}(T(S_n)) = \frac{6n^2-3n-3}{2},$$
$$\widehat{W}(Q(S_n)) = 4n^2-2n-2,$$
$$\widehat{W}(R(S_n)) = \frac{8n^2-2n-3}{2}.$$

For the proof of last equality, we assume that

$$V(S_n) = \{v_0, v_1, v_2, \ldots, v_n\} \text{ and } E(S_n) = \{e_i = v_0v_i \mid 1 \leq i \leq n\}.$$

The automorphism group of $R(S_n)$ has automorphisms τ_i such that $\tau_i : v_i \mapsto e_i$ and τ_i fixes other vertices of the graph. Suppose $A_i = \langle \tau_i \rangle$. Then $A_i \cong \mathbb{Z}_2$ and

$$K = \underbrace{\mathbb{Z}_2 \times \ldots \times \mathbb{Z}_2}_{n \text{ times}}$$

is isomorphic to a subgroup of $\mathrm{Aut}(R(S_n))$. On the other hand, $\mathrm{Sym}(n)$ acts on K by $\alpha(a_i) = (a_{\alpha^{-1}i})$. Hence $\mathrm{Aut}(R(S_n)) \cong \mathbb{Z}_2 \wr \mathrm{Sym}(n)$.

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On the inertia of weighted $(k-1)$-cyclic graphs*

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Abstract

Let G_w be a weighted graph. The inertia of G_w is the triple $\mathrm{In}(G_w) = (i_+(G_w), i_-(G_w), i_0(G_w))$, where $i_+(G_w), i_-(G_w), i_0(G_w)$ are, respectively, the number of the positive, negative and zero eigenvalues of the adjacency matrix $A(G_w)$ of G_w including their multiplicities. A simple n-vertex connected graph is called a $(k-1)$-cyclic graph if its number of edges equals $n+k-2$. Let $\theta(r_1, r_2, \ldots, r_k)_w$ be an n-vertex simple weighted graph obtained from k weighted paths $(P_{r_1})_w, (P_{r_2})_w, \ldots, (P_{r_k})_w$ by identifying their initial vertices and terminal vertices, respectively. Set $\Theta_k := \{\theta(r_1, r_2, \ldots, r_k)_w : r_1 + r_2 + \cdots + r_k = n + 2k - 2\}$. The inertia of the weighted graph $\theta(r_1, r_2, \ldots, r_k)_w$ is studied. Also, the weighted $(k-1)$-cyclic graphs that contain $\theta(r_1, r_2, \ldots, r_k)_w$ as an induced subgraph are studied. We characterize those graphs among Θ_k that have extreme inertia. The results generalize the corresponding results obtained by Tan and Liu in 2013 and Yu et al., 2014.

Keywords: Weighted k-cyclic graph, adjacency matrix, inertia.

Math. Subj. Class.: 05C50, 15A18

1 The first section

In this paper, we only consider simple weighted graphs on positive weight set. Let G_w be a weighted graph with vertex set $\{v_1, v_2, \ldots, v_n\}$, edge set $E(G_w) \neq \emptyset$ and weight set $W(G_w) = \{w(e) > 0, e \in E(G)\}$. The function $w : E(G_w) \to W(G_w)$ is called a weight function of G_w. It is obvious that each weighted graph corresponds to a weight function. The *adjacency matrix* of G_w is defined as the matrix $A(G_w) = (a_{ij})$ such that $a_{ij} = w(v_iv_j)$ if $v_iv_j \in E(G_w)$ and 0 otherwise. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of

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$A(G_w)$ are said to be the eigenvalues of the weighted graph G_w. The *inertia* of G_w is defined to be the triple $\mathrm{In}(G_w) = (i_+(G_w), i_-(G_w), i_0(G_w))$, where $i_+(G_w), i_-(G_w)$ and $i_0(G_w)$ are the numbers of the positive, negative and zero eigenvalues of $A(G_w)$ including multiplicities, respectively. $i_+(G_w)$ and $i_-(G_w)$ are called the *positive, negative index of inertia* (for short, *positive, negative index*) of G_w, respectively. The number $i_0(G_w)$ is called the *nullity* of $A(G_w)$. The nullity and the rank of $A(G_w)$ are also called the nullity and the rank of G_w, and denoted by $\eta(G)$ and $\mathrm{R}(G)$, respectively. Obviously, $\mathrm{R}(G_w) = i_+(G_w) + i_-(G_w)$ and $i_+(G_w) + i_-(G_w) + i_0(G_w) = n$. For convenience, in the whole context, we let G denote the unweighted graph with respect to the weighted graph G_w; G can be also viewed as a trivial weighted graph in which the weight for each edge is 1.

An *induced subgraph* of G_w is an induced subgraph of G having the same weights with those of G_w. For an induced weighted subgraph H_w of G_w, let $G_w - H_w$ be the subgraph obtained from G_w by deleting all vertices of H_w and all incident edges. A *m-cyclic graph* is a simple connected graph in which the number of edges equals the number of vertices plus $m-1$. A weighted path and a weighted cycle of order n are denoted by $(P_n)_w$, $(C_n)_w$, respectively. An isolated vertex is denoted by K_1.

The study of eigenvalues of graph has been received a lot of attention due to its applications in chemistry (see [2, 7, 10, 15] for details). Gregory et al. [8] studied the subadditivity of the positive, negative indices of inertia and developed certain properties of Hermitian rank which were used to characterize the biclique decomposition number. Gregory et al. [9] investigated the inertia of a partial join of two graphs and established a few relations between the inertia and biclique decompositions of partial joins of graphs. Daugherty [3] characterized the inertia of unicyclic graphs in terms of matching number and obtained a linear-time algorithm for computing it. Yu et al. [19] investigated the minimal positive index of inertia among all unweighted bicyclic graphs of order n with pendants, and characterized the bicyclic graphs with positive index 1 or 2. Very recently, it is interesting to see that Marina et al. [1] studied the inertia set of a signed graph in algebraic approach.

The nullity of unweighted graphs has been studied extensively in the literature. Tan and Liu [18] gave the nullity set of unicyclic graphs and characterized the unicyclic graphs with maximum nullity. In addition, Nath and Sarma [17] presented another version of characterization of an acyclic or unicyclic graph to be singular. One of the present authors [13] studied the nullity of graphs with pendant vertices. Fan and Qian [6] characterized the bipartite graphs with the second largest nullity and the regular bipartite graphs with the third largest nullity. Fan and Wang [5] characterized the unicyclic signed graphs of order n with nullity $n-2, n-3, n-4, n-5$, respectively.

Our paper is motivated directly by [4, 11, 13, 19, 20, 21]. On the one hand, Fan et al. [4] studied the nullity of signed bicyclic graph (which is, in fact, the bicyclic graph with edge weight 1 or -1); Li [13] and Hu [11] studied the nullity of unweighted bicyclic graph. On the other hand, Yu et al. [20] characterized all n-vertex weighted uicyclic graphs with positive index 1 or 2; Tan and Liu [21] studied the nullity of unweighted $(k-1)$-cyclic graphs. It is natural and interesting for us to consider the extremal problems on the inertia of weighted $(k-1)$-cyclic graphs, which may generalize the corresponding results obtained in [20, 21].

This paper is organized as follows. In Section 2, some preliminaries are presented. In Section 3, we define two classes of weighted $(k-1)$-cyclic graph, denoted by Θ_k and $\Gamma_{n,k-1}$. Moreover, we give a method to determine the inertia of a weighted graph in Θ_k.

In Section 4, we characterize all weighted $(k-1)$-cyclic graphs in $\Gamma_{n,k-1}$ having just one or two positive (resp. negative) eigenvalues. In Section 5, we characterize all weighted $(k-1)$-cyclic graphs in $\Gamma_{n,k-1}$ of rank $2,3,4$, respectively.

2 Preliminaries

In this section, we list some lemmas which will be used to prove our main results. Suppose M, N are two Hermitian matrices of order n, if there exists an invertible matrix Q of order n such that $QMQ^T = N$, where Q^T denotes the conjugate transpose of Q, then we say that M is *congruent to* N, denoted by $M \cong N$.

Lemma 2.1 ([12]). *Let M, N be two Hermitian matrices of order n satisfying $M \cong N$. Then $i_+(M) = i_+(N)$, $i_-(M) = i_-(N)$ and $i_0(M) = i_0(N)$.*

Let M be a Hermitian matrix. We denote three types of elementary congruence matrix operations (ECMOs) on M as follows:

(1) interchanging i-th and j-th rows of M, while interchanging i-th and j-th columns of M;

(2) multiplying i-th row of M by a non-zero number k, while multiplying i-th column of M by k;

(3) adding i-th row of M multiplied by a non-zero number k to j-th row, while adding i-th column of M multiplied by k to j-th column.

By Lemma 2.1, the ECMOs do not change the inertia of a Hermitian matrix.

Lemma 2.2 ([14]). *Let H_w be an induced subgraph of G_w. Then $i_+(H_w) \leqslant i_+(G_w)$ and $i_-(H_w) \leqslant i_-(G_w)$.*

Lemma 2.3 ([14]). *Let G_w be a weighted graph containing a pendant vertex v with its unique neighbor u. Then $i_+(G_w) = i_+(G_w - u - v) + 1$ and $i_-(G_w) = i_-(G_w - u - v) + 1$.*

The following result is a direct consequence of Lemma 2.3.

Lemma 2.4. *Let $(P_n)_w$ be a weighted path of order n. Then $\mathrm{In}((P_n)_w) = (\frac{n}{2}, \frac{n}{2}, 0)$ if n is even and $(\frac{n-1}{2}, \frac{n-1}{2}, 1)$ otherwise.*

By Lemma 2.4, we can show that the adjacency matrix of $(P_{2k})_w$ is invertible. In fact, let $\{v_1, v_2, \ldots, v_{2k}\}$ be the vertex set of the weighted path $(P_{2k})_w$ such that $v_i v_{i+1} \in E((P_{2k})_w)\,(i = 1, \ldots, 2k-1)$ and $w_{ii} = w(v_{2i-1}v_{2i})\,(i = 1, \ldots, k)$, $w_{i,i+1} = w(v_{2i}v_{2i+1})\,(i = 1, \ldots, k-1)$. Then the adjacency matrix of $(P_{2k})_w$ has the following block form:

$$A = \begin{pmatrix} A_{11} & A_{12} & \ldots & \mathbf{0} & \mathbf{0} \\ A_{21} & A_{22} & \ldots & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \ldots & A_{k-1,k-1} & A_{k-1,k} \\ \mathbf{0} & \mathbf{0} & \ldots & A_{k,k-1} & A_{k,k} \end{pmatrix}$$

where $A_{ii} = \begin{pmatrix} 0 & w_{ii} \\ w_{ii} & 0 \end{pmatrix}, (i = 1, \ldots, k)$ and

$$A_{i+1,i}^T = A_{i,i+1} = \begin{pmatrix} 0 & 0 \\ w_{i,i+1} & 0 \end{pmatrix}, (i = 1, \ldots, k-1).$$

Let $B = (B_{ij})_{i,j=1}^{k}$, where

$$B_{ij} = \begin{cases} \begin{pmatrix} 0 & \dfrac{1}{w_{ii}} \\ \dfrac{1}{w_{ii}} & 0 \end{pmatrix} & \text{if } i = j; \\ \begin{pmatrix} 0 & \dfrac{w_{i,i+1} \dots w_{j-1,j}}{w_{i,i} \dots w_{j,j}} \\ 0 & 0 \end{pmatrix} & \text{if } i < j \text{ and } j - i \equiv 0 \pmod 2; \\ \begin{pmatrix} 0 & -\dfrac{w_{i,i+1} \dots w_{j-1,j}}{w_{i,i} \dots w_{j,j}} \\ 0 & 0 \end{pmatrix} & \text{if } i < j \text{ and } j - i \equiv 1 \pmod 2; \\ B_{ji}^T, & \text{if } i > j. \end{cases}$$

Lemma 2.5. *Let A and B be the matrices defined as above. Then $AB = I$.*

Proof. Let $C = (C_{ij})_{i,j=1}^{k} = AB$. It suffices to show that $C_{ii} = I_2$ for $i = 1, \dots, k$, where I_2 is the identity matrix of order 2, and $C_{ij} = \mathbf{0}$ if $i \neq j$. Note that the first (resp. last) row of A contains just two non-zero blocks, whereas each of the rest rows of A contains just three non-zero blocks, the proofs are a little different between them. First we consider the cases that $i \neq 1, k$.

If $1 < i = j < k$, then

$$\begin{aligned} C_{ii} &= \sum_{s=1}^{k} A_{is}B_{si} = A_{i,i-1}B_{i-1,i} + A_{ii}B_{ii} + A_{i,i+1}B_{i+1,i} \\ &= \begin{pmatrix} 0 & w_{i-1,i} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\dfrac{w_{i-1}}{w_{i-1,i-1}w_{i,i}} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & w_{ii} \\ w_{ii} & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{w_{ii}} \\ \frac{1}{w_{ii}} & 0 \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 & 0 \\ w_{i,i+1} & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ -\dfrac{w_{i,i+1}}{w_{ii}w_{i+1,i+1}} & 0 \end{pmatrix} \\ &= I_2. \end{aligned}$$

If $1 < i < j < k$, we distinguish the following three possible cases to prove our result.

Case 1: $j - i \equiv 0 \pmod 2$. In this case, we have

$$\begin{aligned} C_{ij} &= \sum_{s=1}^{k} A_{is}B_{sj} = A_{i,i-1}B_{i-1,j} + A_{i,i}B_{i,j} + A_{i,i+1}B_{i+1,j} \\ &= \begin{pmatrix} 0 & w_{i-1,i} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\frac{w_{i-1,i} \dots w_{j-1,j}}{w_{i-1,i-1} \dots w_{jj}} \\ 0 & 0 \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 & w_{ii} \\ w_{ii} & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{w_{i,i+1} \dots w_{j-1,j}}{w_{i,i} \dots w_{jj}} \\ 0 & 0 \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 & 0 \\ w_{i,i+1} & 0 \end{pmatrix} \begin{pmatrix} 0 & -\frac{w_{i+1,i+2} \dots w_{j-1,j}}{w_{i+1,i+1} \dots w_{jj}} \\ 0 & 0 \end{pmatrix} \\ &= \mathbf{0}. \end{aligned}$$

Case 2: $j-i=1$. In this case, we have

$$\begin{aligned}C_{ij}&=\sum_{s=1}^{k}A_{is}B_{sj}=A_{i,i-1}B_{i-1,j}+A_{i,i}B_{i,j}+A_{i,i+1}B_{i+1,j}\\&=\begin{pmatrix}0&w_{i-1,i}\\0&0\end{pmatrix}\begin{pmatrix}0&\dfrac{w_{i-1,i}w_{i,j}}{w_{i-1,i-1}w_{ii}w_{jj}}\\0&0\end{pmatrix}+\begin{pmatrix}0&w_{ii}\\w_{ii}&0\end{pmatrix}\begin{pmatrix}0&-\dfrac{w_{ij}}{w_{i,i}w_{jj}}\\0&0\end{pmatrix}\\&\quad+\begin{pmatrix}0&0\\w_{i,i+1}&0\end{pmatrix}\begin{pmatrix}0&\dfrac{1}{w_{jj}}\\\dfrac{1}{w_{jj}}&0\end{pmatrix}\\&=\mathbf{0}.\end{aligned}$$

Case 3: $j-i\equiv 1 \pmod 2$ and $j-i>1$. In this case, we have

$$\begin{aligned}C_{ij}&=\sum_{s=1}^{k}A_{is}B_{sj}=A_{i,i-1}B_{i-1,j}+A_{i,i}B_{i,j}+A_{i,i+1}B_{i+1,j}\\&=\begin{pmatrix}0&w_{i-1,i}\\0&0\end{pmatrix}\begin{pmatrix}0&\dfrac{w_{i-1,i}\cdots w_{j-1,j}}{w_{i-1,i-1}\cdots w_{jj}}\\0&0\end{pmatrix}\\&\quad+\begin{pmatrix}0&w_{ii}\\w_{ii}&0\end{pmatrix}\begin{pmatrix}0&-\dfrac{w_{i,i+1}\cdots w_{j-1,j}}{w_{i,i}\cdots w_{jj}}\\0&0\end{pmatrix}\\&\quad+\begin{pmatrix}0&0\\w_{i,i+1}&0\end{pmatrix}\begin{pmatrix}0&\dfrac{w_{i+1,i+2}\cdots w_{j-1,j}}{w_{i+1,i+1}\cdots w_{jj}}\\0&0\end{pmatrix}\\&=\mathbf{0}.\end{aligned}$$

For $i=1$ or $i=k$, all the proofs above are still correct if we set the corresponding blocks to be $\mathbf{0}$ whenever one of its subscripts equals 0 or $k+1$, such as $A_{10}=A_{k,k+1}=\mathbf{0}$.

If $1\leqslant j<i\leqslant k$, the proof is similar to the case $1\leqslant i<j\leqslant k$. We omit the procedure here. □

3 The inertia of weighted graphs in Θ_k

For $m\geqslant 1$, a *m-cyclic graph* is a simple connected graph in which the number of edges equals the number of vertices plus $m-1$. Let P_{r_i} be a path of order $r_i\,(r_i\geqslant 2)$ and $\{P_{r_i}|1\leqslant i\leqslant k\}$ be the set of $k\,(k\geqslant 2)$ vertex-disjoint paths, where there exists at most one path of order 2. Identify the k initial vertices as u_0 and terminal vertices as v_0, respectively. The resultant graph, denoted by $\theta(r_1,r_2,\ldots,r_k)$, is called a Θ-*graph*. Denote by Θ_k the set of all n-vertex weighted Θ-graphs having form $\theta(r_1,r_2,\ldots,r_k)_w$. Note that any weighted Θ-graph is also a weighted $(k-1)$-cyclic graph. Denote the set of all weighted $(k-1)$-cyclic graphs of order n, which contain a weighted Θ-graph as an induced subgraph, by $\Gamma_{n,k-1}$. In this section, we'll give a method to determine the inertia of weighted graphs in Θ_k.

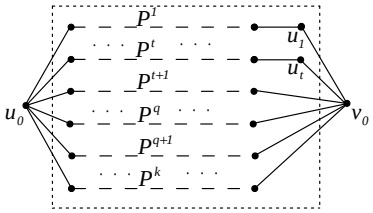

Figure 1: The structure of $\theta(r_1, r_2, \ldots, r_k)$

Let $G_w := \theta(r_1, r_2, \ldots, r_k)_w$ be a graph of order n. Let n_i be the number of r_j's which satisfy $r_j - 2 \equiv i \pmod 4$, $1 \leqslant j \leqslant k$, $0 \leqslant i \leqslant 3$ and set $t := n_1 + n_3$ and $q := t + n_2$. It is easy to see that $G_w \in \Theta_k$, we arrange the structure of G_w as follows: First come the paths $P_{r_1}, \ldots, P_{r_{n_1}}$ with $r_1 \leqslant r_2 \leqslant \ldots \leqslant r_{n_1}$ and $r_i \equiv 3 \pmod 4$, $i = 1, 2, \ldots, n_1$; next $P_{r_{n_1+1}}, \ldots, P_{r_t}$ with $r_{n_1+1} \leqslant r_{n_1+2} \leqslant \ldots \leqslant r_t$ and $r_i \equiv 1 \pmod 4$, $i = n_1 + 1, n_1 + 2, \ldots, t$; then $P_{r_{t+1}}, \ldots, P_{r_q}$ with $r_{t+1} \leqslant r_{t+2} \leqslant \ldots \leqslant r_q$ and $r_i \equiv 2 \pmod 4$, $i = t + 1, t + 2, \ldots, q$; finally $P_{r_{q+1}}, \ldots, P_{r_k}$ with $r_{q+1} \leqslant r_{q+2} \leqslant \ldots \leqslant r_k$ and $r_i \equiv 0 \pmod 4$, $i = q + 1, q + 2, \ldots, k$. Let u_i be the neighbor of v_0 in the odd path P_{r_i}, $i = 1, 2, \ldots, t$. Let $P^i = u_1^i u_2^i \ldots u_{2s_i}^i$ $(1 \leqslant i \leqslant k)$ be the path in P_{r_i} $(1 \leqslant i \leqslant k)$ obtained by deleting u_0, v_0 and u_i if r_i is odd; see Fig. 1. Further on we will label the weight for each edge of G_w according to the following possible cases.

Case 1: $\min\{r_1, r_2, \ldots, r_k\} = 4$**.** In this case, partition the vertex set of G_w as follows: $\{u_0\}, V(P^1), \ldots, V(P^k), \{u_1, \ldots, u_t\}, \{v_0\}$. Let $a_i = w(u_0 u_1^i)$ $(i = 1, \ldots, k)$, $b_i = w(u_i u_{2s_i}^i)$ $(i = 1, \ldots, t)$, $b_j = w(v_0 u_{2s_j}^j)$ $(j = t + 1, \ldots, k)$, $d_i = w(v_0 u_i)$ $(i = 1, \ldots, t)$, $w_{jj}^i = w(u_{2j-1}^i u_{2j}^i)$ $(i = 1, \ldots, k; j = 1, \ldots, \frac{1}{2}|V(P^i)|)$ and $w_{j,j+1}^i = w(u_{2j}^i u_{2j+1}^i)$ $(i = 1, \ldots, k; j = 1, \ldots, \frac{1}{2}|V(P^i)| - 1)$. Then the adjacency matrix of G_w has the following form:

$$A(G_w) = \left(\begin{array}{c|c|c|c|c} 0 & \alpha_1^T \ldots \alpha_t^T & \alpha_{t+1}^T \ldots \alpha_k^T & \mathbf{0} & 0 \\ \hline \alpha_1^T & A_1 & & \beta_1 & \\ \vdots & \ddots & \mathbf{0} & \ddots & \mathbf{0} \\ \alpha_t^T & & A_t & & \beta_t \\ \hline \alpha_{t+1}^T & & A_{t+1} & & \beta_{t+1}^T \\ \vdots & \mathbf{0} & \ddots & \mathbf{0} & \vdots \\ \alpha_k^T & & & A_k & \beta_k^T \\ \hline & \beta_1^T & & & d_1 \\ \mathbf{0} & \ddots & \mathbf{0} & \mathbf{0} & \vdots \\ & & \beta_t^T & & d_t \\ \hline 0 & \mathbf{0} & \beta_{t+1}^T \ldots \beta_k^T & d_1 \ldots d_t & 0 \end{array}\right),$$

where $\alpha_i^T = (a_i, 0, \ldots, 0)$ and $\beta_i^T = (0, \ldots, 0, b_i)$.

We apply the ECMOs on $A(G_w)$: using $-\alpha_i^T A_i^{-1}$ to multiply the $(i+1)$-th row, then adding it to the first row, we can cancel $\alpha_i^T (i = 1, \ldots, k)$ in the first row. Similarly,

using $-\beta_i^T A_i^{-1}$ to multiply the $(i+1)$-th row, then adding it to $(k+i+1)$-th row if $i \leqslant t$, and adding it to the last row if $t+1 \leqslant i \leqslant k$, we can cancel $\beta_i^T (i = 1, \ldots, k)$. After that, column operations are applied so that each α_i and β_i are reduced to $\mathbf{0}$s. By Lemma 2.5, $-\alpha_i^T A_i^{-1} \alpha_i = -\beta_i^T A_i^{-1} \beta_i = 0$ and $c_i = -\alpha_i^T A_i^{-1} \beta_i = -\beta_i^T A_i^{-1} \alpha_i$, where

$$c_i = \begin{cases} -\dfrac{a_i b_i w_{12}^i w_{23}^i \ldots w_{s_i-1,s_i}^i}{w_{11}^i w_{22}^i \ldots w_{s_i,s_i}^i}, & \text{if } |A_i| = 2s_i \equiv 2 \pmod 4; \\ \dfrac{a_i b_i w_{12}^i w_{23}^i \ldots w_{s_i-1,s_i}^i}{w_{11}^i w_{22}^i \ldots w_{s_i,s_i}^i}, & \text{if } |A_i| = 2s_i \equiv 0 \pmod 4. \end{cases}$$

So $A(G_w)$ can be reduced to the following matrix:

$$B = \left(\begin{array}{c|c|c|c|c} 0 & \mathbf{0} & \mathbf{0} & c_1 \ldots c_t & s \\ \hline \mathbf{0} & \begin{matrix} A_1 & & \\ & \ddots & \\ & & A_t \end{matrix} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \begin{matrix} A_{t+1} & & \\ & \ddots & \\ & & A_k \end{matrix} & \mathbf{0} & \mathbf{0} \\ \hline \begin{matrix} c_1 \\ \vdots \\ c_t \end{matrix} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \begin{matrix} d_1 \\ \vdots \\ d_t \end{matrix} \\ \hline s & \mathbf{0} & \mathbf{0} & d_1 \ldots d_t & 0 \end{array}\right),$$

where $s = \sum_{i=t+1}^{k} c_i$.

Define

$$D = \left(\begin{array}{cc|ccc} 0 & s & c_1 & \ldots & c_t \\ s & 0 & d_1 & \ldots & d_t \\ \hline c_1 & d_1 & & & \\ \vdots & \vdots & & \mathbf{0} & \\ c_t & d_t & & & \end{array}\right). \tag{3.1}$$

After interchanging rows and columns, we get the equivalent matrix of B:

$$\begin{pmatrix} D & & & \\ & A_1 & & \\ & & \ddots & \\ & & & A_k \end{pmatrix}. \tag{3.2}$$

It follows that

$$\begin{aligned} i_+(G_w) &= i_+(D) + \sum_{j=1}^{k} i_+(A_k) = i_+(D) + \frac{1}{2}\sum_{j=1}^{k}|A_i| \\ &= i_+(D) + \frac{1}{2}\left(\sum_{j=1}^{t}(r_i-3) + \sum_{j=t+1}^{k}(r_i-2)\right) \\ &= i_+(D) + \frac{1}{2}\left(\sum_{j=1}^{k}(r_i-2) - t\right) \\ &= i_+(D) + \frac{1}{2}(n-2-t). \end{aligned}$$

Similarly, $i_-(G_w) = i_-(D) + \frac{1}{2}(n-2-t), i_0(G_w) = t+2-\mathrm{R}(D)$.

Case 2.: $\min\{r_1, r_2, \ldots, r_k\} = 3$**.** We suppose, without loss of generality, that the first ℓ paths $P_i = u_0u_iv_0$ $(i = 1, \ldots, \ell)$ are of length 3. Partition the vertex of G_w as follows: $\{u_0\}, V(P^{\ell+1}), \ldots, V(P^k), \{u_1, \ldots, u_\ell\}, \{u_{\ell+1}, \ldots, u_t\}, \{v_0\}$. Then we label the weight for each edge of G_w as follows: $c_i = w(u_0u_i)\,(i = 1, \ldots, \ell)$, $d_i = w(v_0u_i)\,(i = 1, \ldots, t)$, $a_i = w(u_0u_1^i)\,(i = \ell+1, \ldots, k)$, $b_i = w(u_iu_{2s_i}^i)\,(i = \ell+1, \ldots, t)$, $b_j = w(v_0u_{2s_j}^j)\,(j = t+1, \ldots, k)$ and $w_{jj}^i = w(u_{2j-1}^iu_{2j}^i)\,(i = \ell+1, \ldots, k; j = 1, \ldots, \frac{1}{2}|V(P^i)|)$, $w_{j,j+1}^i = w(u_{2j}^iu_{2j+1}^i)\,(i = \ell+1, \ldots, k; j = 1, \ldots, \frac{1}{2}|V(P^i)| - 1)$. Then the adjacency matrix of G_w has the following form:

$$A(G_w) = \left(\begin{array}{c|c|c|c|c|c} 0 & \alpha_{\ell+1}^T \ldots \alpha_t^T & \alpha_{t+1}^T \ldots \alpha_k^T & c_1 \ldots c_\ell & \mathbf{0} & 0 \\ \hline \alpha_{\ell+1}^T & A_{\ell+1} & & & \beta_{\ell+1} & \\ \vdots & \ddots & \mathbf{0} & \mathbf{0} & \ddots & \mathbf{0} \\ \alpha_t^T & & A_t & & & \beta_t \\ \hline \alpha_{t+1}^T & & A_{t+1} & & & \beta_{t+1}^T \\ \vdots & \mathbf{0} & \ddots & \mathbf{0} & \mathbf{0} & \vdots \\ \alpha_k^T & & & A_k & & \beta_k^T \\ \hline c_1 & & & & & d_1 \\ \vdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \vdots \\ c_\ell & & & & & d_\ell \\ \hline & \beta_{\ell+1}^T & & & & d_{\ell+1} \\ \mathbf{0} & \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \vdots \\ & & \beta_t^T & & & d_t \\ \hline 0 & \mathbf{0} & \beta_{t+1}^T \ldots \beta_k^T & d_1 \ldots d_\ell & d_{\ell+1} \ldots d_t & 0 \end{array}\right).$$

After applying ECMOs on the above matrix, we can get a diagonal matrix similar to (3.2), hence the result is still holds in this case.

Case 3: $\min\{r_1, r_2, \ldots, r_k\} = 2$**.** Let $c_{t+1} = w(u_0v_0)$, then we only need to delete the row and the column corresponding to A_{t+1} and replace the upper right and the lower left elements of $A(G_w)$ with c_{t+1}, and the rest arguments are similar.

Theorem 3.1. *Let $G_w = \theta(r_1, r_2, \ldots, r_k)_w$ be a weighted graph of order n. Denote by n_i the number of r_j's which satisfy $r_j - 2 \equiv i \pmod 4$ $(1 \leqslant j \leqslant k, 0 \leqslant i \leqslant 3)$ and let $t = n_1 + n_3$. The matrix D is defined as in* (3.1)*. Then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \Big(i_+(D) + \frac{1}{2}(n-2-t), i_-(D) + \frac{1}{2}(n-2-t), t+2-\mathrm{R}(D)\Big). \quad (3.3)$$

In particular,

(i) *if $n_1 + n_3 = 0$, $s = 0$, then* $(i_+(G_w), i_-(G_w), i_0(G_w)) = \big(\frac{1}{2}n - 1, \frac{1}{2}n - 1, 2\big)$.

(ii) *if $n_1 + n_3 = 0$, $s \neq 0$, then* $(i_+(G_w), i_-(G_w), i_0(G_w)) = \big(\frac{1}{2}n, \frac{1}{2}n, 0\big)$.

(iii) *if $n_1 n_3 > 0$, then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \left(\frac{1}{2}(n-t) + 1, \frac{1}{2}(n-t) + 1, t-2\right).$$

(iv) *if $n_1 + n_3 \neq 0$, $n_1 n_3 = 0$ and $d_i c_t \neq c_i d_t$ holds for some $i \in \{1, 2, \ldots, t-1\}$, then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \left(\frac{1}{2}(n-t) + 1, \frac{1}{2}(n-t) + 1, t-2\right).$$

(v) *if $n_1 + n_3 \neq 0$, $n_1 n_3 = 0$, $s > 0$ and $d_i c_t = c_i d_t$ holds for $i = 1, 2, \ldots, t$, then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \begin{cases} \big(\frac{1}{2}(n-t), \frac{1}{2}(n-t) + 1, t-1\big), & \text{if } n_1 > 0, n_3 = 0; \\ \big(\frac{1}{2}(n-t) + 1, \frac{1}{2}(n-t), t-1\big), & \text{if } n_3 > 0, n_1 = 0. \end{cases}$$

(vi) *if $n_1 + n_3 \neq 0$, $n_1 n_3 = 0$, $s = 0$ and $d_i c_t = c_i d_t$ holds for $i = 1, 2, \ldots, t$, then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \left(\frac{1}{2}(n-t), \frac{1}{2}(n-t), t\right).$$

(vii) *if $n_1 + n_3 \neq 0$, $n_1 n_3 = 0$, $s < 0$ and $d_i c_t = c_i d_t$ holds for $i = 1, 2, \ldots, t$, then*

$$(i_+(G_w), i_-(G_w), i_0(G_w)) = \begin{cases} \big(\frac{1}{2}(n-t) + 1, \frac{1}{2}(n-t), t-1\big), & \text{if } n_1 > 0, n_3 = 0; \\ \big(\frac{1}{2}(n-t), \frac{1}{2}(n-t) + 1, t-1\big), & \text{if } n_3 > 0, n_1 = 0. \end{cases}$$

Proof. By the discussion of Cases 1-3 above, the first part of Theorem 3.1 follows directly. Furthermore, by the first part of Theorem 3.1 it is routine to check that (i) and (ii) hold.

(iii) If $n_1n_3 > 0$, applying ECMOs on D yields the following matrix:

$$\left(\begin{array}{cc|ccc} 0 & s & 0 & \dots & c_t \\ s & 0 & \alpha_1 & \dots & d_t \\ \hline 0 & \alpha_1 & & & \\ \vdots & \vdots & & \mathbf{0} & \\ c_t & d_t & & & \end{array}\right),$$

where $\alpha_i = d_i - \frac{d_t}{c_t}c_i$. Noted that $c_1 > 0$ and $c_t < 0$, hence $\alpha_1 \neq 0$, which implies that $i_+(D) = i_-(D) = 2$ and $\mathrm{R}(D) = 4$. By (3.3), we have $(i_+(G_w), i_-(G_w), i_0(G_w)) = (\frac{1}{2}(n-t), \frac{1}{2}(n-t)+1, t-1)$. By a similar discussion as in the proof of (iii), we can show that (iv) also holds.

(v) In this case, applying ECMOs to D yields the following matrix:

$$\left(\begin{array}{cc|ccc} 0 & s & 0 & \dots & 0 \\ s & 0 & 0 & \dots & 0 \\ \hline 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \dots & -\frac{2c_td_t}{s} \end{array}\right).$$

If $n_1 > 0, n_3 = 0$, then $-\frac{2c_td_t}{s} < 0$ for $c_t > 0$, hence $i_+(D) = 1, i_-(D) = 2$ and $\mathrm{R}(D) = 3$. In view of (3.3), we have $(i_+(G_w), i_-(G_w), i_0(G_w)) = (\frac{1}{2}(n-t), \frac{1}{2}(n-t)+1, t-2)$. If $n_1 = 0, n_3 > 0$, then $-\frac{2c_td_t}{s} > 0$ for $c_t < 0$, hence $i_+(D) = 2, i_-(D) = 1$ and $\mathrm{R}(D) = 3$. In view of (3.3), we have $(i_+(G_w), i_-(G_w), i_0(G_w)) = (\frac{1}{2}(n-t)+1, \frac{1}{2}(n-t), t-2)$. By a similar discussion, we can also show that (vi) and (vii) hold.

This completes the proof. □

4 Characterization of weighted graphs in $\Gamma_{n,k-1}$ with small positive (negative) indices

In this section, we'll characterize all the weighted graphs in $\Gamma_{n,k-1}$ with 1 or 2 positive (negative) indices.

Theorem 4.1. *Let $G_w \in \Gamma_{n,k-1}$. Then $i_+(G_w) = 1$ if and only if G_w is one of the following graphs: the weighted graph $\theta(3,\dots,3)_w$ with $c_kd_i = c_id_k$, $i = 1,2,\dots,k$; the weighted graph $\theta(3,\dots,3,2)_w$ with $c_{k-1}d_i = c_id_{k-1}$, $i = 1,2,\dots,k-1$.*

Proof. The sufficiency follows directly from Theorem 3.1. Here we only show the necessity in what follows.

Note that if $G_w \in \Gamma_{n,k-1}$ with pendants, then assume, without loss of generality, that x is a pendent vertex of G_w. Let $N(x) = \{y\}$ and $G'_w = G_w - \{x, y\}$. It's routine to check that G'_w is not a weighted empty graph, which contradicts to the fact that $i_+(G_w) = 1$.

Now we consider the case that G_w contains no pedants and $i_+(G_w) = 1$. In view of Theorem 3.1,

• $t = 0$ and $s = 0$. In this subcase, we have $i_+(G_w) = \frac{1}{2}n - 1 = 1$ holds for $n = 4$. Then $G_w = \theta(2,4)_w$ with weighted condition $c_1w_{11}^2 = a_2b_2$ for $s = 0$. Note that the

weighted graph $\theta(2,4)_w$ with $c_1w_{11}^2 = a_2b_2$ is, in fact, the weighted graph $\theta(3,3)_w$ with $c_2d_i = c_id_2$, $i = 1, 2$.

• $t = 0$ and $s \neq 0$. In this subcase, we have $n \geqslant 4$, hence $i_+(G_w) = \frac{n}{2} \geqslant 2$.

• $n_1 > 0$ and $n_3 > 0$. In this subcase, we have $n - t \geqslant 4$, hence $i_+(G_w) = \frac{1}{2}(n-t) + 1 \geqslant 3$.

• Just one of n_1 and n_3 is 0, and $d_ic_t \neq c_id_t$ holds for some $i \in \{1, 2, \ldots, t\}$. In this subcase, we have $n - t \geqslant 2$ if $n_3 = 0$ and $n - t \geqslant 6$ if $n_1 = 0$. Hence $i_+(G_w) = \frac{1}{2}(n-t) + 1 \geqslant 2$.

• Just one of n_1 and n_3 is 0, $s = 0$ and $d_ic_t = c_id_t$ holds for $i = 1, 2, \ldots, t$. In this subcase, we have $n - t \geqslant 2$ if $n_3 = 0$ and $n - t \geqslant 6$ if $n_1 = 0$. Hence, $i_+(G_w) = 1$ if and only if $n - t = 2$ and $n_3 = 0$. This gives that G_w must be the weighted graph $\theta(3, \ldots, 3)_w$ with $c_kd_i = c_id_k$ holding for $i = 1, 2, \ldots, k$.

• Just one of n_1 and n_3 is 0, $s > 0$ and $d_ic_t = c_id_t$ holds for $i = 1, 2, \ldots, t$. In this subcase, we have $n - t \geqslant 2$ if $n_3 = 0$ and $n - t \geqslant 4$ if $n_1 = 0$. Hence, $i_+(G_w) = 1$ if and only if $n - t = 2$ and $n_3 = 0$. This gives that G_w must be the weighted graph $\theta(3, \ldots, 3, 2)_w$ with $c_{k-1}d_i = c_id_{k-1}$ holding for $i = 1, 2, \ldots, k-1$.

• Just one of n_1 and n_3 is 0, $s < 0$ and $d_ic_t = c_id_t$ holds for $i = 1, 2, \ldots, t$. In this subcase, we have $n - t \geqslant 4$ if $n_3 = 0$ and $n - t \geqslant 6$ if $n_1 = 0$, which implies that $i_+(G_w) = \frac{1}{2}(n-t) + 1 > 1$.

Hence, we conclude that $i_+(G_w) = 1$ if and only if G_w is the weighted graph $\theta(3, \ldots, 3)_w$ with $c_kd_i = c_id_k$ holding for $i = 1, 2, \ldots, k$ or, G_w is the weighted graph $\theta(3, \ldots, 3, 2)_w$ with $c_{k-1}d_i = c_id_{k-1}$ holding for $i = 1, 2, \ldots, k-1$. □

Theorem 4.2. *Let $G_w \in \Theta_k$. Then $i_+(G_w) = 2$ if and only if G_w is one of the following graphs: the weighted graph $\theta(2,4,4)_w$ with $c_1 = \frac{a_2b_2}{w_{11}^2} + \frac{a_3b_3}{w_{11}^3}$; the weighted graph $\theta(3, \ldots, 3)_w$ with $d_ic_t \neq c_id_k$ for some $i \in \{1, 2, \ldots, k\}$; the weighted graph $\theta(3, \ldots, 3, 2)_w$ with $d_ic_{k-1} \neq c_id_{k-1}$ for some $i \in \{1, 2, \ldots, k-1\}$; the weighted graph $\theta(3, \ldots, 3, 2, 4)_w$ with $c_{k-2}d_i = c_id_{k-2}$, $i = 1, 2, \ldots, k-2$ and $c_{k-1}w_{11}^k \geqslant a_kb_k$.*

Proof. The sufficiency is clear by Theorem 3.1. To prove the necessity, suppose that $G_w \in \Theta_k$ with $i_+(G_w) = 2$. We proceed by distinguishing the following subcases.

• $t = 0$ and $s = 0$. In this subcase, $i_+(G_w) = \frac{1}{2}n - 1 = 2$, hence we have $n = 6$. Then G_w may be $\theta(2,4,4)_w$, $\theta(2,6)_w$ or $\theta(4,4)_w$. If G_w is the weighted graph $\theta(2,4,4)_w$, then $c_1w_{11}^2 = a_2b_2$ for $s = 0$, whereas the s of $\theta(2,6)_w$ is positive and the s of $\theta(4,4)_w$ is negative, which contradicts the assumption that $s = 0$.

• $t = 0$ and $s \neq 0$. In this subcase, $i_+(G_w) = \frac{1}{2}n = 2$, hence we have $n = 4$. Then G_w is just the weighted graph $\theta(2,4)_w$ with $c_1w_{11}^2 \neq a_2b_2$. In fact, the weighted graph $\theta(2,4)_w$ with $c_1w_{11}^2 \neq a_2b_2$ is also the weighted graph $\theta(3,3)_w$ with $c_kd_i \neq c_id_k$ for $i = 1, 2$.

• $n_1 > 0, n_3 > 0$. In this subcase, we have $n - t \geqslant 4$. Hence, $i_+(G_w) = \frac{1}{2}(n-t) + 1 \geqslant 3$, which implies that there does not exist such weighted graph G_w.

• Just one of n_1 and n_3 is 0, and $d_ic_t \neq c_id_t$ holds for some $i \in \{1, 2, \ldots, t\}$. In this subcase, by a similar discussion in the proof of Theorem 4.1, $i_+(G_w) = 2$ holds only if

$n_3 = 0$ in which $i_+(G_w) = \frac{1}{2}(n-t)+1$. So we have $n-t = 2$. Hence G_w must be the weighted graph $\theta(3,\ldots,3)_w$ with $d_ic_t \neq c_id_k$ for some $i \in \{1,2,\ldots,k\}$, or the weighted graph $\theta(3,\ldots,3,2)_w$ with $d_ic_{k-1} \neq c_id_{k-1}$ for some $i \in \{1,2,\ldots,k-1\}$.

• Just one of n_1 and n_3 is 0, $s = 0$ and $d_ic_t = c_id_t$ holds for $i = 1,2,\ldots,t$. In this subcase, $i_+(G_w) = \frac{1}{2}(n-t)$. Hence, by a similar discussion in the proof of Theorem 4.1, $i_+(G_w) = 2$ if and only if $n-t = 4$ and $n_3 = 0$, which implies that G_w must be the weighted graph $\theta(3,\ldots,2,4)_w$ with $c_{k-2}d_i = c_id_{k-2}$ $i = 1,2,\ldots,k-2$ and $c_{k-1}w_{11}^k = a_kb_k$.

• Just one of n_1 and n_3 is 0, $s > 0$ and $d_ic_t = c_id_t$ holds for $i \in \{1,2,\ldots,t\}$. In this subcase, $i_+(G_w) = \frac{1}{2}(n-t)$. Hence, by a similar discussion in the proof of Theorem 4.1, $i_+(G_w) = 2$ if and only if $n-t = 4$ and $n_3 = 0$, which implies that G_w must be the weighted graph $\theta(3,\ldots,2,4)_w$ with $c_{k-2}d_i = c_id_{k-2}$ for $i \in \{1,2,\ldots,k-2\}$ and $c_{k-1}w_{11}^k > a_kb_k$.

• Just one of n_1 and n_3 is 0, $s < 0$ and $d_ic_t = c_id_t$ holds for $i \in \{1,2,\ldots,t\}$. In this subcase, by a similar discussion in the proof of Theorem 4.1, we have $n-t \geqslant 4$ if $n_3 = 0$ and $n-t \geqslant 6$ if $n_1 = 0$. Hence, we have $i_+(G_w) = \frac{1}{2}(n-t)+1 > 2$.

This completes the proof. □

Theorem 4.3. *Let $G_w \in \Gamma_{n,k}$ with pedants. Then $i_+(G_w) = 2$ if and only if $G \cong G^1, G^2, \ldots, G^9$ or G^{10} (see Fig. 2) and the corresponding weighted conditions are as shown in Table 1, where the empty cell means that there is no correlation between the inertia index of G_w and its weight set.*

Table 1: The weighted condition for each $G_w \in \Gamma(n,k)$ with pedants satisfying $i_+(G_w) = 2$.

weighted graph G_w	weighted conditions of G_w
$G_w^1, G_w^2, G_w^3, G_w^4$	
G_w^5	$c_{k-1}d_i = c_id_{k-1}$ $(1 \leqslant i \leqslant k-1)$
G_w^6, G_w^7	$c_kd_i = c_id_k$ $(1 \leqslant i \leqslant k)$
G_w^8	$c_{k-1}d_i = c_id_{k-1}$ $(2 \leqslant i \leqslant k-1)$
G_w^9, G_w^{10}	$c_{k-1}d_i = c_id_{k-1}$ $(1 \leqslant i \leqslant k-1)$

Proof. It is routine to check that $i_+(G_w^i) = 2$ holds for $i = 1,2,\ldots,10$. To show the converse, suppose that $i_+(G_w) = 2$. Since G_w has at least one pendent x, let $N(x) = \{y\}$ and $G'_w = G_w - \{x,y\} = H_w + pK_1$, where H_w is obtained from G'_w by deleting all the isolated vertices. By Lemma 2.3 we have $2 = i_+(G_w) = i_+(G'_w)+1 = i_+(H_w)+1$. Hence, $i_+(H_w) = 1$. Recall that G_w contains a Θ-graph as an induced subgraph, we conclude that H_w is either isomorphic to a weighted star or one of the weighted graphs described in Theorem 4.1. If H_w is a star, then G must be isomorphic to $G^i, i = 1,2,3,4$. If H_w is the weighted graph $\theta(3,\ldots,3)_w$, then G must be isomorphic to G^i, $i = 5,6,7$ and if H_w is the weighted graph $\theta(3,\ldots,3,2)_w$, then G must be isomorphic to G^i, $i = 8,9,10$.

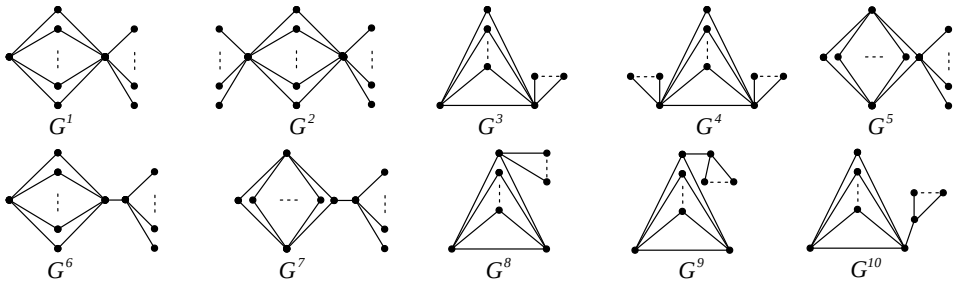

Figure 2: Graphs $G^1, G^2, \ldots, G^9$ and G^{10}.

If G is isomorphic to G^5, without loss of generality, assume that x is adjacent to the internal vertex of the k-th path P_3 (see Fig. 2), so the weighted condition is that $c_{k-1}d_i = c_i d_{k-1}$ holds for $i = 1, 2, \ldots, k-1$. If G is isomorphic to G^6 or G^7, the weighted condition is $c_k d_i = c_i d_k$ for $i = 1, 2, \ldots, k$.

If G is isomorphic to G^8, without loss of generality, assume that x is adjacent to the internal vertex of the first path P_3 (see Fig. 2), so the weighted condition is that $c_{k-1}d_i = c_i d_{k-1}$ holds for $i = 2, 3, \ldots, k-1$. If G is isomorphic to G^9 or G^{10}, the weighted condition is $c_{k-1}d_i = c_i d_{k-1}$ for $i = 1, 2, \ldots, k-1$. □

Similarly, we can have the following theorems:

Theorem 4.4. *Let $G_w \in \Gamma_{n,k-1}$. Then $i_-(G_w) = 1$ if and only if G_w is the weighted $\theta(3, \ldots, 3)_w$ with the weighted condition that $c_k d_i = c_i d_k$ holds for $i = 1, 2, \ldots, k$.*

Theorem 4.5. *Let $G_w \in \Theta_k$. Then $i_-(G_w) = 2$ if and only if G_w is one of the following graphs: the weighted graph $\theta(3, \ldots, 3, 2)_w$ with an arbitrary weighted condition; the weighted graph $\theta(2, 4, 4)_w$ with weighted condition $c_1 = \frac{a_2 b_2}{w_{11}^2} + \frac{a_3 b_3}{w_{11}^3}$; the weighted graph $\theta(3, \ldots, 3)_w$ with the weighted condition that $d_i c_k \neq c_i d_k$ holds for some $i \in \{1, 2, \ldots, k\}$; the weighted graph $\theta(3, \ldots, 3, 2, 4)_w$ with the weighted condition that $c_{k-2}d_i = c_i d_{k-2}$ holds for $i = 1, 2, \ldots, k-2$ and $c_{k-1}w_{11}^k \leqslant a_k b_k$; the weighted graph $\theta(3, \ldots, 3, 4)_w$ with the weighted condition that $c_{k-1}d_i = c_i d_{k-1}$ holds for $i = 1, 2, \ldots, k-1$.*

Theorem 4.6. *Let $G_w \in \Gamma_{n,k-1}$ with pedants. Then $i_-(G_w) = 2$ if and only if G_w is one of the following graphs: the weighted graph G_w has G^1 (resp. G^2, G^3, G^4) as its unweighted graph and its weight set is arbitrary; the weighted graph G_w has G^5 as its unweighted graph satisfying the weighted condition $c_{k-1}d_i = c_i d_{k-1}$, $i = 1, 2, \ldots, k-1$; the weighted graph G_w has G^6 (resp. G^7) as its unweighted graph satisfying the weighted condition $c_k d_i = c_i d_k$, $i = 1, 2, \ldots, k$.*

5 Weighted graphs in $\Gamma_{n,k-1}$ with rank $2, 3,$ or 4

In this section, we characterize all the weighted $(k-1)$-cyclic graphs in $\Gamma_{n,k-1}$ with rank 2, 3, 4, respectively.

Theorem 5.1. *Let $G_w \in \Gamma_{n,k-1}$. Then $\mathrm{R}(G_w) = 2$ if and only if G_w is the weighted $\theta(3,\ldots,3)_w$ with the weighted condition $c_k d_i = c_i d_k$ holding for $i = 1,2,\ldots,k$.*

Proof. Let $G_w \in \Gamma_{n,k-1}$, $i_+(G_w) \geqslant 1$ and $i_-(G_w) \geqslant 1$ since it contains P_2 as an induced subgraph. Then $r(G_w) = 2$ if and only if $i_+(G_w) = i_-(G_w) = 1$. By Theorems 4.1–4.6, we know G_w must be the weighted $\theta(3,\ldots,3)_w$ satisfying the weighted condition that $c_k d_i = c_i d_k$ for any $1 \leqslant i \leqslant k$. □

Theorem 5.2. *Let $G_w \in \Gamma_{n,k-1}$. Then $\mathrm{R}(G_w) = 3$ if and only if G_w is the weighted $\theta(3,\ldots,3,2)_w$ with the weighted condition that $c_{k-1} d_i = c_i d_{k-1}$ holds for $i = 1,2,\ldots,k-1$.*

Proof. Let $G_w \in \Gamma_{n,k-1}$, $i_+(G_w) \geqslant 1$ and $i_-(G_w) \geqslant 1$ since it contains P_{2w} as an induced subgraph. Then $\mathrm{R}(G_w) = 3$ if and only if $i_+(G_w) = 1, i_-(G_w) = 2$ or $i_+(G_w) = 2, i_-(G_w) = 1$. Note that either $i_+(G_w)$ or $i_-(G_w)$ equals 1, hence by Theorems 4.1 and 4.4 we know G_w must be the weighted graph $\theta(3,\ldots,3)_w$ satisfying $c_k d_i = c_i d_k$ for $1 \leqslant i \leqslant k$. □

Theorem 5.3. *Let $G_w \in \Theta_k$. Then $\mathrm{R}(G_w) = 4$ if and only if G_w is one of the following graphs: the weighted graph $\theta(2,4,4)_w$ with weighted condition $c_1 = \frac{a_2 b_2}{w_{11}^2} + \frac{a_3 b_3}{w_{11}^3}$; the weighted graph $\theta(3,\ldots,3)$ with the weighted condition that $d_i c_k \neq c_i d_k$ holds for some $i \in \{1,2,\ldots,k\}$; the weighted graph $\theta(3,\ldots,3,2)_w$ with the weighted condition that $d_i c_{k-1} \neq c_i d_{k-1}$ holds for some $i \in \{1,2,\ldots,k-1\}$; the weighted graph $\theta(3,\ldots,3,2,4)_w$ with the weighted condition that $c_{k-2} d_i = c_i d_{k-2}$ holds for $i = 1,2,\ldots,k-2$ and $c_{k-1} w_{11}^k = a_k b_k$.*

Proof. Let G_w be a weighted $(k-1)$-cyclic graph, it is routine to check that $i_+(G_w) \geqslant 1$ and $i_-(G_w) \geqslant 1$. Then $\mathrm{R}(G_w) = 4$ if and only if $(i_+(G_w), i_-(G_w)) = (1,3)$ or $(i_+(G_w), i_-(G_w)) = (3,1)$ or $(i_+(G_w), i_-(G_w)) = (2,2)$. If one of $i_+(G_w)$ and $i_-(G_w)$ equals 1, by Theorems 4.1 and 4.4, G_w must be the weighted graph $\theta(3,\ldots,3)_w$ or $\theta(3,\ldots,3,2)_w$. In this case, by Theorems 4.1, 4.2, 4.4 and 4.5 we know the rank of such graph G_w is no less than 3. Hence, it should only consider that $(i_+(G_w), i_-(G_w)) = (2,2)$. In this case, based on Theorems 4.2 and 4.5, $(i_+(G_w), i_-(G_w)) = (2,2)$ if and only if G_w is one of the weighted graphs characterized in the above result. □

Similarly, we can have the following theorem:

Theorem 5.4. *Let $G_w \in \Gamma_{n,k-1}$ with pedants. Then $\mathrm{R}(G_w) = 4$ if and only if $G \cong G^1,\ldots,G^7$, what's more, the weighted condition of G_w^1 (resp. G_w^2, G_w^3, G_w^4) is arbitrary; G_w^5 satisfies the weighted condition that $c_{k-1} d_i = c_i d_{k-1}$ holds for $i = 1,2,\ldots,k-1$; while G_w^6 (resp. G_w^7) satisfies the weighted condition that $c_k d_i = c_i d_k$ holds for $i = 1,2,\ldots,k$.*

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Matchings in m-generalized fullerene graphs

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Abstract

A connected planar graph is called m-generalized fullerene if two of its faces are m-gons and all other faces are pentagons and hexagons. In this paper we first determine some structural properties of m-generalized fullerenes and then use them to obtain new results on the enumerative aspects of perfect matchings in such graphs. We provide both upper and lower bounds on the number of perfect matchings in m-generalized fullerene graphs and state exact results in some special cases.

Keywords: Perfect matching, Pfaffian graph, fullerene graph, Hadamard-Fischer inequality.

Math. Subj. Class.: 05C30, 05C70, 15A15

1 Introduction

Classical fullerene graphs have been intensely researched since the discovery of buckminsterfullerene in the fundamental paper [20], which appeared in 1985. This paper gave rise to the whole new area of fullerene science. Most of the research has been driven by a need

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to find a reliable predictor of fullerene stability. It became clear very early that the most stable (i.e., the experimentally observed) isomers all have isolated pentagons (IP). The main focus since has been on the invariants that could further distinguish between the isolated pentagon isomers. Several graph-theoretic invariants have been tested in this capacity and none of them was found completely satisfactory. In the meantime, the experimental evidence appeared indicating that for larger number of atoms some non-IP isomers might be energetically preferable to the IP ones, and even that some non-classical cages (i.e., with faces that are neither pentagons nor hexagons) are favored over the classical ones. Those observations motivated various generalizations of fullerene graphs. One such generalization is the subject of the present study.

A **fullerene graph** is a cubic, planar, 3-connected graph with only pentagonal and hexagonal faces. It follows easily from the Euler's formula that there must be exactly 12 pentagonal faces, while the number of hexagonal faces can be zero or any natural number greater than one. The smallest possible fullerene graph is the dodecahedron on 20 vertices, while the existence of fullerene graphs on an even number of vertices greater than 22 follows from a result by Grünbaum and Motzkin [12] obtained long before the discovery of fullerenes. Analogous results for IP fullerenes was obtained by Klein *et al.* [18].

A connected 3-regular planar graph $G = (V, E)$ is called an **m-generalized fullerene** if exactly two of its faces are m-gons and all other faces are pentagons and/or hexagons. (We also count the outer (unbounded) face of G.) In the rest of the paper we only consider $m \geq 3$; note that for $m = 5, 6$ an m-generalized fullerene graph is a classical fullerene graph. As for the classical fullerenes it is easy to show that the number of pentagons is fixed, while the number of hexagons is not determined. The smallest m-generalized fullerene has $4m$ vertices and no hexagonal faces. Such graphs are sometimes called **m-barrels**. They have two m-gons and $2m$ pentagons and they can be elongated by inserting $k \geq 0$ layers of m hexagons between two half-barrels. The elongated barrels are one of the main subjects of the present paper, since their highly symmetric structure allows for obtaining good bounds and even exact results on the number of perfect matchings in them.

A **matching** M in a graph G is a collection of edges of G such that no two edges of M share a vertex. If every vertex of G is incident to an edge of M, the matching M is called **perfect**. Perfect matchings have played an important role in the chemical graph theory, in particular for benzenoid graphs, where their number correlates with the compound's stability. Although it turned out that for fullerenes they do not have the same role as for benzenoids, there are many results concerning their structural and enumerative properties.

The paper is organized as follows. In the next section we state and prove some structural results about m-generalized fullerene graphs. In particular, we show that the number of hexagons is not necessarily an integer multiple of m. In section 3 we examine the diameter, the hamiltonicity and the leapfrog transformation of the elongated barrels, while in section 4 we obtain the upper bounds on the number of their perfect matchings. In section 5 we refine the results of section 4 by using the transfer matrix method. Finally, in the concluding section we state some conjectures about the entropy of the family of elongated barrels.

2 m-generalized fullerene graphs

In this introductory section we consider some structural properties of m-generalized fullerenes. For the beginning, we show that the number of pentagonal faces must be fixed.

Lemma 2.1. *Let $m \geq 3$ be a non-negative integer different from 5. Then an m-generalized*

fullerene $G = (V, E)$ has exactly $2m$ pentagonal faces.

Proof. Let v, e, f be the number of vertices, edges and faces, respectively, of an m-generalized fullerene G. From the Euler formula, $v - e + f = 2$, and 3-regularity of G we obtain $3v = 2e$. Let p and h denote the number of pentagonal and hexagonal faces, respectively, of G. Since every edge appears in exactly two faces, and every vertex in exactly 3 faces, we have the equality $2e = 2m + 5p + 6h$. By plugging it into Euler formula we obtain

$$\frac{2m + 5p + 6h}{3} - \frac{2m + 5p + 6h}{2} + (2 + p + h) = 2,$$

and hence $p = 2m$. □

The above proof works also for the case $m = 5$, yielding the familiar value of 12 pentagonal faces for classical fullerenes.

It is clear from the definition of elongated barrels that the number of hexagons in such graphs must be divisible by m. Here we show that there are also m-generalized fullerenes in which this is not the case. Take a hemi-dodecahedral cap shown in Fig. 1 left and truncate it at two non-adjacent vertices of the central pentagon. (A hemi-dodecahedral

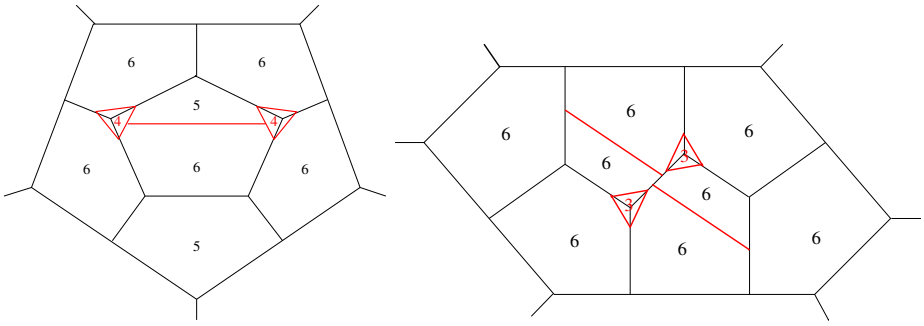

Figure 1: Nanotube caps with the number of hexagons not divisible by m.

cap is a pentagon surrounded by five other pentagons. Without any hexagons, two such caps make a dodecahedron, while by inserting a number of hexagonal layers one obtains a narrow nanotube.) The central pentagon now becomes a heptagon, and four out of five surrounding pentagons become hexagons. Now insert a vertex on both new edges in the heptagon and join them by an edge. The heptagon gives rise to a pentagon and a hexagon. We have obtained a cap with 21 vertices consisting of 2 quadrangles, 2 pentagons and 5 hexagons. We can now construct an infinite sequence of m-generalized fullerenes by taking another hemi-dodecahedral cap and connecting it with our cap using $\ell \neq 4i - 1$ layers of hexagons. The total number of hexagons in such a graph will not be divisible by $m = 4$. Another example, this time of a cap with two triangles and eight hexagons giving rise to an infinite sequence of nanotubes of circumference six, is shown in Fig. 1 right.

Lemma 2.2. *Let $G = (V, E)$ be an m-generalized fullerene with h hexagons. If G has an m-gonal face surrounded by m pentagons, then there exists an m-generalized fullerene G' with $h + m$ hexagons in which one m-gonal face is surrounded by m pentagons.*

Proof. Add additional m vertices in the middle of each edge of the m-gon to make it C_{2m}. Each of the m surrounding pentagons becomes a hexagon. Now connect the new m vertices to a new m-gon. □

So if there exists G satisfying the above lemma, where $h \neq 0$ modulo m, then we can create a sequence of generalized m-fullerene with $h + lm$ hexagons for $l \in \mathbb{N}$.

From a given fullerene graph G its **leapfrog transform** $Le(G)$ is obtained by first taking the dual of G and then truncating it. It is easy to see that $Le(G)$ is again a fullerene graph, with the number of vertices three times that of the original graph. Leapfrog fullerenes have many important properties; in particular, they are always IP, and they are rich in perfect matchings [7, 8]. It follows from the above results that the class of m-generalized fullerenes is also closed under the leapfrog transform.

Lemma 2.3. *The leapfrog of an m-generalized fullerene is again an m-generalized fullerene.*

3 The elongated barrels $F(m, k)$

In this section we describe a special family of m-generalized fullerenes, the elongated barrels, and list their properties. Recall that an **elongated barrel** $F(m, k)$ is obtained from the corresponding barrel by inserting $k \geq 0$ layers (or rings) of m hexagons between two halves of the barrel. For $m = 5$ and $m = 6$ we obtain classical fullerene nanotubes. Most of the nanotube properties are also preserved by elongated barrels. Note that $F(m, k)$ has $n = 2m(k + 2)$ vertices.

Elongated barrels can be neatly represented graphically using a sequence of $k + 3$ concentric circles with monotonically increasing radii such that the innermost and the outermost circle each have m vertices (representing, hence, two m-gons), while all other circles have $2m$ vertices each. An example is shown in Fig. 3. It follows that all elongated barrels are circular graphs in the sense of ref. [5]. (A graph G is **circular** if all its vertices can be placed on a number of concentric circles with increasing radii so that the edges are either arcs of the circles or connect vertices on neighboring circles without intersections between circles. A graph is **semi-circular** if there is a set V_0 of its vertices that cannot be placed on the circles in the above manner; instead, the subgraph induced by V_0 is placed

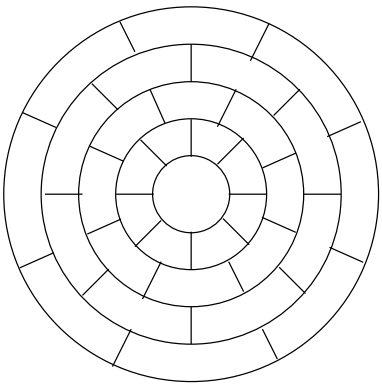

Figure 2: Elongated barrel $F(8, 2)$.

within the innermost circle. Since any connected planar graph without bridges is trivially semi-circular, of interest are graphs for which V_0 is either empty or small.)

Theorem 3.1. *Let $m \geq 3$ and k be non-negative integers. Then the diameter $d(F(m,k))$ of the elongated barrel $F(m,k)$ is given by $d(F(m,k)) = 2k+3$ for large enough k.*

Proof. It is clear that for $k = 0$ the diameter is equal to m and that it is achieved along the circumference. The effect of circumference is still felt for small k; for large k, however, (where large means $k \geq m$), the effect vanishes as the diameter is achieved between two vertices in antipodal caps. So, take a vertex v in one of antipodal m-gons. There are three vertices at distance one from v, one of them already at the first layer of hexagons, the other two in the same m-gon. Two more steps are needed to reach the second layer of hexagons; however, two more steps from other vertices at distance one from v will also advance along the m-gon and along the concentric circle of the first layer of hexagons. It is clear that after some (roughly) $2m$ steps the advances along concentric circles will meet on the opposite side, and from there on, all vertices on the i-th concentric circle will be at the distance of either $2i$ or $2i+1$ from v. The antipodal ring of pentagon is reached after $2k+1$ steps, and additional two steps are needed to reach any vertex in the antipodal m-gon. □

For $m = 5, 6$, i.e., for fullerene nanotubes, the above result is consistent with results of [2, 3].

The problem of hamiltonicity of fullerene graphs had been open for a long time. There were several partial results [17, 19, 21], until this special case of Barnette's conjecture was settled by Kardoš, who provided a computer-assisted proof [15].

Theorem 3.2. *For all natural numbers $m \geq 3$ and k, $F(m,k)$ is Hamiltonian.*

Proof. We construct a Hamiltonian cycle in $F(m,k)$ in the following way. Start from the innermost m-gon. Label its vertices clockwise by $v_{0,1}, \ldots, v_{0,m}$. Connect them by the path $P_0 = v_{01}v_{02}\ldots v_{0,m-1}v_{0,m}$. Each of the end-vertices of this path has exactly one neighbor not in the m-gon. Moreover, those neighbors both lie in the same pentagon and they are not adjacent. Hence, they both lie on C_{2m}. Label the vertices of C_{2m} by

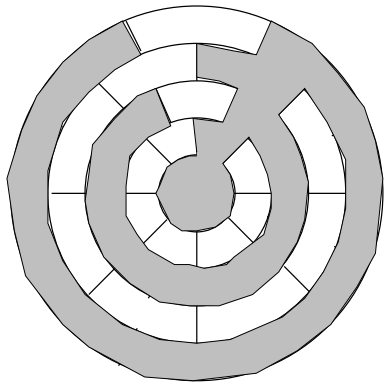

Figure 3: A Hamilton cycle in $F(8,2)$.

$v_{1,1}, \ldots, v_{1,2m-1}, v_{1,2m}$ clockwise so that $v_{1,1}$ is adjacent to $v_{0,1}$ and $v_{1,2m-1}$ is adjacent to $v_{0,m}$. Extend the path on one end by edges $v_{0,m}v_{1,2m-1}$ and $v_{1,2m-1}v_{1,2m}$, and on the

other side by the path $v_{0,1}v_{1,1}v_{1,2}\dots v_{1,2m-2}$ and denote the new path by P_1. Proceed in the same manner toward next concentric circle. After $k+1$ steps the end-vertices of P_{k+1} will be adjacent each to one of two adjacent vertices, $v_{k+2,1}$ and $v_{k+2,m}$, on the outer C_m, and hence, those two edges, together with all edges of the outer C_m except $v_{k+2,m}v_{k+2,1}$, will form a Hamilton cycle when added to P_{k+1}. □

The existence of Hamiltonian cycles has several consequences important for matchings-related properties of elongated barrels.

Corollary 3.3. *$F(m,k)$ has at least three different perfect matchings. Moreover, each edge of $F(m,k)$ is contained in some perfect matching of $F(m,k)$.*

The first claim is obvious – there are two perfect matchings formed by taking every other edge in a Hamiltonian cycle, and the third one formed by the edges that do not participate in it. The second claim of the above corollary says that all elongated barrels are 1-extendable. (A graph G is 1-extendable if each its edge is contained in a perfect matching of G.) This fact gives us a linear lower bound on the number of perfect matchings in $F(m,k)$, but we will derive much better lower bounds later. A bit better linear bounds would also follow for $m \geq 5$ by using the fact that all $F(m,k)$ are also 2-extendable, i.e., that any two independent edges are contained in (and hence can be extended to) a perfect matching. The 2-extendability follows from the fact that for $m \geq 5$ all $F(m,k)$ are cyclically 5-edge connected, i.e., they cannot be separated into two components, each containing a cycle, by deleting fewer than 5 edges [6], and result by Holton and Plummer [14] which claims that a cubic 3-connected planar graph which is cyclically 4-edge connected and has no faces of size 4 is 2-extendable.

Another consequence is 3-edge-colorability of $F(m,k)$. It means that its edges can be partitioned into 3 perfect matchings. As perfect matchings are also known as 1-factors, we have the following result.

Corollary 3.4. *$F(m,k)$ is 1-factorizable.*

An interesting perspective of elongated barrels has been offered by recently introduced concept of **altans**. Let G be a planar graph and S a cyclically ordered set of k vertices of degree 2 incident with its unbounded side. Altan $A(G)$ is obtained by encircling G by C_{2k} and connecting every other vertex of C_{2k} to a vertex of S respecting the cyclical order. The obtained graph can serve itself as input for another round of the altan transform; in that way we obtain iterated altans $A^n(G)$ for $n \geq 0$. The above definition is very informal, but it captures the most important aspects; we refer the reader to [4, 13] for formal definition of altans and exhaustive survey of their properties.

Starting from $G = C_m$ and taking $S = V(C_m)$, the altan transform will result in one half of barrel $F(m,0)$. Further iterations will result in adding successive layers of hexagons, so that $k+1$ iterations will give us $F(m,k)$ without one of its two caps.

An interesting property of altan transform is that it exactly doubles the number of perfect matchings of the starting graph [4].

Theorem 3.5. *Let $\Phi(G)$ denote the number of perfect matchings in G. Then $\Phi(A(G)) = 2\Phi(G)$. Hence, $\Phi(A^n(G)) = 2^n\Phi(G)$.*

The above result gives us an exponential lower bound on the number of perfect matchings in $F(m,k)$ for an even m.

Corollary 3.6. *Let m be even. Then*

$$\Phi F(m,k) \geq 2^{k+3}.$$

It is clear that the above result underestimates $\Phi(F(m,k))$, since it does not take into account perfect matchings containing some (or even all) edges connecting $A^{k+1}(C_m)$ with the other cap. We will later compare this bound with some more precise bounds obtained using transfer matrices. For odd m the above result is of no use, since all iterated altans of C_m have an odd number of vertices for odd m.

It would be interesting to see if similar exponential lower bounds could be established for all m-generalized fullerenes. A similar long-standing open problem for fullerenes was settled recently in [16].

Another consequence of being Hamiltonian is the following upper bound on the number of perfect matchings in $F(m,k)$. It is a direct consequence of Corollary 11 of [5].

Corollary 3.7. *Let $\Phi(F(m,k))$ denote the number of perfect matchings in $F(m,k)$. Then $\Phi(F(m,k)) \leq 8^{n/8}$ for mk even and $\Phi(F(m,k)) \leq \sqrt{3} \cdot 8^{(n-2)/8}$ for mk odd. Here n denotes the number of vertices of $F(m,k)$.*

Since $8^{1/8} \approx 1.29684 < 1.34801 \approx 6^{1/6}$, our result improves the upper bound of $6^{n/6}$ of reference [1].

The last result of this section shows that the property of circularity is preserved under the leapfrog transform for even k and not preserved for odd k.

Theorem 3.8. *The leapfrog transform of $F(m,k)$ is circular if and only if k is even. In that case, the circular structure of $Le(F(m,k))$ is as follows. The first inner circle is C_m, the second circle is C_{3m}, then there are $\frac{3k}{2}+1$ circles C_{4m}, then follows the circle C_{3m}, and the last circle is C_m. If k is odd then $Le(F(m,k))$ is semi-circular and has the following structure. The first circle is C_m, then the next $\frac{3k+3}{2}$ circles are C_{4m}. The next to the last circle is C_{3m}, and the last circle is C_m. Inside the first circle there are m vertices.*

The proof follows along the same lines as for Theorem 15 of [5] and we omit the details.

4 Improved upper bounds on the number of perfect matchings in $F(m,k)$

In this section we use the Hadamard–Fischer inequality to improve the upper bounds on $\Phi(F(m,k))$ from the previous section. To this end, we consider two orientations of C_m. In the first one, all edges are oriented clockwise; in the second one, one edge is oriented anti-clockwise, while all other edges are oriented clockwise. The first orientation we denote by $1 \to 2 \to \ldots \to n \to 1$, the second one by $1 \to 2 \to \ldots \to n, 1 \to n$. Let $T_{n,-}, T_{n,+}$ be the skew symmetric matrices obtained from the first and from the second orientation, respectively. We will need the following result (Lemma 18 of ref. [5]).

Lemma 4.1. *For $n \geq 3$*

$$\begin{cases} \det(I_n - T_{n,+}^2) = \det(I_n - T_{n,-}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n)^2 & \text{if } n \text{ is odd;} \\ \det(I_n - T_{n,+}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n + 2)^2 & \text{if } n \text{ is even;} \\ \det(I_n - T_{n,-}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n - 2)^2 & \text{if } n \text{ is even.} \end{cases}$$

Furthermore, for $n \geq 3$ the odd-indexed subsequence of $(\det(I_n - T^2_{n,+}))^{\frac{1}{n}}$ is increasing, while the even-indexed subsequence is decreasing. Both subsequences converge to $(\frac{1+\sqrt{5}}{2})^2 \approx 2.6180$.

Now we combine the lemma with the Hadamard-Fischer inequality to establish an upper bound on $\Phi(F(m,k))$ better than those of the previous section.

Theorem 4.2. *The number of perfect matchings in $F(m,k)$ is bounded from above by*

$$\begin{cases} \left(\left(\frac{1+\sqrt{5}}{2}\right)^m + \left(\frac{1-\sqrt{5}}{2}\right)^m\right)\left(\left(\frac{1+\sqrt{5}}{2}\right)^{2m} + \left(\frac{1-\sqrt{5}}{2}\right)^{2m} + 2\right)^{\frac{k+1}{2}} & \text{if } m \text{ is odd;} \\ \left(\left(\frac{1+\sqrt{5}}{2}\right)^m + \left(\frac{1-\sqrt{5}}{2}\right)^m + 2\right)\left(\left(\frac{1+\sqrt{5}}{2}\right)^{2m} + \left(\frac{1-\sqrt{5}}{2}\right)^{2m} + 2\right)^{\frac{k+1}{2}} & \text{if } m \text{ is even.} \end{cases}$$

Proof. The proof is along the lines of the proof of Theorem 9 of [5]. We use the Hadamard-Fischer inequality to estimate from above the determinant of $B := -S^2(F(m,k))$, which is equal to $\Phi(F(m,k))^4$. Let $V_i, i \in [k+3]$ be all vertices of $F(m,k)$ on the $i-th$ circle. So V_1 and V_{k+3} have m vertices, while all other V_i have $2m$ vertices. Recall the Hadamard-Fischer inequality

$$\det B \leq \prod_{i \in [k+3]} \det B[V_i].$$

Note that since the path of distance 2 between any two edges on each V_i can be obtained only using the edges on the cycle $F(m,k)(V_i)$, it follows that $B[V_i] = I_{|V_i|} - S(F(m,k+1)(V_i))^2$. Here $S(F(m,k)(V_i))$ is a skew symmetric matrix induced by the Pfaffian orientation of $F(m,k)$ on the cycle $F(m,k)(V_i)$. (See [24] for more on Pfaffian graphs.) The arguments in Section 5 of [5] yield that $\det B(V_i) = \det(I_{|V_i|} - T^2_{|V_i|,+})$. The theorem now follows by applying Lemma 4.1. □

Theorem 4.2 gives better upper bounds than Corollary 3.7. It is only to be expected, since it fully draws on the information stored in the structure of $F(m,k)$, while Corollary 3.7 uses only its hamiltonicity and regularity. While the asymptotic behavior of Corollary 3.7 is of the type $8^{n/8} \approx 1.29684^n$ and does not depend on m, Theorem 4.2 yields the asymptotic $(\varphi^{2m}+2)^{\frac{n}{4m}}$, that is roughly of the order of $\sqrt{\varphi}^n \approx 1.2720^n$ for large m.

5 The transfer matrix method for counting perfect matchings in $F(m,k)$

In this section we provide some explicit formulas and some asymptotics result of the type $\Phi(F(m,k)) \sim C\rho(m)^k$, where $\rho(m)$ is the spectral radius of certain nonnegative irreducible matrix associated with $F(m,k)$. We use the transfer matrix method to count the matchings as in [10].

Consider the cycle C_{2m}. Fix a vertex on C_{2m} and call this vertex 1. View 1 as colored in white. Then color other vertices of C_{2m} black and white so we get a bipartite partition of C_{2m}, where the edges connect white and black vertices. Delete a black neighbor vertex to the left of 1 on C_{2m} to obtain the path P_{2m-1}. Then the vertex i for $i = 2, \ldots, m$ is the white vertex of distance $2(i-1)$ from 1 on P_{2m-1}. The black vertex i on C_{2m} is located to the right of the white vertex i. So the distance between the white vertex 1 and the black vertex $i \in [m-1]$ is $2i-1$ on P_{2m-1}. The distance between the white vertex 1 and the

black vertex m is 1 on C_{2m}. Let $S \subset [m] = \{1, 2, \ldots, m\}$. Then $\alpha(S), \beta(S)$ are the sets of those white vertices and black vertices on C_{2m} whose indices belong to S, respectively.

Let $A(m) = [a_{ST}]$ be the following $2^m \times 2^m$ matrix with nonnegative integer entries. Each S, T is a subset of $[m] = \{1, \ldots, m\}$. (S, T are allowed to be empty.) Then a_{ST} is the number of perfect matchings in the subgraph of C_{2m} obtained by deleting the vertices $\alpha(S) \cup \beta(T)$. We assume that $a_{[m][m]} = 1$.

Lemma 5.1. *Let $m \geq 3$ be an integer, and assume that $A(m) = [a_{ST}]_{S,T \subset [m]}$ is defined as above. Then $a_{ST} = 0$ if $|S| \neq |T|$. In particular, A is a direct sum of $m+1$ submatrices $A_{i,m} = [a_{ST}]_{S,T \subset [m], |S|=|T|=i}$ for $i = 0, \ldots, m$.*

Proof. Let $S, T \subset [m]$. Delete the vertices from $\alpha(S), \beta(T)$ in C_{2m} to obtain the subgraph G. Then G has $m - |S|, m - |T|$ white and black vertices, respectively. To have a perfect matching in G we need the equality $|S| = |T|$. Hence $A(m) = \mathrm{diag}(A_{0,m}, \ldots, A_{m,m})$. □

As an illustration, we construct matrix A for the smallest case $m = 3$. Here by $i \pm 1$ we mean modulo 3. So $3 + 1 = 1$ and $1 - 1 = 3$. Note that $a_{ST} = 0$ if $|S| + |T|$ is odd. Then the following elements of A are nonzero:

$$a_{\emptyset\emptyset} = 2, a_{\{i\}\{i\}} = a_{\{i\}\{i+1\}} = a_{\{i\}\{i+2\}} = a_{\{i,j\}\{i,j\}} = a_{\{i,j\}\{i-1,j-1\}} = a_{[3][3]} = 1.$$

Hence $A(3)$ is an 8×8 matrix whose rows and columns are indexed by the subsets of $[3]$ in the following way: $\emptyset, \{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}, \{1,2,3\}$.

$$A(3) = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

We can see that $A(3)$ is the direct sum of the following matrices:

$$A_{0,3} = [2],\ A_{1,3} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix},\ A_{2,3} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix},\ A_{3,3} = [1].$$

Let now $m \geq 3$ and k be nonnegative integers. In $F(m, k)$ we label each vertex on O_i for $i = 1, \ldots, k + 3$ as follows. Choose a vertex on O_1, which is C_m, and call it vertex 1. Then the right neighbor of i is $i+1$ for $i = 1, \ldots, m-1$. Assume that all m vertices of C_m are colored in black. Now the white vertex indexed i on O_2, which is C_{2m}, is connected to the vertex i in O_1. Now label the black vertices on O_2 as above and connect black vertices in O_2 to white vertices in O_3, which have the same index $i \in [m]$. Continue in the same manner until we color and label all vertices of $F(m, k)$. Note that the color of all vertices on O_{k+3}, which is C_m, is white. Furthermore, the only edges that connect two vertices with the same color in $F(m, k)$ lie on O_1 and O_{k+3}.

Let $\mathbf{x} = (x_S), S \subset [m]$ be the following vector with $0, 1, 2$ coordinates. Consider the cycle C_m, which is either O_1 or O_{k+3}, where the vertices are marked as above. Then x_S is the number of perfect matchings in the subgraph of C_m induced by the set of vertices $[m] \setminus S$.

Theorem 5.2.

$$\Phi(F(m,k)) = \mathbf{x}^\top A(m)^{k+1}\mathbf{x}.$$

Proof. The right-hand side of the above formula can be written as

$$\mathbf{x}^\top A(m)^{k+1}\mathbf{x} = \sum_{S_1,\ldots,S_{k+2}\subset[m]} x_{S_0}x_{S_{k+2}} \prod_{j\in[k]} a_{S_jS_{j+1}}. \tag{5.1}$$

One summand $x_{S_1}x_{S_{k+1}} \prod_{i\in[k]} a_{S_iS_{i+1}}$ counts perfect matchings in which S_1 vertices in C_m are matched with S_1 corresponding white vertices in the adjacent C_{2m}, while the remaining vertices on C_m are matched between themselves. The number of such matchings is x_{S_1}. The black vertices i, where $i \in S_2$, in C_{2m}, are matched with the white vertices next level in C_{2m}, which is the third circle of the circular graph $F(m,k)$. (We assumed for simplicity that $k > 1$.) Continue in this way until the last white vertices in the set S_{k+2} of O_{k+2}, which is C_{2m}, are matched with the black vertices in the set S_{k+1} of O_{k+1}. The set of black vertices on O_{k+2}, denoted by S_{k+2} are connected to the cycle C_m, which is the last circle O_{k+3}. Observe that $a_{S_kS_{k+1}}$ is the number of perfect matchings in the subgraph C_{2m} when we remove the white vertices S_k and the black vertices S_{k+1}. Finally, $x_{S_{k+3}}$ is the number of perfect matchings in the subgraph C_m after removing vertices S_{k+3}. To summarize, the summand $x_{S_1}x_{S_{k+1}} \prod_{i\in[k]} a_{S_iS_{i+1}}$ counts the total number of perfect matchings in $F(m,k)$ where for each $j \in [k+2]$, S_j is the set of white vertices on O_{j+1} which is matched to the black vertices in O_j. □

Now we use the above result to count perfect matchings in $F(m,k)$ for small values of m.

Corollary 5.3. $\Phi(F(3,k)) = 3^{k+2} + 1$.

Proof. Note that $\mathbf{x}$ has 8 coordinates. There are 4 nonzero coordinates. First $x_{[3]} = 1$. This corresponds to the situation where we match all three vertices in C_3 in the circle O_1 to 3 vertices in C_6 in the circle O_2. But then to have a nonzero perfect matching we need to match the remaining 3 vertices on C_6 to 3 vertices in the next level. Continuing in this fashion we deduce that we have only one such perfect matching corresponding to the matching whose edges consist of all edges between different circles. The corresponding summand in the right hand side of formula (5.1) is the contribution of the matrix $A_{3,3} = [1]$ in $A(3)$. The three nonzero coordinates correspond to $x_{\{i\}} = 1$ for $i = 1, 2, 3$. These 3 coordinates correspond to the matrix $A_{1,3}$ in $A(3)$. Clearly $A_{1,3}^k = 3^{k-1}A_{1,3}$. Hence the contribution of all such terms in (5.1) is equal to 3^{k+2}. □

Corollary 5.4.

$$\Phi(F(4,k)) = 2(2+\sqrt{2})^{k+1} + 2(2-\sqrt{2})^{k+1} + 2^{k+3} + 1.$$

Proof. We need to consider only the cases when S has cardinality $0, 2, 4$. If $S_1 = \emptyset$, then $x_{S_1} = 2$. In this case we need to choose $S_1 = \ldots = S_{k+2} = \emptyset$. So we match the edges on the circles $O_1, \ldots, O_{k+3}$. The number of perfect matchings for each even cycle is 2.

Hence the total number of such matchings is 2^{k+3}. Now suppose that $S_1 = [4]$. Then $S_1 = \ldots = S_{k+1}$. So we match only the vertices between the circles $O_1, \ldots, O_{k+3}$. The number of such perfect matchings is 1. Suppose finally that $|S_1| = 2$. So $x_{S_1} = 1$ if and only if the two vertices in S_1 are neighbors. In other words, two vertices in S_1 form an edge in C_4. Let us write down the 6×6 matrix $A_{2,4}$ with rows and columns indexed by 2-element subsets of $[4]$ in the following order: $\{1,2\}, \{1,3\}, \{1,4\}, \{2,3\}, \{2,4\}, \{3,4\}$.

$$A_{2,4} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix} \tag{5.2}$$

So $A_{2,4}$ is an irreducible matrix with a positive diagonal. Its characteristic polynomial $x^6 - 6x^5 + 14x^4 - 24x^3 + 28x^2 - 24x + 8$ factors as $(x^2 - 4x + 2)(x^2 - 2x + 2)(x^2 + 2)$. It has two real eigenvalues, $2 + \sqrt{2}$ and $2 - \sqrt{2}$, and two pairs of conjugated complex eigenvalues. Hence, $\Phi(F(4,k))$ will be dominated by the $(k+1)$-st power of the spectral radius, $(2 + \sqrt{2})^{k+1}$, with the correction term $(2 - \sqrt{2})^{k+1}$. The claim now follows by adding all contributions. □

Corollary 5.5.

$$\Phi(F(5,k)) = 5^{k+2} + 5\left[\left(\frac{5+\sqrt{5}}{2}\right)^k + \left(\frac{5-\sqrt{5}}{2}\right)^k\right] + 1.$$

Proof. Note that $x_S > 0$ if and only if $|S| = 1, 3, 5$. For $|S| = 5$, i.e. $S = [5]$ we deduce that the number of perfect matchings is 1, which is achieved by matching the adjacent vertices on different circles. This gives us the last term in the right hand side. Consider now the case $|S| = 1$. First choose any vertex on O_1, which is C_5. There are 5 choices. Connect this vertex to a white vertex on O_2, which is C_{10}. Now choose any black vertex on O_2. Delete these two vertices. We obtain one or two paths of even length which have 1 perfect matching. That is, $a_{\{i\},\{j\}} = 1$ for any $i, j \in [5]$. Continuing in this manner we obtain the number of perfect matchings to be 5^{k+2}, the dominant term on the right hand side. The middle term is obtained by considering the eigenvalues of $A_{3,5}$, the 10 by 10 matrix whose row and columns are indexed by lexicographically ordered 3-element subsets of $[5]$.

$$A_{3,5} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix} \tag{5.3}$$

□

Corollary 5.6.

$$\Phi(F(6,k)) \sim (2(2+\sqrt{3}))^{k+2}.$$

Proof. The dominant term is the power of the spectral radius of $A_{2,6}$, a matrix of order 15 that we omit. □

Results of Corollaries 5.3 and 5.4 are new. Corollary 5.5 is in agreement with results of Sachs, Hansen and Zheng from [23], while Corollary 5.6 agrees with findings in [22].

6 The entropy of the family $F(m,k), k \in \mathbb{N}$

Recall that the graph $F(m,k)$ has $2m(k+2)$ vertices. The **dimer entropy** $h(m)$ of the family $F(m,k)$ is defined as

$$h(m) := \limsup_{k\to\infty} \frac{\log \Phi(F(m,k))}{2m(k+2)}.$$

(See [9–11].) From the previous section we deduce

$$h(m) = \frac{\log \rho(m)}{2m}.$$

Equivalently, it says that the number of perfect matchings in $F(m,k)$ for m fixed and $k \gg 1$ is of order $e^{kh(m)}$.

Empirical results suggest that narrow nanotubes have the largest number of perfect matchings among all fullerene graphs on $10k$ vertices. That motivates us to advance the following conjecture.

Let n be an integer number greater than 11 so that there is a fullerene with $2n$ vertices. Denote by μ_{2n} the maximal number of perfect matchings in all fullerene graphs with $2n$ vertices. Define

$$h_F := \limsup_{n\to\infty} \frac{\log \mu_{2n}}{2n}.$$

We conjecture that $h_F = h(5)$.

Similar claim seems plausible also for m-generalized fullerenes. Fix an integer $m \geq 3, m \neq 5, 6$. Let $\mu_{2m(k+2),m}$ be the maximal number of perfect matchings in all m-generalized fullerene graphs with $2m(k+2)$ vertices. Define

$$h_F(m) := \limsup_{k\to\infty} \frac{\log \mu_{2m(k+2),m}}{2m(k+2)}.$$

We conjecture that $h_F(m) = h(m)$.

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Bipartite graphs with at most six non-zero eigenvalues

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Abstract

In this paper we characterize all bipartite graphs with at most six non-zero eigenvalues. We determine the eigenvalues of bipartite graphs that have at most four non-zero eigenvalues.

Keywords: Eigenvalues of graphs, bipartite graphs.

Math. Subj. Class.: 05C31, 05C50

1 Introduction and Main Results

Throughout this paper we will consider only simple graphs. A graph with no isolated vertices is called reduced (also called canonical in the literature) if no two non-adjacent vertices have the same neighborhood. It is well known that the number of vertices of reduced graphs are bounded by some functions of the rank, see [7]. It is not hard to see if a reduced graph has exactly m non-zero eigenvalues, then G has at most $2^m - 1$ vertices. Therefore the number of non-isomorphic reduced graphs with a given number m of non-zero eigenvalues (counted by their multiplicities) is finite. So it is natural to look for a classification of reduced graphs with a given number of non-zero eigenvalues. Note that the number of non-zero eigenvalues of a graph is equal to the rank of the graph which by definition is the rank of the adjacency matrix of the graph. It is not hard to characterize the reduced graphs with rank r, for $r \leq 3$. The classification of reduced graphs of rank 4 and rank 5 can be found in [8] and also in [1] and [2], respectively. Thus it is natural to classify all reduced graphs of rank 6 (see [8] for a characterization according to minimal subgraphs

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of nullity one). Recently, in [9], triangle-free graphs of rank 6 are claimed to be classified in Theorem 4.1. But we find that the graphs G_2 and G_3 in the main result in [9], have rank 8. On the other hand, the main step to find a classification for triangle-free graphs of rank 6 is first to classify bipartite graphs of the same rank (see [9]). In this paper, in a different way from [5] and [9], we completely characterize all bipartite graphs with rank r, where $r \in \{2, 4, 6\}$. In other words, we find all bipartite graphs with at most six non-zero eigenvalues. Also we find the eigenvalues of bipartite graphs of rank 4.

2 Notation and Preliminaries

Let $G = (V, E)$ be a graph. The *order* of G denotes the number of vertices of G. For two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, the *disjoint union* of G_1 and G_2 denoted by $G_1 + G_2$ is the graph with vertex set $V_1 \cup V_2$ and edge set $E_1 \cup E_2$. The graph rG denotes the disjoint union of r copies of G. Let u and v be two vertices of a graph G. By uv we mean an edge between u and v. For every vertex $v \in V$, the *open neighborhood* of v is the set $N(v) = \{u \in V : uv \in E\}$. An independent set in a graph is a set of pairwise non-adjacent vertices. For every vertex $v \in V(G)$, the *degree* of v that is denoted by $deg(v)$ is the number of edges incident with v. We denote by K_n, $K_{m,n}$, C_n, and P_n, the complete graph of order n, the complete bipartite graph with part sizes m, n, the cycle of order n, and the path of order n, respectively.

If $\{v_1, \ldots, v_n\}$ is the set of vertices of a graph G, then the *adjacency matrix* of G, $A(G) = (a_{ij})$, is an $n \times n$ matrix where a_{ij} is 1 if v_i is adjacent to v_j, otherwise $a_{ij} = 0$. Thus $A(G)$ is a symmetric matrix with zeros on the diagonal and all the eigenvalues of $A(G)$ are real. By $[v]$ we mean the column of $A(G)$ that correspond to a vertex v of G, that is the vector of neighbors of v. By the eigenvalues of G we mean those of its adjacency matrix. The multiset of eigenvalues of G is denoted by $Spec(G)$. We let $Spec(G) = \{\lambda_1, \ldots, \lambda_n\}$, where $\lambda_1 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. The rank of G, denoted by $rank(G)$, is the rank of $A(G)$. In fact, $rank(G)$ is the number of all non-zero eigenvalues of G. We consider the rank of graphs over the field of real numbers. Let H be a bipartite graph with parts X and Y. Suppose that $X = \{u_1, \ldots, u_m\}$ and $Y = \{v_1, \ldots, v_n\}$. By $B(G) = (b_{ij})$ we mean the $(0, 1)$ matrix of size $m \times n$ such that $b_{ij} = 1$ if and only if u_i and v_j are adjacent, otherwise $b_{ij} = 0$. We note that the rank of any bipartite graph is even. More precisely:

Remark 2.1. Let H be a bipartite graph with parts X and Y. Let $B = B(H)$, as mentioned above. Then we have $rank(H) = 2\, rank(B)$.

Definition 2.2. A graph G is called *reduced* or *canonical* if it has no isolated vertex and for any two non-adjacent vertices u and v, $N(u) \neq N(v)$. Equivalently, any row of the adjacency matrix is non-zero and no two rows of the adjacency matrix of G are equal.

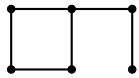
Definition 2.3. Let G be a graph. We say G is *neighbor-reduced* if G has no isolated vertex and there are no three vertices u, v and w satisfying all the following conditions:

1) $\{u, v, w\}$ is an independent set.
2) $N(u) \cap N(v) = \varnothing$.
3) $N(w) = N(u) \cup N(v)$.

Equivalently, any row of the adjacency matrix is non-zero and no row of the adjacency matrix of G is the sum of two other rows.

Definition 2.4. A graph G is called *strongly reduced*, if G is reduced and neighbor-reduced.

We note that there is no connection between Definitions 2.2 and 2.3. For example the path P_5 is reduced but it is not neighbor-reduced while the cycle C_4 is not reduced but it is neighbor-reduced. The cycle C_6 is reduced and neighbor-reduced graph, that is C_6 is strongly reduced. Also the graph H which is shown in Figure 1 is neither reduced (because it has a duplicate vertex) nor neighbor-reduced (because it has P_5 as an induced subgraph (Table 1 of [8])).



H

Figure 1: A non-reduced and non-neighbor-reduced bipartite graph.

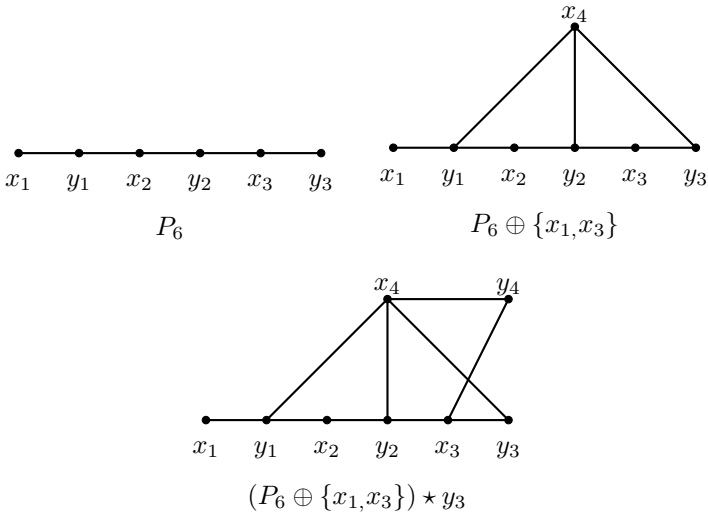


Figure 2: Three bipartite graphs with rank 6 obtained from P_6 with operations $\star$ and $\oplus$.

Let G be a graph and v be a vertex of G. Suppose that $N(v) = \{v_1, \ldots, v_k\}$. By $G \star v$, this operation is well known in the literature as adding a duplicate vertex, we mean the graph obtained by adding a new vertex w and new edges $\{wv_1, \ldots, wv_k\}$ to G. Thus in $G \star v$, $N(w) = N(v)$, that is $G \star v$ is not reduced (see Figure 2). Let S be an independent set of G which is ordered as $S = \{u_1, \ldots, u_t\}$ and $t \geq 2$. We inductively define $G \star S$ as $(G \star u_1) \star S \setminus \{u_1\}$. We note that the operation has the effect of adding even cycles and no odd cycles to the graph; therefore G is bipartite if and only if $G \star v$ is bipartite.

Suppose that u and v are non-adjacent vertices of G such that $N(u) \cap N(v) = \varnothing$. By $G \oplus \{u, v\}$ we mean the graph obtained by adding a new vertex w to G and new edges

$\{wx : x \in N(u)\} \cup \{wy : y \in N(v)\}$. Thus in $G \oplus \{u, v\}$, $N(w) = N(u) \cup N(v)$. See Figure 2. It is easy to prove the following theorem:

Theorem 2.5. *Let G be a graph and u and v be two non-adjacent vertices of G. Then*

$$rank(G) = rank(G \star v) = rank(G \oplus \{u, v\}).$$

Theorem 2.5 shows that for classifying the graphs of rank r it is sufficient to classify the reduced graphs (or the neighbor-reduced graphs) of rank r. Thus in sequel we consider the reduced graphs.

3 Graphs of Rank 2

In this section we characterize all graphs with rank 2. We note that $rank(G) = 0$ if and only if $G = nK_1$, for some natural number n. By the fact that the sum of all eigenvalues of a graph is zero, there is no graph with rank 1.

Remark 3.1. Let G be a graph of rank 2. Thus $Spec(G) = \{\alpha, 0, \ldots, 0, \beta\}$, for some non-zero real numbers α and β. Since for any graph H, $\sum_{\lambda \in Spec(H)} = 0$, we obtain $\beta = -\alpha$. Thus G is bipartite (see Theorem 3.11 of [4]). In the other words, any graph of rank 2 is bipartite.

Theorem 3.2. *Let G be a reduced graph. Then $rank(G) = 2$ if and only if $G = P_2$.*

Proof. Assume that $rank(G) = 2$. By Remark 3.1, G is bipartite. Let X and Y be the parts of G and $B = B(G)$. By Remark 2.1, $rank(B) = 1$. This shows that all columns of B are the same. In the other words, all vertices of part X have the same neighbors. Since G is reduced, we conclude that $|X| = 1$. Similarly, $|Y| = 1$. Thus $G = P_2$. □

Theorem 3.3. *Let G be a graph. Then $rank(G) = 2$ if and only if $G = K_{m,n} + tK_1$, for some natural numbers m and n and a non-negative integer t.*

Proof. First suppose that $rank(G) = 2$. If G is reduced, then by Theorem 3.2, $G = P_2 + tK_1$, for some $t \geq 0$. Assume that G is not reduced. By deleting some vertices from G, one can obtain a reduced graph H. By Theorem 2.5, $rank(H) = 2$. Thus by the connected case, $H = K_2 + tK_1$. Since $G = H \star S$, for some independent set S of G, we obtain that $G = K_{m,n} + tK_1$, for some integers $m, n \geq 1$. The second part of assertion is trivial. □

4 Bipartite Graphs of Rank 4 and their Eigenvalues

In this section we investigate about the bipartite graphs with rank 4. We note that by a different method in [5], the bipartite graphs of rank 4 are classified.

Theorem 4.1. *Let G be a reduced bipartite graph. Then $rank(G) = 4$ if and only if $G = 2P_2$ or $G = P_4$ or $G = P_5$.*

Proof. One can easily see that $rank(2P_2) = rank(P_4) = rank(P_5) = 4$. It remains to prove the other part. Suppose that G is a reduced bipartite graph. Let X and Y be the parts of G and $B = B(G)$. By Remark 2.1, $rank(B) = 2$. Let $u, v \in Y$. Suppose that $[u]$ and $[v]$ are two columns of B correspondence to u and v, respectively. Assume that $[u] = \alpha[v]$,

for some real α. It is trivial that $\alpha \in \{0,1\}$. If $\alpha = 0$, then u is an isolated vertex, a contradiction. Thus $\alpha = 1$. This shows that $N(u) = N(v)$, a contradiction. Therefore very two columns of B are independent.

Let x_1, x_2, x_3 be three vertices of X. Since $rank(B) = 2$ and any two columns of B are independent, for some non-zero real numbers a and b we have

$$[x_3] = a[x_1] + b[x_2]. \tag{4.1}$$

By multiplying the vector j (all components are 1) to both sides of Equation 4.1, we obtain that:

$$deg(x_3) = a\, deg(x_1) + b\, deg(x_2). \tag{4.2}$$

Since $N(x_1) \neq N(x_2)$, without losing the generality let $N(x_1) \not\subseteq N(x_2)$. Assume that $u \in N(x_1) \setminus N(x_2)$. Considering the entries correspondence to u in the vectors $[x_1], [x_2]$ and $[x_3]$ in the Equality (4.1), we obtain $a \in \{0,1\}$. Since a is non-zero, $a = 1$. Let w be a neighbor of x_2. Considering the entries correspondence to w in the Equality (4.1), we have $b \in \{-1,0,1\}$. Since $b \neq 0$, $b = \pm 1$. Thus for any three columns X_1, X_2 and X_3 of B, one of the following holds:

$$X_1 = X_2 + X_3 \quad \text{or} \quad X_2 = X_1 + X_3 \quad \text{or} \quad X_3 = X_1 + X_2. \tag{4.3}$$

We claim that $|X|, |Y| \leq 3$. By contradiction suppose that $|X| \geq 4$. Let x_1, x_2, x_3, x_4 be the vertices of X with have the minimum degree among all vertices of X. Suppose that $deg(x_1) \geq deg(x_2) \geq deg(3) \geq deg(x_4)$. Since the sets $\{[x_1], [x_2], [x_3]\}$ and $\{[x_2], [x_3], [x_4]\}$ are dependent, by Equations 4.2 and 4.3, we obtain $[x_1] = [x_2] + [x_3]$ and $[x_2] = [x_3] + [x_4]$. Therefore $[x_1] = 2[x_3] + [x_4]$, a contradiction (by Equation 4.3). Similarly, $|Y| \leq 3$. Since $|X|, |Y| \leq 3$, G has at most 6 vertices. It is not hard to see that G is isomorphic to one of the graphs $2P_2$ or P_4 or P_5. The proof is complete. □

Let $V(2P_2) = \{x_1, y_1, x_2, y_2\}$ and $E(2P_2) = \{x_1y_1, x_2y_2\}$. Thus $P_5 = 2P_2 \oplus \{x_1, x_2\}$. Therefore P_5 is not neighbor-reduced. Using this fact and Theorem 4.1 we obtain the following:

Theorem 4.2. *Let G be a strongly reduced bipartite graph. Then $rank(G) = 4$ if and only if $G = 2P_2$ or $G = P_4$.*

Using Theorems 2.5 and 4.1 (similar to proof of Theorem 3.3), one can characterize all bipartite graphs of rank 4.

Theorem 4.3 (Theorem 7.1 of [8])**.** *Let G be a bipartite graph with no isolated vertex. Then $rank(G) = 4$ if and only if G is obtained from $2P_2$ or P_4 or P_5 with the operation $\star$.*

We finish this section by computing the eigenvalues of bipartite graphs of rank 4. First we prove the following lemma. For other proofs, see also page 115 of [4], page 54 of [3] and page 115 of [6].

Lemma 4.4. *Let G be a bipartite graph. Let $Spec(G) = \{\lambda_1, \ldots, \lambda_n\}$. Then*

$$\lambda_1^4 + \cdots + \lambda_n^4 = 2m + 8q + 4 \sum_{v \in V(G)} \binom{deg(v)}{2},$$

where m and q are the number of edges and the number of cycles of length 4 of G, respectively.

Proof. It is well-known that for any natural number k, $\lambda_1^k + \cdots + \lambda_n^k$ is equal to the number of closed walks of G with length k (page 81 of [4]). Since G is bipartite, all closed walks of length 4 appear in the subgraphs of G that are isomorphic to P_2, P_3 or C_4. We note that in any P_2, P_3 and C_4 there are $2, 4$ and 8 closed walks of length 4 (which cover all vertices of P_2, P_3 and C_4), respectively. On the other hand, the number of P_3 in G is $\sum_{v\in V(G)} \binom{deg(v)}{2}$. This completes the proof. □

Theorem 4.5. *Let G be a bipartite graph of rank 4. Let $Spec(G) = \{\alpha, \beta, 0, \ldots, 0, -\beta, -\alpha\}$. Suppose that v is a vertex of G with $deg(v) = t$. Then $Spec(G\star v) = \{\gamma, \theta, 0, \ldots, 0, -\theta, -\gamma\}$, where γ and θ are as following:*

$$\gamma, \theta = \sqrt{\frac{\alpha^2 + \beta^2 + t \pm \sqrt{2(\alpha^4 + \beta^4 + L) - (\alpha^2 + \beta^2 + t)^2}}{2}}.$$

Also,

$$\gamma, \theta = \sqrt{\frac{m + t \pm \sqrt{2(m^2 - 2\alpha^2\beta^2 + L) - (m + t)^2}}{2}},$$

where $L = t + 6\binom{t}{2} + 2\sum_{w\in N(v)} deg(w)$.

Proof. Assume that m and m' are the number of edges of G and $G \star v$, respectively. Suppose that q and q' are the number of cycles of length 4 of G and $G\star v$, respectively. Thus $m' = m + t$ and $q' = q + \binom{t}{2}$. Since G is bipartite, $G\star v$ is bipartite, too. By Theorem 2.5, $rank(G \star v) = 4$. Therefore we have $Spec(G \star v) = \{\gamma, \theta, 0, \ldots, 0, -\theta, -\gamma\}$, for some non-zero real numbers γ and θ. Using Lemma 4.5 we obtain

$$\begin{aligned} 2(\gamma^4 + \theta^4) = {} & 2(m + t) + 8\left(q + \binom{t}{2}\right) \\ & + 4\sum_{w\in V(G)\setminus N(v)} \binom{deg(w)}{2} + 4\sum_{w\in N(v)} \binom{deg(w) + 1}{2} + 4\binom{t}{2}. \quad (4.4) \end{aligned}$$

Since for any integer $k \geq 0$, $\binom{k+1}{2} = \binom{k}{2} + k$, using Lemma 4.5 we conclude that:

$$\gamma^4 + \theta^4 = \alpha^4 + \beta^4 + t + 6\binom{t}{2} + 2\sum_{w\in N(v)} deg(w). \quad (4.5)$$

On the other hand, by the fact that for every graph H, $\sum_{\lambda\in Spec(H)} \lambda^2 = 2|E(H)|$, we obtain that $\alpha^2 + \beta^2 = m$ and $\gamma^2 + \theta^2 = m + t$. These equalities imply that

$$\gamma^2 + \theta^2 = \alpha^2 + \beta^2 + t. \quad (4.6)$$

Let $L = t + 6\binom{t}{2} + 2\sum_{w\in N(v)} deg(w)$. Suppose that $p = \gamma^2$ and $q = \theta^2$. Using Equations 4.5 and 4.6 we obtain

$$pq = \frac{(\alpha^2 + \beta^2 + t)^2 - (\alpha^4 + \beta^4 + L)}{2}, \quad \text{and} \quad p + q = \alpha^2 + \beta^2 + t.$$

The latter equalities show that p and q are roots of the following polynomial:

$$x^2 - (\alpha^2 + \beta^2 + t)x + \frac{(\alpha^2 + \beta^2 + t)^2 - (\alpha^4 + \beta^4 + L)}{2}.$$

The proof is complete. □

Remark 4.6. Let $f(G,\lambda)$ be the characteristic polynomial of G. Suppose that G is a bipartite graph of order n with rank 4 and with $Spec(G)=\{\alpha,\beta,0,\ldots,0,-\beta,-\alpha\}$. Let m be the number of edges of G. Thus $f(G,x)=x^{n-4}(x^4-mx^2+\alpha^2\beta^2)$. Assume that v is a vertex of G with $deg(v)=t$ and $L=t+6\binom{t}{2}+2\sum_{w\in N(v)}deg(w)$. Then by the proof of Theorem 4.5

$$f(G\star v,x)=x^{n-3}(x^4-(\alpha^2+\beta^2+t)x^2+\frac{(\alpha^2+\beta^2+t)^2-(\alpha^4+\beta^4+L)}{2}).$$

5 Bipartite Graphs of Rank 6

In this section we characterize all bipartite graphs of rank 6. We note that all the singular graphs of rank 6 are characterized in [8]. In addition the bipartite singular (reduced) graphs of nullity one are those corresponding to the last four lines of Table 2 in [8], that is the graphs shown in Figure 7 in [8]. These are the graphs G_8 to G_{12} of our paper. The graphs G_1 to G_7 are non-singular and G_{13} has nullity two. As we mentioned in the introduction, in [9] the authors consider the triangle-free graphs of rank 6. But we find that the graphs G_2 and G_3 in Theorem 4.1 of [9], have rank 8. On the other hand, the main step to find a classification for triangle-free graphs of rank 6 is first to classify bipartite graphs of the same rank [9]. In this section by a different way from [9], we completely characterize all bipartite graphs of rank 6. In other words, we find all bipartite graphs with exactly six non-zero eigenvalues.

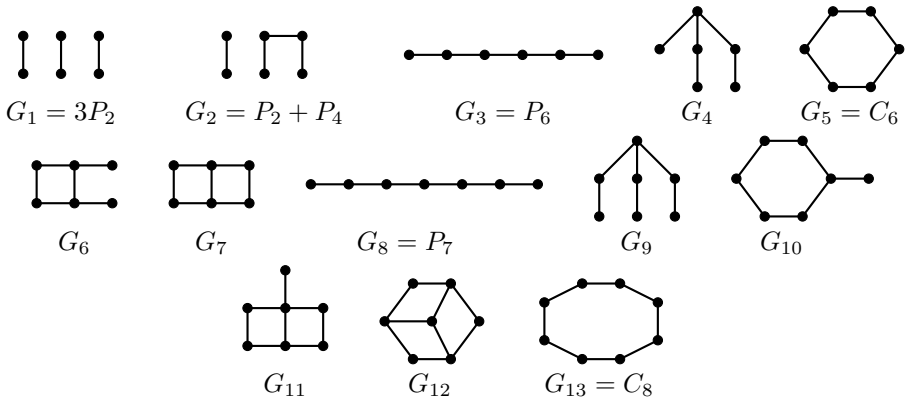


Figure 3: All strongly reduced bipartite graphs of rank 6.

Theorem 5.1. *Let G be a strongly reduced bipartite graph. Then $rank(G)=6$ if and only if G is one of the graphs which are shown in Figure 3.*

Proof. Let X and Y be the parts of G and $B=B(G)$. Since $rank(G)=6$, by Theorem 2.1, $rank(B)=3$. We show that $|X|,|Y|\leq 4$ (that is G has at most 8 vertices). Let y,y_1,y_2,y_3 be four vertices of Y. Since $rank(B)=3$, there exist some real numbers a,a_1,a_2 and a_3 such that $a[y]+a_1[y_1]+a_2[y_2]+a_3[y_3]=0$. We claim that all the numbers a,a_1,a_2 and a_3 are non-zero. If two coefficients are zero, for example $a_2=a_3=0$, then $N(y)=N(y_1)$, a contradiction (because G is reduced). If one of the coefficients is zero, say $a=0$, then as we see in the proof of Theorem 4.2, one of the following holds:

$[y_1] = [y_2] + [y_3]$ or $[y_2] = [y_1] + [y_3]$ or $[y_3] = [y_1] + [y_2]$, a contradiction (since G is neighbor-reduced). Thus the claim is proved.

Suppose that $deg(y) \geq deg(y_1) \geq deg(y_2) \geq deg(y_3)$. One can see that $N(y) \not\subseteq N(y_i)$, for $i = 1, 2, 3$. Let

$$[y] = \alpha[y_1] + \beta[y_2] + \gamma[y_3], \text{ where } \alpha, \beta, \gamma \neq 0. \tag{5.1}$$

Since $N(y) \setminus N(y_1) \neq \varnothing$, by Equation (5.1) we obtain $\beta l_1 + \gamma l_2 = 1$, where $l_1, l_2 \in \{0, 1\}$. This shows that $\beta = 1$ or $\gamma = 1$ or $\beta + \gamma = 1$. Similarly, since $N(y) \not\subseteq N(y_i)$ for $i = 2, 3$, we have $\alpha = 1$ or $\gamma = 1$ or $\alpha + \gamma = 1$ and $\alpha = 1$ or $\beta = 1$ or $\alpha + \beta = 1$. It is not hard to see that the multiset $\{\alpha, \beta, \gamma\}$ is one of the following:

$$\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\},\ \{1, 1, 1\},\ \{-1, 1, 1\}, \{-2, 1, 1\},\ \{-1, 1, 2\}, \{-1, -1, 1\}.$$

Therefore $[y]$ satisfying in one of the following equations:

$\mathbf{L_1}$: $2[y] = [y_1]+[y_2]+[y_3]$. $\mathbf{L_2}$: $[y] = [y_1]+[y_2]+[y_3]$. $\mathbf{L_3}$: $[y] = [y_1]+[y_2]-[y_3]$.
$\mathbf{L_4}$: $[y] = [y_1]-[y_2]+[y_3]$. $\mathbf{L_5}$: $[y] = -[y_1]+[y_2]+[y_3]$. $\mathbf{L_6}$: $[y] = [y_1]+[y_2]-2[y_3]$.
$\mathbf{L_7}$: $[y] = [y_1]-2[y_2]+[y_3]$. $\mathbf{L_8}$: $[y] = -2[y_1]+[y_2]+[y_3]$. $\mathbf{L_9}$: $[y] = 2[y_1]+[y_2]-[y_3]$.
$\mathbf{L_{10}}$: $[y] = 2[y_1]-[y_2]+[y_3]$. $\mathbf{L_{11}}$:$[y] = [y_1]+2[y_2]-[y_3]$. $\mathbf{L_{12}}$:$[y] = -[y_1]+2[y_2]+[y_3]$.
$\mathbf{L_{13}}$: $[y] = [y_1]-[y_2]+2[y_3]$. $\mathbf{L_{14}}$:$[y] = -[y_1]+[y_2]+2[y_3]$. $\mathbf{L_{15}}$: $[y] = [y_1]-[y_2]-[y_3]$.
$\mathbf{L_{16}}$: $[y] = -[y_1] + [y_2] - [y_3]$. $\mathbf{L_{17}}$: $[y] = -[y_1] - [y_2] + [y_3]$.

By multiplying the vector j (all components are 1) to both sides of Equation (5.1) we conclude that

$$deg(y) = \alpha\, deg(y_1) + \beta\, deg(y_2) + \gamma\, deg(y_3). \tag{5.2}$$

Suppose that y_1, y_2, y_3 have the minimum degree among all vertices of Y. Let $deg(y_1) \geq deg(y_2) \geq deg(y_3)$. By Equation (5.2) the cases $L_8, L_{15}, L_{16}, L_{17}$ cannot happen. On the other hand one can see that the cases L_7, L_9, L_{10}, L_{11} can not occur. For example suppose that L_7 holds. So there exists a vertex $y \neq y_1, y_2, y_3$ in Y such $[y] = [y_1] - 2[y_2] + [y_3]$. This shows that $N(y_2) \subseteq N(y_1) \cap N(y_3)$. Since $deg(y_2) \geq deg(y_3)$, $N(y_2) = N(y_3)$, a contradiction (because G is reduced).

Now we claim that $|Y| \leq 4$. By contradiction let $|Y| \geq 5$. Assume that y_1, y_2, y_3 have the minimum degree among all vertices of Y and $deg(y_1) \geq deg(y_2) \geq deg(y_3)$. Suppose that y and y_0 are two vertices of Y (distinct from y_1, y_2, y_3). Thus $[y]$ and $[y_0]$ are satisfying in one of the equations $L_1, L_2, L_3, L_4, L_5, L_6, L_{12}, L_{13}, L_{14}$. We show that it is impossible. For example suppose that $[y]$ satisfying in the equation L_i and y_0 in L_j. Clearly, $i \neq j$. For instance let $i = 3$ and $j = 4$. That is $[y] = [y_1] + [y_2] - [y_3]$ and $[y_0] = [y_1] - [y_2] + [y_3]$. Thus $[y] + [y_0] = 2[y_1]$, a contradiction (because every three columns of B is independent). As other manner let $i = 1$ and $j = 2$. Thus $[y_0] = -2[y]+2[y_2]+2[y_3]$, a contradiction (because it does not appear in equations $L_1, \ldots, L_{17}$). As a last manner let $i = 12$ and $j = 14$. The condition L_{12} implies that $N(y_2) \subseteq N(y_1)$ and $N(y_2) \cap N(y_3) = \varnothing$. On the other hand L_{14} shows that $N(y_3) \subseteq N(y_1)$. Since G is neighbor-reduced, $N(y_1) \neq N(y_2) \cup N(y_3)$. Let $x \in N(y_1) \setminus N(y_2) \cup N(y_3)$. By the equality $[y] = -[y_1] + 2[y_2] + [y_3]$, we find that the component correspondences to x in $[y]$ is -1, a contradiction. Similarly one can check the other value for i and j, where

$i, j \in \{1, 2, 3, 4, 5, 6, 12, 13, 14\}$. The claim is proved. That is $|Y| \leq 4$. Similarly $|X| \leq 4$. Thus G has at most 8 vertices. One can see that all of the strongly reduced graphs of rank 6 and with at most 8 vertices are given in Figure 3. The proof is complete. □

Remark 5.2. Let b_n and c_n be the number of connected bipartite graphs and connected strongly reduced bipartite graphs of order n, respectively. Then

$$b_1 = b_2 = b_3 = 1,\ b_4 = 3,\ b_5 = 5,\ b_6 = 17,\ b_7 = 44,\ b_8 = 182,$$

$$c_1 = c_2 = 1,\ c_3 = 0,\ c_4 = 1,\ c_5 = 0,\ c_6 = 5,\ c_7 = 5,\ c_8 = 36.$$

We note that among all connected strongly reduced bipartite graphs of order 8, the cycle C_8 is the only graph with rank 6 and the others have rank 8.

Using Theorems 2.5 and 5.1 (similar to proof of Theorems 3.3 and 4.3) we characterize all bipartite graphs of rank 6. See also Theorem 8.3 of [8].

Theorem 5.3. *Let G be a bipartite graph with no isolated vertex. Then $rank(G) = 6$ if and only if G is obtained from one of the graph which is shown in Figure 3 with the operations $\star$ and $\oplus$.*

Now we characterize all bipartite reduced graphs of rank 6.

Theorem 5.4. *Let G be a reduced bipartite graph. Then $rank(G) = 6$ if and only if G is one of the graphs which are shown in Figurer 4.*

Proof. It is easy to check that all graphs of Figure 4 are reduced of rank 6. Thus it remains to prove the other part. Let G be a reduced bipartite graph of rank 6. If G is strongly reduced, then by Theorem 5.1, G is one of the graphs $G_1, \ldots, G_{13}$ which are shown in Figure 3. Otherwise, by Theorem 5.3, G is obtained from one of the graphs $G_1, \ldots, G_{13}$ by the operations $\star$ and $\oplus$. Since G is reduced, G is obtained only by the operation $\oplus$ from $G_1, \ldots, G_{13}$ (note that if H is a non-reduced graph, then for any independent set S of H, $H \star S$ is also non-reduced).

Thus to obtain G it is sufficient to apply the operation $\oplus$ on the graphs $G_1, \ldots, G_{13}$. Since there is no non-adjacent vertices u and v in $G_5, G_6, G_7, G_{11}, G_{12}$ such that $N(u) \cap N(v) = \varnothing$, we can not apply $\oplus$ on the graphs $G_5, G_6, G_7, G_{11}, G_{12}$.

For the other graphs, one can see the following:

1) The graphs $G_{1,1}, G_{1,2}, G_{1,3}, G_{1,4}, G_{1,5}, G_{1,6}, G_{1,7}$ and $G_{1,8}$ are obtained from G_1.
2) The graphs $G_{2,1}, G_{2,2}, G_{2,3}$ and $G_{2,4}$ are obtained from G_2.
3) The graph $G_{3,1}$ is obtained from G_3.
4) The graph $G_{4,1}$ is obtained from G_4.
5) The graphs $G_{8,1}, G_{8,2}, G_{8,3}$ and $G_{8,4}$ are obtained from G_8.
6) The graphs $G_{9,1}, G_{9,2}$ and $G_{9,3}$ that are isomorphic to $G_{1,4}, G_{1,6}$ and $G_{1,8}$, respectively, are obtained from G_9.
7) The graph $G_{10,1}$ is obtained from G_{10}.
8) The graph $G_{13,1}$ is obtained from G_{13}.

Therefore we obtain 20 reduced graphs from $G_1, G_2, G_3, G_4, G_8, G_9, G_{10}$ and G_{13}. Since $G_1, \ldots, G_{13}$ are also reduced, there are exactly 33 bipartite reduced graphs of rank 6 (see Figure 4). □

Similar to other theorems like Theorem 5.3 we can prove one of the main result of this paper.

Theorem 5.5. *Let G be a bipartite graph with no isolated vertex. Then $rank(G) = 6$ if and only if G obtained from one of the graphs which are shown in Figurer 4 with the operation $\star$.*

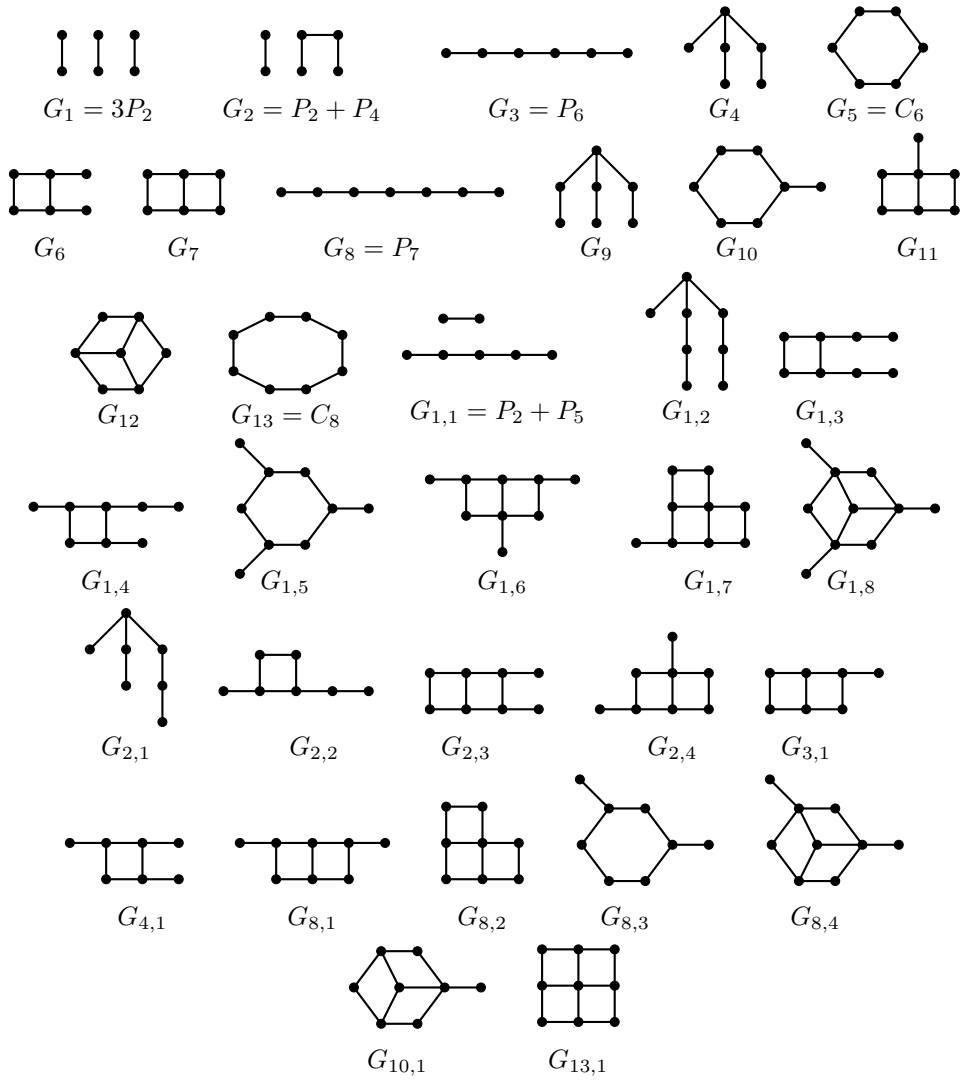


Figure 4: All reduced bipartite graphs of rank 6.

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Mathematical aspects of Wiener index

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Abstract

The Wiener index (i.e., the total distance or the transmission number), defined as the sum of distances between all unordered pairs of vertices in a graph, is one of the most popular molecular descriptors. In this article we summarize some results, conjectures and problems on this molecular descriptor, with emphasis on works we were involved in.

Keywords: Graph distance, Wiener index, average distance, topological index, molecular descriptor, chemical graph theory.

Math. Subj. Class.: 05C12, 05C05, 05C20, 92E10

1 Introduction

Having a molecule, if we represent atoms by vertices and bonds by edges, we obtain a molecular graph, [87, 88]. Graph theoretic invariants of molecular graphs, which predict properties of the corresponding molecule, are known as topological indices. The oldest topological index is the Wiener index [107], which was introduced in 1947 as the path number.

At first, the Wiener index was used for predicting the boiling points of paraffins [107], but later a strong correlation between the Wiener index and the chemical properties of a

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compound was found. Nowadays this index is a tool used for preliminary screening of drug molecules [1]. The Wiener index also predicts binding energy of protein-ligand complex at a preliminary stage.

Hence, the Wiener index was used by chemists decades before it attracted attention of mathematicians. In fact, it was studied long time before the branch of discrete mathematics, which is now known as Graph Theory, was developed. Many years after its introduction, the same quantity has been studied and referred to by mathematicians as the gross status [48], the distance of graphs [29] and the transmission [93]. A great deal of knowledge on the Wiener index is accumulated in several survey papers [13, 16, 24, 67, 109]. This paper is also of similar kind and it appears in a volume dedicated to A. Graovac, whose wide research opus of mathematical chemistry includes also works of the Wiener index, e.g., see [34, 84, 90, 99, 100].

Let $d(u, v)$ denote the distance between vertices u and v in G. The *Wiener index* of a graph G, denoted by $W(G)$, is the sum of distances between all (unordered) pairs of vertices of G

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v). \tag{1.1}$$

Though, the Wiener index is the most common topological index, nowadays we know over 200 topological indices used in chemistry. Here we mention three of them, those, which can be considered as weighted versions of the Wiener index.

For an edge $e = ij$, let $n_e(i)$ be the number of vertices of G being closer to i than to j and let $n_e(j)$ be the number of vertices of G lying closer to j than to i. The *Szeged index* of a graph G is defined by

$$\mathrm{Sz}\,(G) = \sum_{e=ij\in E(G)} n_e(i)n_e(j).$$

This invariant was introduced by Gutman [37] during his stay at the Attila Jozsef University in Szeged, and he named it after this place.

In 1989, lead by the idea of characterizing the alkanes, Schultz [89] defined a new index $\mathrm{MTI}(G)$ that is degree and distance based. Gutman decomposed this index into two parts and called one of them *Schultz index (of the first kind)*, which is defined by

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u) + d(v))\, d(u, v)\,,$$

where $d(v)$ denotes the degree of v. The same invariant was independently and simultaneously introduced by Dobrynin and Kochetova [17].

Gutman [36] also introduced a new index,

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)d(v)d(u, v)\,,$$

and named it the *Schultz index of the second kind*. Nowadays this index is also known as the *Gutman index*.

In this paper we consider mathematical aspects of the Wiener index. This is not a typical survey. We summarize our mathematical work on this molecular descriptor over the past years and, what is more important, we integrate some conjectures, problems, thoughts, and ideas for possible future work that we find interesting. We include also a couple of related open problems that have been considered by other authors.

2 Some fundamental properties of Wiener index

Already in 1947, Wiener has shown that the Wiener index of a tree can be decomposed into easily calculable edge–contributions. In what follows, by $n(G)$ we denote the number of vertices of G. Let F be a graph with p components, $T_1, T_2, \ldots, T_p$. Then we set

$$N_2(F) = \sum_{1 \le i < j \le p} n(T_i)\, n(T_j)\,.$$

If $p = 1$, that is if F is connected, then $N_2(F) = 0$.

Theorem 2.1 (Wiener, 1947)**.** *For a tree T the following holds*

$$W(T) = \sum_{e \in E(T)} N_2(T - e). \tag{2.1}$$

Since T is a tree, for every edge $e = ij$ of T, the forest $T - e$ is comprised of two components, one of size $n_e(i)$ and the other of size $n_e(j)$, which gives $N_2(T - e) = n_e(i)n_e(j)$. Thus, one can restate (2.1) as

$$W(T) = \sum_{e=ij \in E(T)} n_e(i)n_e(j). \tag{2.2}$$

So the Szeged and Wiener indices coincide on trees. In fact, the Szeged index was defined from (2.2) by relaxing the condition that the graph is a tree.

In analogy to the classical Theorem 2.1, we have the following vertex version (see [44]):

Theorem 2.2. *Let T be a tree on n vertices. Then*

$$W(T) = \sum_{v \in V(T)} N_2(T - v) + \binom{n}{2}. \tag{2.3}$$

An interesting theorem of Doyle and Graver [26] is of a similar kind. Let F be a graph with p components, $T_1, T_2, \ldots, T_p$. Then we set

$$N_3(F) = \sum_{1 \le i < j < k \le p} n(T_i)\, n(T_j)\, n(T_k)\,.$$

Note that if $p = 1$ or $p = 2$, then $N_3(F) = 0$. Now we state their result, moreover we give an alternative short proof in the spirit of combinatorial countings, more precisely involving combinations of order 3.

Theorem 2.3 (Doyle and Graver)**.** *Let T be a tree on n vertices. Then*

$$W(T) + \sum_{v \in V(T)} N_3(T - v) = \binom{n+1}{3}. \tag{2.4}$$

Proof. Let $V(T) = \{1, \ldots, n\}$ and let $V^* = V(T) \cup \{\pi\}$. For any path $P = a_0 a_1 a_2 \cdots a_k$ in T with $a_0 < a_k$, assign the 3-set $\{a_0, a_i, a_k\}$ to the edge $a_i a_{i+1}$ for $1 \le i < k$ and $\{a_0, a_k, \pi\}$ to the edge $a_0 a_1$. So we assign k distinct 3-sets to a path P of length k. This

way we assign all together $W(T)$ 3-sets. For any non-assigned 3-set $\{a, b, c\}$ (observe that π does not appear here) of $\binom{V^*}{3}$, T has no path containing them so there is precisely one vertex v (their median) that this 3-set contributes 1 to $N_3(T - v)$. As V^* is of size $n + 1$, the claim is established. □

It is well known that for trees on n vertices, the maximum Wiener index is obtained for the path P_n, and the minimum for the star S_n. Thus, for every tree T on n vertices we have

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3}.$$

Since the distance between any two distinct vertices is at least one, among all graphs on n vertices K_n has the smallest Wiener index. So for any connected graph G on n vertices, it holds

$$\binom{n}{2} = W(K_n) \leq W(G) \leq W(P_n) = \binom{n+1}{3}.$$

Note that the alternative proof of Theorem 2.3 gives us a new proof that $W(P_n) = \binom{n+1}{3}$ and that P_n is the extremal graph for the maximum. Among 2-connected graphs on n vertices the n-cycle has the largest Wiener index

$$W(C_n) = \begin{cases} \frac{n^3}{8} & \text{if } n \text{ is even,} \\ \frac{n^3-n}{8} & \text{if } n \text{ is odd.} \end{cases}$$

3 Inverse Wiener index problem

In 1995 Gutman and Yeh [45] considered an inverse Wiener index problem. They asked for which integers w there exist trees with Wiener index w, and posed the following conjecture:

For all but finitely many integers w there exist trees with Wiener index w. (3.1)

Inspired by the conjecture above, Lepović and Gutman [74] checked integers up to 1206 and found 49 integers that are not Wiener indices of trees. In 2004, Ban, Bereg, and Mustafa [2] computationally proved that for all integers w on the interval from 10^3 to 10^8 there exists a tree with Wiener index w. Finally, in 2006, two proofs of the conjecture were published. First, Wang and Yu [106] proved that for every $w > 10^8$ there exists a caterpillar tree with Wiener index w. The second result is due to Wagner [101], who proved that all integers but 49 are Wiener indices of trees with diameter at most 4.

Surprisingly, it turns out that in most cases the inverse problem has many solutions. Fink, Lužar and Škrekovski [30] showed that the following theorem holds.

Theorem 3.1. *There exists a function $f(w) \in \Omega(\sqrt[4]{w})$ such that for every sufficiently large integer w there exist at least $2^{f(w)}$ trees with Wiener index w.*

In [30] there is also proposed a constant time algorithm, which for a given integer w returns a tree with diameter four and with Wiener index w. It would be interesting to find a better lower bound on $f(w)$ in Theorem 3.1.

However, beside caterpillars and trees with small diameter, it could be interesting to find some other types of trees (or graphs) that solve the inverse Wiener index problem. Li and Wang [75] considered this problem for peptoids, Wagner et. al [103] for molecular

and so-called hexagon type graphs, and Wagner [102] for graphs with small cyclomatic number.

Bereg and Wang [3] experimentally came to the observation that this may hold for binary trees, as stated bellow. Moreover, they observed that the conjecture may hold even when restricting to 2-trees, and even more, they where not able to disprove it for 1-trees (a binary tree of height h is a *k-tree* if every vertex of depth less than $h-k$ has precisely two children).

Conjecture 3.2. *Except for some finite set, every positive integer is the Wiener index of a binary tree.*

In [73] was considered the following problem, so called the *Wiener inverse interval problem*.

Problem 3.3. For given n, find all values w which are Wiener indices of graphs (trees) on n vertices.

Regarding the above problem, let $\mathrm{WG}(n)$ and $\mathrm{WT}(n)$ be the corresponding sets of values w for graphs and trees on n vertices, respectively. Both sets have $\binom{n+1}{3}$ for the maximum element. The smallest value in $\mathrm{WG}(n)$ is $\binom{n}{2}$ and in $\mathrm{WT}(n)$ it is $(n-1)^2$. In [73], the size of the set $\mathrm{WG}(n)$ was considered, and it was shown that it is of order $\frac{1}{6}n^3 + O\left(n^2\right)$. In the same paper the following problems were stated.

Conjecture 3.4. *The cardinality of* $\mathrm{WG}(n)$ *is of order* $\frac{1}{6}n^3 - \frac{1}{2}n^2 + \Theta(n)$.

Conjecture 3.5. *The cardinality of* $\mathrm{WT}(n)$ *equals* $\frac{1}{6}n^3 + \Theta\left(n^2\right)$.

In fact in [73] it was shown that the length of the largest interval of integers which is fully contained in $\mathrm{WG}(n)$ is of size $\frac{1}{6}n^3 + O\left(n^2\right)$. Regarding the length of the largest interval when only trees are considered, the following is conjectured.

Conjecture 3.6. *In the set* $\mathrm{WT}(n)$*, the cardinality of the largest interval of integers equals* $\Theta\left(n^3\right)$.

4 Graphs with prescribed minimum/maximum degree

Here we consider extremal values of the Wiener index in some subclasses of the class of all graphs on n vertices. Recall that the *maximum degree* of a graph G, denoted by $\Delta(G)$, and the *minimum degree* of a graph, denoted by $\delta(G)$, are the maximum and minimum degree of its vertices. As mentioned above, among n-vertex graphs with the minimum degree ≥ 1, the maximum Wiener index is attained by P_n. But when restricting to minimum degree ≥ 2, the extremal graph is C_n. Observe that with the reasonable assumptions $\Delta \geq 2$ and $\delta \leq n-1$, the following holds

$$\max\{W(G);\, G \text{ has maximum degree at most } \Delta \text{ and } n \text{ vertices}\} = W(P_n), \text{ and}$$
$$\min\{W(G);\, G \text{ has minimum degree at least } \delta \text{ and } n \text{ vertices}\} = W(K_n).$$

Analogous reasons motivate the following two problems.

Problem 4.1. What is the maximum Wiener index among n-vertex graphs with the minimum degree at least δ?

Problem 4.2. What is the minimum Wiener index among n-vertex graphs with the maximum degree at most Δ?

A related problem was considered by Fischermann et al. [31], and independently by Jelen and Trisch in [52, 53], who characterized the trees which minimize the Wiener index among all n-vertex trees with the maximum degree at most Δ. They also determined the trees which maximize the Wiener index, but in a much more restricted family of trees which have two distinct vertex degrees only. Later Stevanović [94] determined the trees which maximize the Wiener index among all graphs with the maximum degree Δ, and originally Problem 4.2 was proposed by him in an equivalent form which requires that the maximum degree is precisely Δ.

Restricting to $\Delta = \delta = r$, i.e., restricting to regular graphs, could be especially interesting. In general, introducing (resp. removing) edges in a graph decreases (resp. increases) the Wiener index, but in the class of r-regular graphs on n vertices we have fixed number of $r \cdot n/2$ edges. Thus, more important role is played by the diameter. Recall that in the case of trees, where the number of edges is fixed as well, the maximum Wiener index is attained by P_n which has the largest diameter, and the minimum Wiener index is attained by S_n, which has the smallest diameter. Let us start with the first nontrivial case $r = 3$, i.e. with cubic graphs.

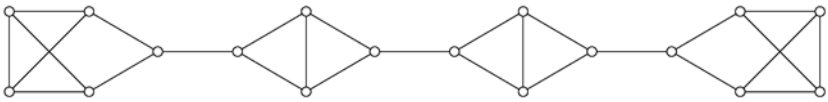

Figure 1: The graph L_{18}.

Let n be even and $n \geq 10$. If $4 \nmid n$, then L_n is obtained from $(n-10)/4$ copies of $K_4 - e$ joined to a path by edges connecting the vertices of degree 2, to which at the ends we attach two pendant blocks, each on 5 vertices, see Figure 1 for L_{18}.

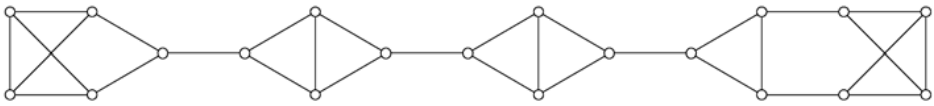

Figure 2: The graph L_{20}.

On the other hand if $4 \mid n$, then L_n is obtained from $(n-12)/4$ copies of $K_4 - e$, joined into a path by edges connecting the vertices of degree 2, to which ends we attach two pendant blocks, one on 5 vertices and the other on 7 vertices, see Figure 2 for L_{20} [68]. We have the following conjecture.

Conjecture 4.3. *Among n-vertex cubic graphs, L_n has the largest Wiener index.*

We believe that similar statements hold also for higher $r \geq 4$, with intermediate repetitive gadget $K_4 - e$ replaced by $K_{r+1} - e$, where on both ends we attach suitable gadgets so that the resulting graph will have n vertices. Actually, these graphs are those with the

maximum diameter, see [58], where the problem of finding a regular graph of given order and degree with maximum diameter is studied from a different point of view.

The cubic graphs with the minimum Wiener index are hard to describe for us but it seems that they have the smallest diameter. For suitable n, good candidates are the cage graphs, e.g. Petersen graph and Heawood graph. Guided by our intuition, we believe that the following may hold.

Conjecture 4.4. *Among all r-regular graphs on n vertices, the maximum Wiener index is attained by a graph with the maximum possible diameter.*

Conjecture 4.5. *Among all r-regular graphs on n vertices, the minimum Wiener index is attained by a graph with the minimum possible diameter.*

5 Graphs with prescribed diameter/radius

The *eccentricity* $\mathrm{ecc}(v)$ of a vertex v in G is the largest distance from v to another vertex of G; that is, $\max\{d(v,w) \mid w \in V(G)\}$. The *diameter* of G, denoted by $\mathrm{diam}(G)$, is the maximum eccentricity in G. Similarly, the *radius* of G, denoted by $\mathrm{rad}(G)$, is the minimum eccentricity in G.

Plesník [86] obtained the graphs with minimum Wiener index in the class of graphs of order n and diameter d ($d \leq n-1$). When $d < n-1$, they are cycle-containing graphs. In 1975 he [85] addressed the following problem.

Problem 5.1. What is the maximum Wiener index among graphs of order n and diameter d?

This problem remains unsolved even under additional restrictions. DeLaViña and Waller [9] conjectured the following.

Conjecture 5.2. *Let G be a graph with diameter $d > 2$ and order $2d+1$. Then $W(G) \leq W(C_{2d+1})$, where C_{2d+1} denotes the cycle of length $2d+1$.*

Wang and Guo [105] determined the trees with maximum Wiener index among trees of order n and diameter d for some special values of d, $2 \leq d \leq 4$ or $n-3 \leq d \leq n-1$. Independently, Mukwembi [83] considered the diameter up to 6 and showed that bounds he obtained are best possible. It could be also interesting to find a sharp upper bound on the Wiener index for trees of given order and larger diameter.

For any connected graph G, $\mathrm{rad}(G) \leq \mathrm{diam}(G) \leq 2\,\mathrm{rad}(G)$. By considering the close relationship between the diameter and the radius of a graph, it is natural to consider the above problem with radius instead of diameter [5].

Problem 5.3. What is the maximum Wiener index among graphs of order n and radius r?

Chen et al. [5] characterized graphs with the maximum Wiener index among all graphs of order n with radius two. Analogous problem for the minimum Wiener index was posed by You and Liu [110].

Problem 5.4. What is the minimum Wiener index among all graphs of order n and radius r?

Regarding this problem, Chen et al. [5] stated the following conjecture. For integers n, r, and s with $n \geq 2r$, $r \geq 3$, and $n - 2r + 1 \geq s \geq 1$, construct a graph $G_{n,r,s}$ from a $2r$-cycle $v_1v_2 \cdots v_{2r}$ so that v_1 is replaced by K_s and v_2 is replaced by $K_{n-2r+2-s}$, connect v_{2r} to each vertex of K_s, connect each vertex of K_s to each vertex of $K_{n-2r+2-s}$, and connect each vertex of $K_{n-2r+2-s}$ to v_3 (in other words v_1 is replicated $s-1$ times, and v_2 is replicated $n-2r+1-s$ times). Notice that the resulting graph has n vertices and radius r.

Conjecture 5.5. *Let n and r be two positive integers with $n \geq 2r$ and $r \geq 3$. Then graphs $G_{n,r,s}$ for $s \in \{1, \ldots, r-1\}$ attain the minimum Wiener index in the class of graphs on n vertices and with radius r.*

6 Congruence relations for Wiener index

It was of interest to several authors to obtain congruence relations for the Wiener index. The first result of this kind was proved by Gutman and Rouvray [43]. They established the congruence relation for the Wiener index of trees with perfect matchings.

Theorem 6.1 (Gutman and Rouvray)**.** *Let T and T' be two trees on the same number of vertices. If both T and T' have perfect matchings, then $W(T) \equiv W(T') \pmod 4$.*

A *segment* of a tree is a path contained in the tree whose terminal vertices are branching or pendant vertices of the tree. Dobrynin, Entringer and Gutman [13] obtained a congruence relation for the Wiener index in the class of *k-proportional trees*. Trees of this class have the same order, the same number of segments, and the lengths of all segments are multiples of k.

Theorem 6.2 (Dobrynin, Entringer and Gutman)**.** *Let T and T' be two k-proportional trees. Then*

$$W(T) \equiv W(T') \pmod{k^3}.$$

Theorem 6.1 was recently generalized by Lin in [76] by establishing the congruence relation for the Wiener index of trees containing T-factors. A graph G has a *T-factor* if there exist vertex disjoint trees $T_1, T_2, \ldots, T_p$ such that $V(G) = V(T_1) \cup V(T_2) \cup \cdots \cup V(T_p)$ and each T_i is isomorphic to a tree T on r vertices. If T is a path on r vertices, we say that the graph G has a P_r-factor. In this sense the well-known perfect matching is a P_2-factor.

Theorem 6.3 (Lin)**.** *If T and T' are two trees on the same number of vertices, both with P_r-factors, then*

$$W(T) \equiv W(T') \pmod r \quad \textit{for odd } r,$$

and

$$W(T) \equiv W(T') \pmod{2r} \quad \textit{for even } r.$$

Recently Gutman, Xu and Liu [46] showed that the first congruence in the above result is a special case of a much more general result on the Szeged index. As its consequence, for the Wiener index they obtained the following result.

Theorem 6.4 (Gutman, Xu and Liu). *Let Γ_0 be the union of connected graphs $G_1, G_2, \ldots, G_p$, $p \geq 2$, each of order $r \geq 2$, all blocks of which are complete graphs. Denote by Γ a graph obtained by adding $p-1$ edges to Γ_0 so that the resulting graph is connected. Then*

$$W(\Gamma) \equiv \sum_{i=1}^{p} W(G_i) \pmod{r}.$$

In [49] we generalized both the above results. Let r and t be integers, $r \geq 2$ and $0 \leq t < r$. Further, let $\mathcal{H} = \{H_1, H_2, \ldots, H_\ell\}$ be a set of connected graphs, such that for all i, $1 \leq i \leq \ell$, we have $|V(H_i)| \equiv -t \pmod{r}$. Finally, let $\mathcal{F} = \{F_1, F_2, \ldots, F_{\ell-1}\}$ be a set of connected graphs, such that for all j, $1 \leq j \leq \ell - 1$, we have $|V(F_j)| \equiv t + 2 \pmod{r}$. For every F_j, choose vertices $v_j^1, v_j^2 \in V(F_j)$. We remark that the vertices v_j^1 and v_j^2 are not necessarily distinct. Denote by $\mathcal{G} = \mathcal{G}(\mathcal{H}, \mathcal{F})$ the set of all graphs obtained when all the vertices v_j^1 and v_j^2, $1 \leq j \leq \ell - 1$, are identified with some vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that the resulting graph is connected.

Every graph in $\mathcal{G}$ contains ℓ graphs from $\mathcal{H}$, $\ell - 1$ graphs from $\mathcal{F}$, and each graph of $\mathcal{F}$ connects two graphs of $\mathcal{H}$. Since the graphs in $\mathcal{G}$ are connected, if we contract every H_i to a single vertex and we consider F_j's as edges joining pairs of these contracted vertices, then the resulting graph is a tree. In this way, $H_1, H_2, \ldots, H_\ell$ can be regarded as supervertices, $F_1, F_2, \ldots, F_{\ell-1}$ as superedges, and the resulting graph has a tree structure.

In Figure 3 we have one graph G of $\mathcal{G}$ for given parameters r, t and ℓ, and for given sets $\mathcal{H}$, $\mathcal{F}$ and $\{v_j^1, v_j^2\}_{j=1}^{\ell-1}$. The vertices of H_j's are depicted by full circles in Figure 3 and the edges of H_i's are thick.

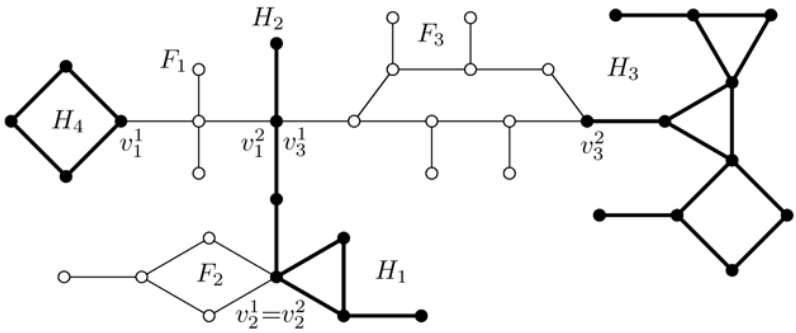

Figure 3: A graph of $\mathcal{G}$ for $r = 7$, $t = 3$, $\ell = 4$ and given H_i's, F_j's and v_j^k's.

Theorem 6.5. *Let $G_1, G_2 \in \mathcal{G}$. Then $W(G_1) \equiv W(G_2) \pmod{r}$.*

Now we generalize the second part of Theorem 6.3. Let r be an even number, $r \geq 2$. Further, let $\mathcal{H} = \{H_1, H_2, \ldots, H_\ell\}$ be a set of trees, such that for all i, $1 \leq i \leq \ell$, we have $|V(H_i)| \equiv 0 \pmod{r}$. Finally, let $\mathcal{F} = \{F_1, F_2, \ldots, F_{\ell-1}\}$ be a set of trees, such that for all j, $1 \leq j \leq \ell - 1$, we have $|V(F_j)| \equiv 2 \pmod{r}$. For every F_j, choose vertices $v_j^1, v_j^2 \in V(F_j)$. Denote by $\mathcal{G}^T$ the set of all graphs obtained when all the vertices v_j^1 and v_j^2, $1 \leq j \leq \ell - 1$, are identified with some vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that the

resulting graph is connected. Hence, $\mathcal{G}^T$ is a restriction of $\mathcal{G}$ when all the graphs in $\mathcal{H}$ and $\mathcal{F}$ are trees and $t = 0$.

Theorem 6.6. *Let r be even and $G_1, G_2 \in \mathcal{G}^T$. Then $W(G_1) \equiv W(G_2) \pmod{2r}$.*

Theorems 6.5 and 6.6 show limits of Theorem 6.3. Note that a segment can be defined on graphs as well, and similarly one can define k-proportional graphs. So, it would be interesting to find analogous limits for Theorem 6.2.

Problem 6.7. Let G and G be two k-proportional graphs. Under which conditions we have $W(G) \equiv W(G') \pmod{k^3}$?

7 Wiener index and line graph operation

Let G be a graph. Its *line graph*, $L(G)$, has vertex set identical with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. *Iterated* line graphs are defined inductively as follows:

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

The main problem here is to determine the relation between $W(L(G))$ and $W(G)$. Particularly, we focuss on graphs G satisfying

$$W(L(G)) = W(G), \tag{7.1}$$

see [8, 22, 21, 40, 42], and in particular see the expository papers [24, 67]. Let us remark that in the literature one easily encounters the term *edge-Wiener index* of G, which is actually the Wiener index of the line graph, sometimes shifted by $\binom{n}{2}$, see [55].

The following remark of Buckley [4] is a pioneering work in this area.

Theorem 7.1 (Buckley, 1981)**.** *For every tree T, $W(L(T)) = W(T) - \binom{n}{2}$.*

By the above result, the Wiener index of a line graph of a tree is strictly smaller than the Wiener index of the original tree. An interesting generalization of this was given by Gutman [38]:

Theorem 7.2. *If G is a connected graph with n vertices and m edges, then*

$$W(L(G)) \geq W(G) - n(n-1) + \frac{1}{2}m(m+1).$$

In addition, regarding Theorem 7.1, Gutman and Pavlović [42] showed that the Wiener index of a line graph is not greater than the Wiener index of the original graph even if we allow a single cycle in the graph.

Theorem 7.3. *If G is a connected unicyclic graph with n vertices, then $W(L(G)) \leq W(G)$, with equality if and only if G is a cycle of length n.*

In connected bicyclic graphs all the three cases $W(L(G)) < W(G)$, $W(L(G)) = W(G)$, and $W(L(G)) > W(G)$ occur [42]. There are 26 bicyclic graphs of order 9 with the property $W(L(G)) = W(G)$ [14, 41], and already 166 ten-vertex vertices with this property, see [24].

The following result tells us that in most cases (7.1) does not hold for graphs of minimum degree at least 2, see [6, 108].

Theorem 7.4. *Let G be a connected graph with $\delta(G) \geq 2$. Then*

$$W(L(G)) \geq W(G).$$

Moreover, the equality holds only for cycles.

7.1 Sandwiching by Gutman index

The following result was proved independently and simultaneously in [6] and [108].

Theorem 7.5. *Let G be a connected graph of size m. Then*

$$\frac{1}{4}(\mathrm{Gut}(G) - m) \leq W(L(G)) \leq \frac{1}{4}(\mathrm{Gut}(G) - m) + \binom{m}{2}.$$

Moreover, the lower bound is attained if and only if G is a tree.

Let $\kappa_i(G)$ denote the number of i-cliques in a graph G. In [65], the lower bound of the above theorem is improved in the following way.

Theorem 7.6. *Let G be a connected graph. Then,*

$$W(L(G)) \geq \frac{1}{4}\mathrm{Gut}(G) - \frac{1}{4}|E(G)| + \frac{3}{4}\kappa_3(G) + 3\kappa_4(G) \tag{7.2}$$

with the equality in (7.2) if and only if G is a tree or a complete graph.

It follows from the above theorem that for a connected graph G of minimal degree $\delta \geq 2$ we have

$$W(L(G)) \geq \frac{\delta^2}{4}W(G) - \frac{1}{4}|E(G)| \geq \delta^2 - \frac{1}{4}W(G).$$

Moreover, this lower bound was improved in [72].

Theorem 7.7. *Let G be a connected graph of minimum degree δ. Then*

$$W(L(G)) \geq \frac{\delta^2}{4}W(G)$$

with equality holding if and only if G is isomorphic to a path on three vertices or a cycle.

7.2 Extremal line graphs

The problem of finding graphs, whose line graph has the maximal Wiener index was given by Gutman [38] (see also [24]).

Problem 7.8. Find an n-vertex graph G whose line graph $L(G)$ has the maximal Wiener index.

We say that a graph is *dumbell* if it is comprised of two disjoint cliques connected by a path, and similarly a graph is *barbell* if it is comprised of two disjoint complete bipartite graphs connected by a path.

Conjecture 7.9. *In the class of graphs G on n vertices, $W(L(G))$ attains maximum for some dumbell graph.*

The above conjecture is supported by a result in [8]. We state a similar one for bipartite graphs.

Conjecture 7.10. *Let n be a large integer. Then in the class of all bipartite graphs G on n vertices $W(L(G))$ attains maximum for some barbell graph.*

7.3 Extremal ratios

Dobrynin and Mel'nikov [24] proposed to estimate the extremal values for the ratio

$$\frac{W(L^k(G))}{W(G)}, \tag{7.3}$$

and explicitly stated the case $k = 1$ as a problem. In [72] this problem was solved for the minimum.

Theorem 7.11. *Among all connected graphs on n vertices, the fraction $\frac{W(L(G))}{W(G)}$ is minimum for the star S_n.*

The problem for the maximum remains open.

Problem 7.12. Find n-vertex graphs G with maximal values of $\frac{W(L(G))}{W(G)}$.

Notice that

$$\frac{W(L(S_n))}{W(S_n)} = \frac{n-2}{2(n+1)}, \quad \frac{W(L(P_n))}{W(P_n)} = \frac{n-2}{n+1}, \quad \text{and} \quad \frac{W(L(K_n))}{W(K_n)} = \binom{n-1}{2}.$$

The line graph of K_n has the greatest number of vertices, and henceforth, it may attain the maximum value. Restricting to bipartite graphs, the almost balanced complete bipartite graphs have most vertices, so in this class of graphs the extreme could be $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Regarding the minimum of (7.3), we expect that for higher iterations $k \geq 2$, it should be P_n, as it is the only graph whose line graph decreases in size. We believe the following holds, as it is proposed and considered in [50].

Conjecture 7.13. *Let $k \geq 2$ and let n be a large integer. Then in the class of graphs G on n vertices $W(L^k(G))/W(G)$ attains the maximum for K_n, and it attains the minimum for P_n.*

7.4 Graphs with given girth

The *girth* of a graph is the length of a shortest cycle contained in the graph. A connected graph G is isomorphic to $L(G)$ if and only if G is a cycle. Thus, cycles provide a trivial infinite family of graphs for which $W(G) = W(L(G))$. In [23], Dobrynin and Mel'nikov stated the following problem.

> *Is it true that for every integer $g \geq 5$ there exists a graph $G \neq C_g$ of girth g, for which $W(G) = W(L(G))$?* (7.4)

The above problem (7.4) was solved by Dobrynin [11] for all girths $g \neq \{5, 7\}$; these last two cases were solved separately. Already in [23], Dobrynin and Mel'nikov [23] constructed infinite families of graphs of girths three and four with the property $W(G) = W(L(G))$. Inspired by their result the following statement was proved in [6].

Theorem 7.14. *For every non-negative integer h, there exist infinitely many graphs G of girth $g = h^2 + h + 9$ with $W(L(G)) = W(G)$.*

The above result encouraged the authors of [6] to state the following conjecture.

Conjecture 7.15. *For every integer $g \geq 3$, there exist infinitely many graphs G of girth g satisfying $W(G) = W(L(G))$.*

7.5 Graphs and cyclomatic number

The *cyclomatic number* $\lambda(G)$ of a graph G is defined as $\lambda(G) = |E(G)| - |V(G)| + 1$. Some attention was devoted to graphs G with prescribed cyclomatic number satysfying the equality $W(L(G)) = W(G)$. As already mentioned, the smallest 26 bicyclic graphs with 9 vertices are reported in [14, 41]. Bicyclic graphs up to 13 vertices are counted in [24] and diagrams of such graphs with 9 and 10 vertices are also given. The smallest 71 tricyclic graphs with 12 vertices are counted in [14]. There are 733 tricyclic graphs of order 13 with this properties [24]. Denote by $n(\lambda)$ the minimal order of graphs with cyclomatic number $\lambda \geq 2$ and $W(L(G)) = W(G)$. Then $n(2) = 9$ and $n(3) = 12$.

Graphs with increasing cyclomatic number were constructed in [15, 21, 22]. To construct graphs from [22], properties of the Pell equation from the number theory were applied. The cyclomatic number λ of graphs from [22] rapidly grows and the order of graphs is asymptotically equal to $(2 + \sqrt{5})\lambda \approx 4.236\lambda$ when $\lambda \to \infty$. The following conjecture was put forward in [22]:

Conjecture 7.16. *The graphs constructed in [22] have the minimal order among all graphs with given cyclomatic number satisfying the property* $W(L(G)) = W(G)$.

Graphs for all possible $\lambda \geq 2$ were constructed in [21]. It is known that $n(\lambda) \leq 5\lambda$ for $\lambda \geq 4$, $n(5) \leq 21$ and $n(7) \leq 29$. The following problem was posed in [14].

Problem 7.17. Find an exact value of $n(\lambda)$ for small $\lambda \geq 4$.

7.6 Quadratic line graphs

The graph $L^2(G)$ is also called the *quadratic line graph* of G. As mentioned above, for non-trivial tree T we cannot have $W(L(T)) = W(T)$. But there are trees T satisfying

$$W(L^2(T)) = W(T), \tag{7.5}$$

see [10, 18, 19, 67]. Obviously, the simplest trees are such which have a unique vertex of degree greater than 2. Such trees are called *generalized stars*. More precisely, *generalized t-star* is a tree obtained from the star $K_{1,t}$, $t \geq 3$, by replacing all its edges by paths of positive lengths, called *branches*. In [23] we have the following theorem.

Theorem 7.18. *Let S be a generalized t-star with q edges and branches of length k_1, $k_2, \ldots, k_t$. Then*

$$W(L^2(S)) = W(S) + \frac{1}{2}\binom{t-1}{2}\left(\sum_{i=1}^{t} k_i^2 + q\right) - q^2 + 6\binom{t}{4}. \tag{7.6}$$

Based on this theorem, it is proved in [23] that $W(L^2(S)) < W(S)$ if S is a generalized 3-star, and $W(L^2(S)) > W(S)$ if S is a generalized t-star where $t \geq 7$. Thus, property (7.5) can hold for generalized t-stars only when $t \in \{4, 5, 6\}$. In [23] and [66], for every $t \in \{4, 5, 6\}$ infinite families of generalized t-stars with property (7.5) were found, see also [67]. These results suggest the following conjecture [20]:

Conjecture 7.19. *Let T be a non-trivial tree such that $W(L^2(T)) = W(T)$. Then there is an infinite family of trees T' homeomorphic to T, such that $W(L^2(T')) = W(T')$.*

Of course, more interesting is the question which types of trees satisfy (7.5). Perhaps such trees do not have many vertices of degree at least 3. Let $\mathcal{T}$ be a class of trees which have no vertex of degree two, and such that $T \in \mathcal{T}$ if and only if there exists a tree T' homeomorphic to T, and such that $W(L^2(T')) = W(T')$. Trees that satisfy (7.5) are in abundance, so perhaps, it is impossible to characterize them, but the characterization of trees from $\mathcal{T}$ could be achievable.

Problem 7.20. Characterize the trees in $\mathcal{T}$.

By the above results, among the stars only $K_{1,4}$, $K_{1,5}$, and $K_{1,6}$ are in $\mathcal{T}$. Recently, the following progress was done by Ghebleh, Kanso, Stevanović [35] regarding the above problem. Note that in [66] it was conjectured that this set is finite.

Theorem 7.21. *$\mathcal{T}$ is infinite.*

Up to our knowledge the trees constructed in [35] may have arbitrary many 3-vertices, but no vertex of higher degree. Possibly, the later can be achieved with combination of all these known constructions. However, we expect that no tree in $\mathcal{T}$ has a vertex of degree exceeding 6 and the number of vertices of degree at least 4 is bounded, and perhaps it is very small, 1 or 2 or so. In order to motivate further research in this direction, we state these expectations as problems.

Conjecture 7.22. *Trees from $\mathcal{T}$ satisfy the following:*

(a) *no tree has a vertex of degree exceeding* 6*;*

(b) *there is a constant* c *such that no tree has more than* c *vertices of degree at least* 4*.*

7.7 Iterated line graphs

As we have seen, there is no non-trivial tree T for which $W(L(T)) = W(T)$ and there are many trees T, satisfying $W(L^2(T)) = W(T)$. However, it is not easy to find a tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$. In [13], Dobrynin, Entringer and Gutman posed the following problem:

$$\textit{Is there any tree } T \textit{ satisfying equality } W(L^i(T)) = W(T) \textit{ for some } i \geq 3? \tag{7.7}$$

Observe that if T is a trivial tree, then $W(L^i(T)) = W(T)$ for every $i \geq 1$, although here the graph $L^i(T)$ is empty. The real question is, if there is a non-trivial tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$. The same question appeared four years later in [23] as a conjecture. Based on the computational experiments, Dobrynin and Mel'nikov expressed their belief that the problem has no non-trivial solution and stated the following conjecture:

$$\textit{There is no tree } T \textit{ satisfying equality } W(T) = W(L^i(T)) \textit{ for any } i \geq 3. \tag{7.8}$$

In a series of papers [59], [60], [61], [62], [63] and [64], conjecture (7.8) was disproved and all solutions of problem (7.7) were found, see also [67]. Let $H_{a,b,c}$ be a tree on $a + b + c + 4$ vertices, out of which two have degree 3, four have degree 1 and the remaining $a + b + c - 2$ vertices have degree 2. The two vertices of degree 3 are connected by a path of length 2. Finally, there are two pendant paths of lengths a and b attached to one vertex of degree 3 and two pendant paths of lengths c and 1 attached to the other vertex of degree 3, see Figure 4 for $H_{3,2,4}$. We have the following statement.

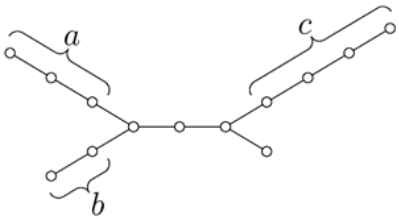

Figure 4: The graph $H_{a,b,c}$.

Theorem 7.23. *For every $j, k \in \mathbb{Z}$ define*

$$\begin{aligned} a &= 128 + 3j^2 + 3k^2 - 3jk + j, \\ b &= 128 + 3j^2 + 3k^2 - 3jk + k, \\ c &= 128 + 3j^2 + 3k^2 - 3jk + j + k. \end{aligned}$$

Then $W(L^3(H_{a,b,c})) = W(H_{a,b,c})$.

Let $\ell \in \{j, k, j+k\}$. Since for every integers j and k the inequality $3j^2 + 3k^2 - 3jk + \ell \geq 0$ holds, we see that $a, b, c \geq 128$ in Theorem 7.23. Therefore, the smallest graph satisfying the assumptions is $H_{128,128,128}$ on 388 vertices, obtained when $j = k = 0$. If we take in mind that there are approximately $7.5 \cdot 10^{175}$ non-isomorphic trees on 388 vertices while the number of atoms in the entire Universe is estimated to be only within the range of 10^{78} to 10^{82}, then to find "a needle in a haystack" is trivially easy job compared to finding a counterexample when using only the brute force of (arbitrarily many) real computers.

The following theorem gives a complete answer to problem (7.7).

Theorem 7.24. *Let T be a tree and $i \geq 3$. Then the equation $W(L^i(T)) = W(T)$ has a solution if and only if $i = 3$ and G is of type $H_{a,b,c}$ as stated in Theorem 7.23.*

We conclude this section with the following problem.

Problem 7.25. Find all graphs (with cycles) G and powers i for which

$$W(L^i(G)) = W(G). \tag{7.9}$$

For $i = 1$ the above problem is very rich with many different solutions, so probably it will not be possible to find all of them. But still, stating it as a problem could serve as a motivation for searching of various graph classes that satisfy the equation. However, we want to emphasize the case $i \geq 2$. In this case the problem is still rich with many solutions, particularly among the trees, but abandoning the class of trees can reduce the solutions significantly. At the moment, cycles are the only known cyclic graphs G for which $W(L^i(G)) = W(G)$ holds for some $i \geq 3$ and we believe that there are no other cyclic graphs satisfying (7.9). This was conjectured independently in [24] and [67].

Conjecture 7.26. *Let $i \geq 3$. There is no graph G, distinct from a cycle and a tree, such that*

$$W(L^i(G)) = W(G).$$

8 Excursion into digraphs

In [69, 70, 71], we have considered the Wiener index of not necessarily strongly connected digraphs. In order to do so, if in a digraph there is no directed path from a vertex u to a vertex v, we follow the convention that

$$d(u, v) = 0, \tag{8.1}$$

which was independently introduced in several studies of directed networks.

A counterpart of the Wiener theorem for *directed trees*, i.e. digraphs whose underlying graphs are trees can be stated in this way.

Theorem 8.1. *Let T be a directed tree with the arc set $A(T)$. Then*

$$W(T) = \sum_{ab \in A(T)} t(a)s(b),$$

where $t(a)$ denotes the number of vertices that can reach a, and $s(b)$ denotes the number of vertices that can be reached by b.

Here we give a counterpart of a relation between the Wiener index and betweenness centrality $B(x)$ for oriented graphs.

Theorem 8.2. *For any digraph D of order n*

$$W(D) = \sum_{x \in V(D)} B(x) + p(D),$$

where $p(D)$ denotes the number of ordered pairs (u, v) such that there exists a directed path from u to v in D.

The above result implies that for strongly connected digraph D on n vertices, we have the relation

$$W(D) = \sum_{x \in V(D)} B(x) + 2\binom{n}{2}.$$

Let $W_{\max}(G)$ and $W_{\min}(G)$ be the maximum possible and the minimum possible, respectively, the Wiener index among all digraphs obtained by orienting the edges of a graph G.

Problem 8.3. For a given graph G find $W_{\max}(G)$ and $W_{\min}(G)$.

The above problem has been considered for strongly connected orientations. Plesník [86] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard. Regarding the problem of finding $W_{\max}(G)$, Plesník and Moon [82, 86] resolved it for complete graphs, under the assumption that the orientation is strongly connected.

We showed [69] that the above mentioned results of Plesník and Moon hold also for non-strongly connected orientations assuming the condition (8.1). One may expect that *for a 2-connected graph G, $W_{\max}(G)$ is attained for some strongly connected orientation.* However, this is not the case as we proved by Θ-graphs $\Theta_{a,b,1}$ for a and b fulfilling certain

conditions. By $\Theta_{a,b,c}$ we denote a graph obtained when two distinct vertices are connected by three internally-vertex-disjoint paths of lengths $a+1$, $b+1$ and $c+1$, respectively. We assume $a \geq b \geq c$ and $b \geq 1$. The orientation of $\Theta_{a,b,c}$ which achieves the maximum Wiener index is not strongly connected if $c \geq 1$. However, we believe that the following holds.

Conjecture 8.4. *Let $a \geq b \geq c$. Then $W_{\max}(\Theta_{a,b,c})$ is attained by an orientation of $\Theta_{a,b,c}$ in which the union of the paths of lengths $a+1$ and $b+1$ forms a directed cycle.*

Analogous results as for Θ-graphs, stating that the orientation of a graph which achieves the maximum Wiener index is not strongly connected, can probably be proved also for other graphs which are not very dense and which admit an orientation with one huge directed cycle without "shortcuts", that is without directed paths shortening the cycle. On the other hand, we were not able to find examples without long induced cycles that makes us wonder if the following holds.

Conjecture 8.5. *Let G be a 2-connected chordal graph. Then $W_{\max}(G)$ is attained by an orientation which is strongly connected.*

Finally, we wonder how hard it is to find $W_{\max}$ and $W_{\min}$.

Problem 8.6. For a given graph G, what is the complexity of finding $W_{\max}(G)$ (resp. $W_{\min}(G)$)? Are these problems NP-hard?

Consider also the following problem for the minimum value.

Conjecture 8.7. *For every graph G, the value $W_{\min}(G)$ is achieved for some acyclic orientation G.*

This is certainly true for bipartite graphs. Namely, by orienting all edges of such a graph G so that the corresponding arcs go from one bipartition to the other, we obtain a digraph D with $W(D) = |E(G)|$. As obviously $W_{\min}(G) \geq |E(G)|$, this case is established.

Now we turn our attention to graphs with higher chromatic number. Our next conjecture is motivated by the Gallai-Hasse-Roy-Vitaver theorem, which states that a number k is the smallest number of colors among all colorings of a graph G if and only if k is the largest number for which every orientation of G contains a simple directed path with k vertices. In other words, the chromatic number $\chi(G)$ is one plus the length of a longest path in a special orientation of the graph which minimizes the length of a longest path. The orientations for which the longest path has the minimum length always include at least one acyclic orientation.

A graph orientation is called *k-coloring-induced*, if it is obtained from some proper k-coloring such that each edge is oriented from the end-vertex with the bigger color to the end-vertex with the smaller color.

Conjecture 8.8. *$W_{\min}(G)$ is achieved for a $\chi(G)$-coloring-induced orientation.*

As mentioned above, Conjecture 8.8 holds for bipartite graphs and trivially it holds for complete graphs. It was shown that holds for graphs with at most one cycle and prisms. By computer it was tested also for the Petersen graph. Observe that Conjecture 8.8 implies Conjecture 8.7.

9 Wiener index for disconnected graphs

Since the formula (1.1) cannot be applied to non-connected graphs, for these graphs we set

$$W(G) = \sum_{\substack{\{x,y\}\subseteq V(G) \\ x-y \text{ path exists in } G}} d(x,y). \tag{9.1}$$

In other words, we ignore pairs of vertices x and y for which the distance $d(u,v)$ can be considered as "infinite" analogously as we ignored such pairs of vertices in the case of digraphs. For example, in [12], the Wiener index has been used in quantitative studies of disconnected hexagonal networks.

Let G be a disconnected graph with components $G_1, G_2, \ldots, G_p$. By (9.1) we get

$$W(G) = W(G_1) + W(G_2) + \cdots + W(G_p)\,.$$

It is interesting to study the problems from the previous sections using the modified definition of Wiener index (9.1). Particularly, we find interesting the analogues of Problems 3.3 and (7.7).

Problem 9.1. For given n, find all values w which are Wiener indices of not necessarily connected graphs (forests) on n vertices.

Let $i \geq 3$. From the proof of Theorem 7.24 one can see that most trees T satisfy $W(L^i(T)) > W(T)$, while paths on $n \geq 2$ vertices satisfy $W(L^i(P_n)) < W(P_n)$. Hence, the following problem is interesting.

Problem 9.2. For $i \geq 3$, find all forests F for which $W(L^i(F)) = W(F)$.

10 Trees with given degree conditions

Lin [77] characterized the trees which maximize and minimize the Wiener index among all trees of given order that have only vertices of odd degrees. An ordering of trees by their smallest Wiener indices for trees of given order that have only vertices of odd degrees was obtained by Furtula, Gutman and Lin [33]. In [32] Furtula further determined the trees with the second up to seventeenth greatest Wiener indices. Lin [77] suggested analogous problems for general graphs.

Problem 10.1. Characterize the graphs with maximal Wiener index in the set of graphs on $2n$ vertices whose vertices are all of odd degree, and in the set of graphs on n vertices whose vertices are all of even degree, respectively.

In [78] Lin characterized the trees which minimize (maximize, respectively) the Wiener index among all trees with given number of vertices of even degree. He proposed the following problems for the class of graphs $E_{n,r}$ of order n with exactly r vertices of even degree, where $r \geq 1$ and $n \equiv r \pmod 2$.

Problem 10.2. Order the trees in $E_{n,r}$ with the smallest or greatest Wiener index.

Problem 10.3. Characterize graphs with maximal and minimal Wiener index in $E_{n,r}$, respectively.

The same author in [79] characterized trees which maximize the Wiener index among all trees of order n with exactly k vertices of maximum degree. For better understanding how the maximum degree vertices influence the Wiener index he proposes to consider analogous problem for the minimum.

Problem 10.4. Characterize the tree(s) with the minimal Wiener index among all trees of order n with exactly k vertices of maximum degree.

Wang [104] and Zhang et al. [96] independently determined the tree that minimizes the Wiener index among trees of given degree sequence. But the following problem from [54, 91, 97] is still open, although it is known for longer time that extremal graphs are caterpillars [92].

Problem 10.5. Which trees maximize the Wiener index among trees of given degree sequence?

11 Few more problems

Here we collect some more problems on Wiener index.

Eulerian graphs. Denote by $\mathcal{E}_n$ the set of all Eulerian graphs of order n. Gutman et al. [39] characterized elements of $\mathcal{E}_n$ having the first few smallest Wiener indices. They proved that for graphs in $\mathcal{E}_n$, C_n attains the maximal value. In addition, they posed a conjecture on the second-maximal Wiener index in $\mathcal{E}_n$.

Conjecture 11.1. *The second-maximal Wiener index between all Eulerian graphs of large enough order n is attained by $C_{n,3}$ (i.e. the graph obtained from disjoint cycles C_{n-2} and C_3 by identifying one vertex in each of them).*

They have also analogous conjecture for small values of n, see [39] for more details.

Fullerene graphs. In [51] the Wiener indices of the $(6, 0)$-nanotubes (tubical fullerenes) is computed. Note that such a graph has $12k$ vertices, for some $k \geq 2$, and the corresponding value of the Wiener index is $48k^3 + 828k - 1632$. These fullerenes have long diameter and consequently big Wiener index. Nevertheless the authors believe that the following may hold.

Conjecture 11.2. *The Wiener index of fullerene graphs on n vertices is of asymptotic order $\theta(n^3)$.*

Wiener index versus Szeged index. Klavžar, Rajapakse and Gutman [56] showed that $\mathrm{Sz}\,(G) \geq W(G)$, and even more, by a result of Dobrynin and Gutman [25], equality $\mathrm{Sz}\,(G) = W(G)$ holds if and only if each block of G is complete. In [80] a classification of graphs with $\eta(G) = \mathrm{Sz}\,(G) - W(G) \leq 3$ is presented. In [81] the authors classify connected graphs which satisfy $\eta(G) = 4$ or 5. Moreover, they state the following conjecture.

Conjecture 11.3. *Let G be a graph of order n with blocks $B_1, \ldots, B_k$ such that none is complete. Let B_i be of order n_i. Then*

$$\mathrm{Sz}\,(G) - W(G) \geq \sum_{i=1}^{k} (2n_i - 6).$$

The difference η was also studied by Klavžar and Nadjafi-Arani [57].

Wiener index of graphs with given matching number. Zhou and Trinajstić [98] determined the minimum Wiener index of connected graphs with $n \geq 5$ vertices and matching number $i \geq 2$, and characterized the extremal graphs. Du and Zhou [28] determined the minimum Wiener indices of trees and unicyclic graphs, respectively, with given number of vertices and matching number. Also, they characterized extremal graphs. For this class of trees Tan [95] et al. determined ordering of trees with the smallest Wiener indices.

Regarding the maximum Wiener index, Dankelmann [7] determined it for connected graphs with $n \geq 5$ vertices and matching number $i \geq 2$, and he characterized the unique extremal graph, which turned out to be a tree. Thus, the maximum Wiener index among trees with given number of vertices and matching number is known, as well as the corresponding unique extremal graph. Finding the maximum Wiener index among unicyclic graphs remains an open problem [28].

Problem 11.4. Find the maximum Wiener index among unicyclic graphs with n vertices and matching number i for $3 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor - 1$.

Graph connectivity. Graphs with higher connectivity have more edges, and henceforth smaller Wiener index. Gutman and Zhang [47] showed that in the class of k-connected graphs on n vertices, the minimum value of Wiener index is attained by $K_k + (K_1 \cup K_{n-k-1})$, i.e. the graph obtained when we connect all vertices of K_k with all vertices of disjoint union of K_1 and K_{n-k-1}. This graph is extremal also in the class of k-edge-connected graphs on n vertices. They pose the following problem.

Problem 11.5. Find the maximum Wiener index among k-connected graphs on n vertices.

Note that P_n is the extremal graph in the class of 1-connected graphs, and C_n is extremal in the class of 2-connected graphs. Of course, similar problem can be posed for k-edge-connected graphs. The authors of [47] ask the following question, which has affirmative answer in the case of the minimum Wiener index.

Problem 11.6. Do the extremal graphs for the maximum Wiener index in the classes of k-connected and k-edge-connected graphs coincide?

Trees and unicyclic graphs with given bipartition. Du [27] considered Wiener index of trees and unicyclic graphs on n vertices with prescribed sizes of bipartitions p and q, where $n = p + q$ and $p \geq q$. He showed that in the case of trees, the extremal graph for the minimum Wiener index is obtained by connecting the centers of disjoint stars $K_{1,p-1}$ and $K_{1,q-1}$, and the extremal graph for the maximum Wiener index is obtained by connecting the end-vertices of a path P_{2q-1} with $\lceil (p-q+1)/2 \rceil$ and $\lfloor (p-q+1)/2 \rfloor$ new vertices, respectively.

Regarding the unicyclic graphs, Du showed that the minimum Wiener index is attained by the graph, which is obtained by connecting $p-2$ vertices to one vertex of a 4-cycle, and connecting $q-2$ vertices to its neighbour on the 4-cycle. Moreover, if $p = q = 3$, then C_6 is also an extremal graph. What remains open, is the maximum value.

Problem 11.7. Find the maximum Wiener index among unicyclic graphs on n vertices with bipartition sizes p and q, where $n = p + q$.

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Mathematical aspects of fullerenes

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Abstract

Fullerene graphs are cubic, 3-connected, planar graphs with exactly 12 pentagonal faces, while all other faces are hexagons. Fullerene graphs are mathematical models of fullerene molecules, i.e., molecules comprised only by carbon atoms different than graphites and diamonds. We give a survey on fullerene graphs from our perspective, which could be also considered as an introduction to this topic. Different types of fullerene graphs are considered, their symmetries, and construction methods. We give an overview of some graph invariants that can possibly correlate with the fullerene molecule stability, such as: the bipartite edge frustration, the independence number, the saturation number, the number of perfect matchings, etc.

Keywords: Fullerene, cubic graph, planar graph, topological indices.

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1 Introduction

The first fullerene molecule, with a structure like a football, was discovered experimentally in 1985 by Kroto et al. [75]. The discovered molecule C_{60}, is comprised only by 60 carbon atoms, and it resembles the Richard Buckminster Fuller's geodetic dome, therefore it was named buckminsterfullerene. Until that moment the only all-carbon structures the modern science was aware of were graphite and diamond. In 1991, the Science magazine pronounced the buckminsterfullerene for the "Molecule of the year", and later in 1996 the discovery of C_{60} was rewarded with the Nobel price for chemistry. Soon after the experimental discovery of the buckminsterfullerene, its existence in the nature was confirmed along with similar structures having 70, 76, 78, 82, 84, 90, 94, or 96 carbon atoms. Each of these all-carbon molecules have polyhedral structure, and all faces of the polyhedron are either pentagons or hexagons. All polyhedral molecules made entirely of carbon atoms are called *fullerenes*. The discovery of the Buckminsterfullerene marked the birth of fullerene chemistry and nanotechnology, but at the same time the fullerenes were studied from different perspectives. The experimental work was paralleled by theoretical investigations, applying the methods of graph theory to the mathematical models of fullerene molecules called *fullerene graphs*.

The study from graph theoretical point of view has been motivated by a search for invariants that will correlate with their stability as a chemical compound. Later graph invariant were used in order to predict the physical and chemical properties of a fullerene compound. A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success [42, 29]. Graph theory invariants that have been considered as possible stability predictors are: the bipartite edge frustration, the independence number, the saturation number, the number of perfect matchings, etc. As a result of those investigations, we have achieved a fairly thorough understanding of fullerene graphs and their properties. However, some problems and questions still remain open [25, 78, 49]. Special place among them have several interesting conjectures made by *Graffiti*, a conjecture making software [41].

2 Fullerene graphs

Fullerenes can also be seen as graphs, vertices represent atoms, and edges represent bonds between atoms. A *fullerene graph* is a 3-connected 3-regular planar graph with only pentagonal and hexagonal faces. In what follows fullerene graphs will be also called fullerenes. Due to Whitney's Theorem (1933) simple planar 3-connected graphs have a unique planar embedding, and therefore the same holds for fullerene graphs. By Euler's formula follows the next property of fullerene graphs.

Proposition 2.1. *The number of pentagonal faces in a fullerene graph is* 12.

The previous result gives no restriction on the number of hexagons. Grünbaum and Motzkin [59] showed that fullerene graphs exist for any number of hexagonal faces except for 1, i.e., they proved the following.

Theorem 2.2. *Fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$.*

Usually in chemistry the fullerene molecule on n vertices is denoted by C_n. Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of the corresponding fullerene molecule. Notice that as

the number of vertices (hexagons) grows, the number of fullerenes increases as well. For example the fullerenes on 20, 24 and 26 vertices have the unique layout, but the fullerene C_{40} has 40 isomers, while the buckminsterfullerene has 1812 different isomers. There is a believe that number of fullerenes on n vertices is of order $\Theta(n^9)$, see Fowler and Manolopoulos in [45] and Cioslowski [22] for more details.

2.1 Types of fullerene graphs

Regarding the position of the pentagons we distinguish several types of fullerene graphs. The fullerene graphs where no two pentagons are adjacent, i.e., each pentagon is surrounded by five hexagons, satisfy the *isolated pentagon rule* or shortly IPR, and they are considered as stable fullerene compounds [76]. Cioslowski [22] stated the following conjecture concerning the number of IPR fullerenes on n vertices.

Conjecture 2.3. *For all $n > 106$, the number of the IPR fullerene isomers with n carbon atoms is bracketed by the total numbers of isomers of the C_{n-50} and C_{n-48} fullerenes.*

If all pentagonal faces are "equally distributed", we obtain fullerene graphs of icosahedral symmetry, whose smallest representative is the dodecahedron. The dodecahedron is the only icosahedral fullerene that does not satisfy the IPR. On the other hand, if the pentagonal faces are grouped in two clusters by six, we obtain nanotubical fullerene graphs. Now, we consider these types of graphs separately.

2.1.1 Icosahedral fullerene graphs

The common feature of all icosahedral fullerenes is their geometrical shape. The simplest icosahedral fullerene graph is the dodecahedron, C_{20}; the next one is the famous buckminsterfullerene C_{60}. Caspar and Klug [21] and Coxeter [23] suggested a method that constructs the duals of the icosahedral fullerene graphs: *geodesic domes*, i.e., triangulations of the sphere with vertices of degree 5 and 6.

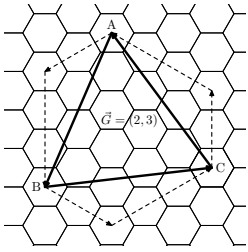

Figure 1: Construction of a $(2,3)$-triangle, a metaface of a $(2,3)$-icosahedral fullerene graph. The vertices of the equilateral triangle ABC are centers of pentagons.

Goldberg [54] observed that all icosahedral fullerene graphs can be obtained by mapping (a part of) the hexagonal grid onto the triangular faces of an icosahedron. He also showed that the number of vertices n in a fullerene of icosahedral symmetry can be determined by two integers i and j by the following equation, conveniently called the *Goldberg equation*

$$n = 20(i^2 + ij + j^2). \tag{2.1}$$

The integers i and j in the Goldberg equation are in fact the components of a two-dimensional *Goldberg vector* $\vec{G} = (i, j)$, sometimes also called *Coxeter coordinates*. We always assume that $0 \leq i \leq j$ and $0 < j$ in order to avoid the mirror effect. This vector determines the distance and positions of the vertices of the (i, j)-triangle in the hexagonal lattice, see Figure 1 for a construction method of an $(2, 3)$-triangle. Precisely 20 such (i, j)-triangles produce an (i, j)-icosahedral fullerene in a manner shown on Figure 2. The vertices of the triangles are centers of the 12 pentagons of the fullerene graph. Observe that the dodecahedron is the $(0, 1)$-icosahedral fullerene, whereas the buckminsterfullerene is the $(1, 1)$-icosahedral fullerene.

If $i = j$ or $j = 0$, then the (i, j)-icosahedral fullerene graph has mirror symmetry, its symmetry group is (isomorphic to) $\mathscr{I}_h$, the full symmetry group of a regular icosahedron. Otherwise, its symmetry group is (isomorphic to) $\mathscr{I}$, the group of rotations of a regular icosahedron.

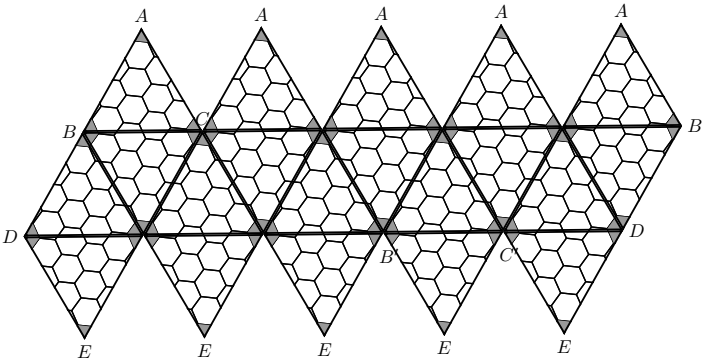

Figure 2: A $(2, 3)$-icosahedral fullerene. Its triangular faces are constructed as on Figure 1. The vertices with the same label coincide.

2.1.2 Fullerenes with other symmetry groups

A symmetry group of a fullerene can contain an m-fold rotational axis only for $m = 2$, 3, 5, and 6. This makes the list of all possible symmetry groups finite; it consists of 36 groups:

$$\begin{aligned}
\text{icosahedral: } & \mathscr{I}_h, \mathscr{I};\\
\text{tetrahedral: } & \mathscr{T}_h, \mathscr{T}_d, \mathscr{T};\\
\text{prismatic: } & \mathscr{D}_{6h}, \mathscr{D}_{5h}, \mathscr{D}_{3h}, \mathscr{D}_{2h};\\
\text{antiprismatic: } & \mathscr{D}_{6d}, \mathscr{D}_{5d}, \mathscr{D}_{3d}, \mathscr{D}_{2d};
\end{aligned}$$

dihedral: $\mathscr{D}_6, \mathscr{D}_5, \mathscr{D}_3, \mathscr{D}_2$;
skewed: $\mathscr{S}_{12}, \mathscr{S}_{10}, \mathscr{S}_6, \mathscr{S}_4$;
rotation-reflection: $\mathscr{C}_{6h}, \mathscr{C}_{5h}, \mathscr{C}_{3h}, \mathscr{C}_{2h}$;
pyramidal: $\mathscr{C}_{6v}, \mathscr{C}_{5v}, \mathscr{C}_{3v}, \mathscr{C}_{2v}$;
rotation only: $\mathscr{C}_6, \mathscr{C}_5, \mathscr{C}_3, \mathscr{C}_2$,
nonaxial: $\mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1$.

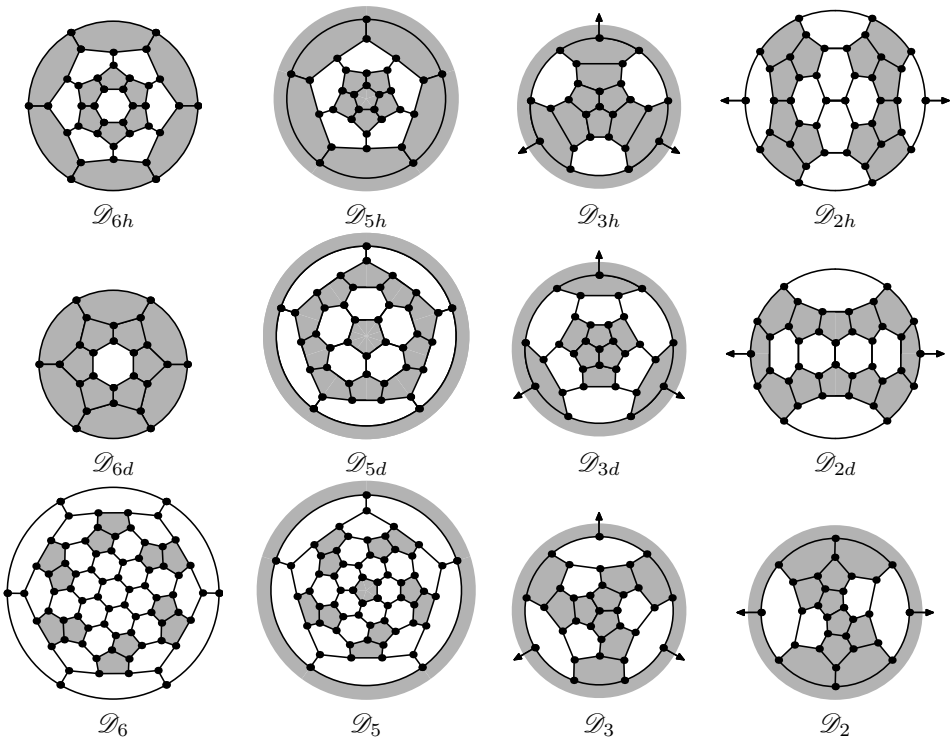

Figure 3: Examples of smallest fullerenes with prismatic, antiprismatic and dihedral symmetry groups.

It was proved that whenever a five-fold or six-fold rotational axis is present, the structure of the fullerene implies a perpendicular twofold rotational axis [46]. This means that the groups $\mathscr{S}_{12}, \mathscr{S}_{10}, \mathscr{C}_{6h}, \mathscr{C}_{5h}, \mathscr{C}_{6v}, \mathscr{C}_{5v}, \mathscr{C}_6$, and $\mathscr{C}_5$ only occur as subgroups of icosahedral, prismatic, antiprismatic, or dihedral groups $\mathscr{I}_h, \mathscr{I}, \mathscr{D}_{6h}, \mathscr{D}_{5h}, \mathscr{D}_{6d}, \mathscr{D}_{5d}, \mathscr{D}_6$, and $\mathscr{D}_5$. The final list of 28 fullerene symmetry groups is therefore:

$$\mathscr{I}_h, \mathscr{I}; \mathscr{T}_h, \mathscr{T}_d, \mathscr{T}; \mathscr{D}_{6h}, \mathscr{D}_{5h}, \mathscr{D}_{3h}, \mathscr{D}_{2h}; \mathscr{D}_{6d}, \mathscr{D}_{5d}, \mathscr{D}_{3d}, \mathscr{D}_{2d};$$
$$\mathscr{D}_6, \mathscr{D}_5, \mathscr{D}_3, \mathscr{D}_2; \mathscr{S}_6, \mathscr{S}_4; \mathscr{C}_{3h}, \mathscr{C}_{2h}; \mathscr{C}_{3v}, \mathscr{C}_{2v}; \mathscr{C}_3, \mathscr{C}_2; \mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1.$$

As shown in [46], fullerenes of each group can be found among all fullerenes on n vertices $20 \leq n \leq 140$. From a fullerene with a given symmetry group, by a leapfrog

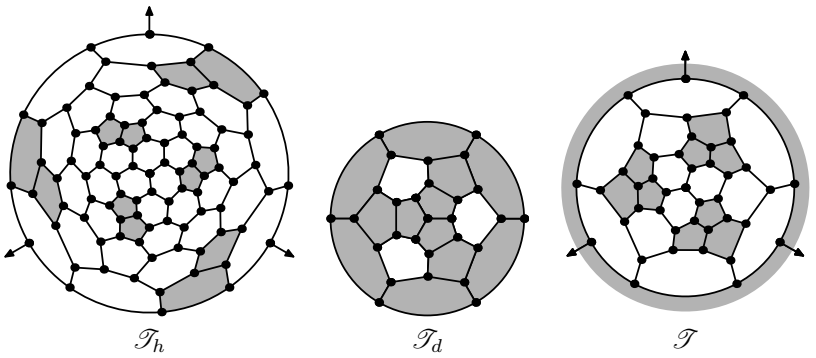

Figure 4: Examples of smallest fullerenes with tetrahedral symmetry groups.

transformation (see Figure 9) one can construct a bigger fullerene with the same symmetry group. Thus, there is an isolated pentagon fullerene for each of the 28 symmetry groups. Symmetry groups for small fullerenes are considered in [8] and [45]. In the later work the smallest fullerene is found for each possible symmetry group, see Figures 3, 4, and 5. All fullerenes with symmetry group of at least 10 elements, i.e., $\mathscr{I}_h$, $\mathscr{I}$, $\mathscr{T}_d$, $\mathscr{T}_h$, $\mathscr{T}$, $\mathscr{D}_{6h}$, $\mathscr{D}_{6d}$, $\mathscr{D}_6$, $\mathscr{D}_{5h}$, $\mathscr{D}_{5d}$ or $\mathscr{D}_5$, are catalogued in [57].

2.1.3 Nanotubical fullerene graphs

While the icosahedral fullerenes have "spherical" shape, there is a class of fullerene graphs of tubular shapes, called *nanotubical* graphs or simply *nanotubes*. From the aspect of mathematics they are not well defined. However, they are cylindrical in shape, with the two ends capped with a subgraph containing six pentagons and possibly some hexagons. The cylindrical part of a nanotube can be obtained by rolling a planar hexagonal grid. The way the grid is wrapped is represented by a Goldberg vector (i, j), called also the *type* of the nanotube. See Figure 6 for an example of the construction of the cylindrical part of a nanotube, also called an *open nanotube*.

For a given nanotube of type (i, j), the sum $i + j$ is called *perimeter* of the nanotube. The smallest possible perimeter is 1, but the open nanotube $(0, 1)$ is not simple. The open nanotubes with perimeter 2 are the nanotubes $(1, 1)$ and $(0, 2)$, but these graphs are not 3-connected. The smallest perimeter such that the graph is 3-connected is 3. On the other side in nature, the thinnest (open) nanotube is $(2, 2)$-nanotube [95]. Since fullerene graphs are cyclically 5-edge connected [28] it is not possible to close an open nanotube with perimeter smaller than 5. Even more there is a cap with six pentagons that closes $(0, 5)$-nanotube, but there are no caps for $(1, 4)$, and $(2, 3)$-nanotube. For all vectors (i, j) with $i + j \geq 6$ there exists a nanotube. A $(0, 5)$-nanotube is depicted on Figure 13.

Notice that the caps of nanotubes are not well defined. One can find (infinitely) many caps for an (i, j)-nanotube by inserting or removing a hexagonal face from a patch with six pentagons that is a subgraph of the nanotube. On the other hand Brinkmann et al. [15] showed that from all possible caps for an (i, j)-nanotube, we can always choose a "nice" cap. We call a cap P *nice* if its boundary can be represented by the sequence $(23)^i(32)^j$, and at least one pentagon is incident to the boundary of P. An edge on the boundary is called i-j *edge* if its end vertices are of degree i and j, respectively. Observe that if

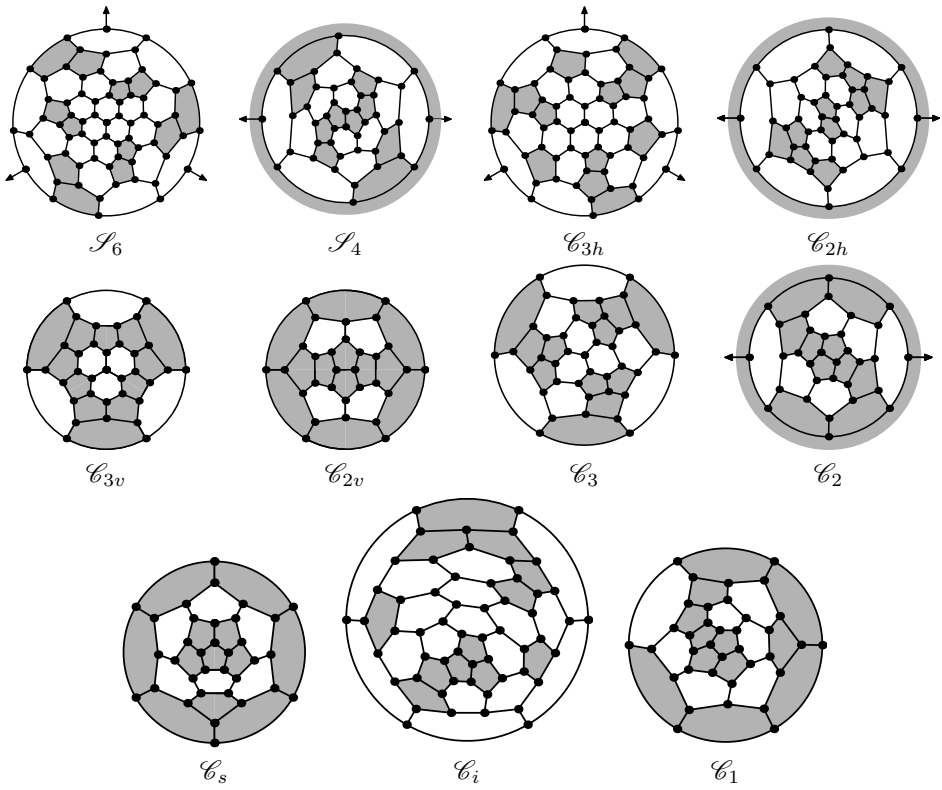

Figure 5: Examples of smallest fullerenes with other symmetry groups.

$i \geq j > 0$ the boundary of a nice cap has precisely one 2-2 edge and one 3-3 edge. If $j = 0$, all the edges on the boundary are 2-3 edges. Starting with any cap, and inserting or removing a finitely many hexagons we can construct a nice cap. If the number of vertices of the nanotube is large enough compared to i and j, we can always choose the two caps such that they are nice and disjoint.

Although the caps are not well defined, a result from Brinkmann et al. [15] provides the existence of "nice" caps.

Theorem 2.4. *Let F be a long enough (i, j)-nanotube. Then, among all possible caps of F, there are caps such that their border can be represented by the sequence $(23)^i(32)^j$.*

Let $\mathcal{P}(i, j)$ be the set of all possible nice caps for an (i, j)-nanotube. A nice cap according to Brinkmann et al. [15] can be transformed into a nice cap according to current definition by inserting less than $i + j$ hexagons. Brinkmann et al. in [15, 13] give a method for constructing all possible nice caps for an (i, j)-nanotubes. Due to this result we have that $\mathcal{P}(i, j)$ is a finite set.

Nanotubes with $i = 0$ are called *zig-zag* nanotubes, and the ones with $i = j$ are called *armchair* nanotubes. These are the only types of nanotubes where the cylindrical part has a mirror symmetry. The buckminsterfullerene C_{60} can be viewed as the smallest nanotube of type $(5, 5)$, see Figure 7. It is also the smallest nanotube with the caps satisfying the IPR.

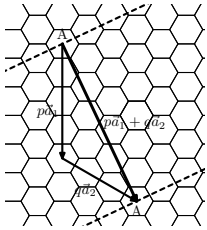

Figure 6: An example of a $(2, 4)$ nanotube. The hexagons denoted equally overlap.

There are IPR nanotubes for all types (i, j) with $i + j \geq 11$ and for $(5, 5)$, $(0, 9)$, $(0, 10)$, $(1, 9)$, and $(2, 8)$.

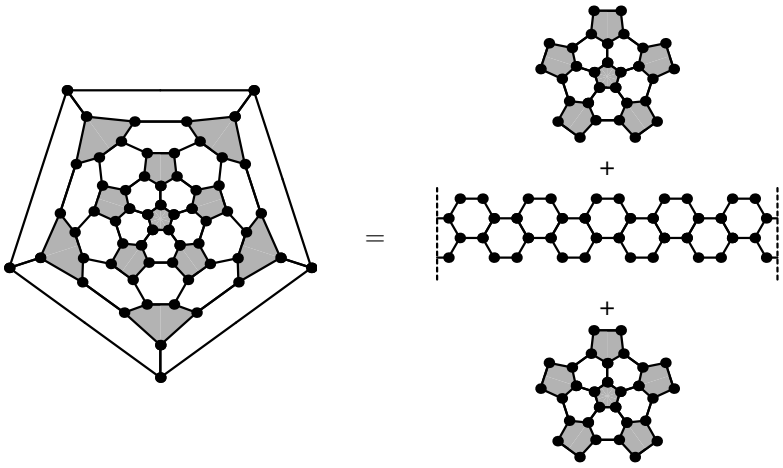

Figure 7: Buckminsterfullerene is the smallest nanotube of type $(5, 5)$.

2.2 Pentagonal-hexagonal patches

Not every fullerene graph is a nanotube. Therefore, subgraphs with similar structure as the nanotube caps were studied in order to facilitate fullerene generation and enumeration.

A *patch* is a 2-connected plane graph with only pentagonal or hexagonal faces, except maybe one (the unbounded) face. All interior vertices of a patch are of degree 3, and all vertices of the exceptional face, which we consider as the *outer* face, are of degree 2 or 3. Let P be a patch with h hexagons and p pentagons. All the vertices incident to the outer face – the *boundary* of P, $b(P)$ – are of degree two or three; let the number of vertices of degree two and three on the border of P be denoted by $n_{2,b}(P)$ and $n_{3,b}(P)$, respectively. Clearly for the size of the border holds $|b(P)| = n_{2,b}(P) + n_{3,b}(P)$. Bornhöft et al. [11], and independently Kardoš et al. [70] give the following relation between the number of vertices on the border and the number of pentagons in the patch.

Proposition 2.5. *Let P be a patch with p pentagons. Then, $|b(P)| = 2n_{3,b}(P) + 6 - p$.*

The last result gives the relation between $n_{2,b}(P)$ and $n_{3,b}(P)$, i.e., $n_{2,b}(P)-n_{3,b}(P)=6-p$. If P is a patch with six pentagons, then the number of vertices of degree 2, and the number of vertices of degree 3 are equal, not depending on the size or shape of P. Observe that if one ring of hexagons around P is added, the length of the border does not change. If P has less than six pentagons, then after adding a ring of hexagons around P, the number of vertices on the outer face will increase, and vice versa if P has more than six pentagons after adding the ring of hexagons the number of vertices on the outer face will decrease. This result confirms that in order to preserve the constant perimeter of the tube in the nanotubes, each cap must have precisely six pentagons.

The degrees of the vertices on the boundary can be regarded as a sequence of length $|b(P)|$ whose elements are 2 and 3.

Inserting a face (pentagon or hexagon) to a patch P means creating a new patch from P with one face more than P such that the new face is incident to at least one edge from the outer face of P. *Removing* a face is an inverse operation of the insertion.

Let the set of all patches with h hexagons and p pentagons be denoted by $\mathcal{P}_{p,h}$. There is a "monotone" method (with respect to the length of the patch boundary) for construction of all possible patches with at most 5 pentagons and given upper bound on the border starting with pentagonal or hexagonal face.

Proposition 2.6. *Each patch P with h hexagons and $p \leq 5$ pentagons can be obtained by adding a pentagon or hexagon to some patch $P' \in \mathcal{P}_{p-1,h} \cup \mathcal{P}_{p,h-1}$ such that $|b(P)| \geq |b(P')|$.*

Bornhöft et al. [11] determined the minimum and maximum possible boundary lengths of pentagon-hexagon patches with h hexagons and $p \leq 6$ pentagons. They show that the minimal boundary length is obtained for a face spiral patch $S_{p,h}$ starting with all p pentagons and continuing with the hexagons. A maximum boundary length is obtained for a patch with a tree as its inner dual. Let $\min(p,h)$ and $\max(p,h)$ be the minimal boundary length and maximal boundary length of a patch with p pentagons and h hexagons respectively. The following theorem from [11] determines which intermediate values can occur as a boundary length of a patch with p pentagons and h hexagons.

Theorem 2.7. *For $p \leq 6$ there exists a patch P with p pentagons and h hexagons and a boundary length b if and only if $\min(p,h) \leq b \leq \max(p,h)$ and $b \equiv p \pmod 2$.*

3 Construction of fullerene graphs

As said before for a fullerene on n vertices, there should be $\Theta(n^9)$ isomers. Searching for an efficient method that constructs all possible isomers on n vertices resulted in several different approaches. Here, we consider the spiral method, Stone-Wales rearrangement, and patch replacement transformation.

By Coxeter and Coldberg constructions, one can construct icosahedral fullerene as described in Section 2. A modification of the same method can be used in order to construct other fullerenes with smaller number of symmetries, but as the number of symmetries decreases, this construction method gets more complicated. When icosahedral fullerenes are constructed all 20 triangles are the same and equilateral, but in the case of fullerenes with lower symmetries the triangles can be isosceles or scalene. This implies that the triangles are not equal, and therefore more parameters are needed, what makes this method compli-

cated. A Coxeter method for construction of tetrahedral and dihedral fullerenes is given in [80].

Fullerenes can be constructed from other fullerenes with two simple techniques; rearranging the faces known as Stone-Wales rearrangement, or by adding two new vertices by Endo-Kroto insertion:

- The *Stone-Wales rearrangement* [90] is a transformation that constructs an isomer of a fullerene graph. This transformation rearranges the pentagons and hexagons in a patch with two pentagons and two hexagons without changing the number of vertices as shown on Figure 8.
- The *Endo-Kroto* $C2$ insertion [38] is a transformation that results a bigger fullerene, i.e., a fullerene on $n+2$ vertices. This transformation is possible only if the fullerene contains a patch as on Figure 8 (c).

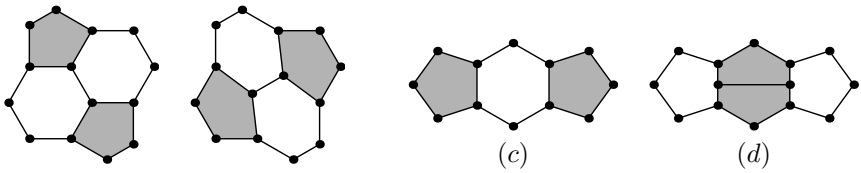

Figure 8: Stone-Wales rearrangement and Endo-Kroto C2 insertion. Stone-Wales rearrangement: replaces the patch (a) by the patch (b). Endo-Kroto C2 insertion: replaces the patch (c) by the patch (d), and inserts two new vertices.

It is easy to see that these two transformations do not allow to construct all the fullerene graphs. Moreover, since the pentagons can be arbitrarily far away from each other, no finite set of transformations can be sufficient to generate all the fullerene graphs. However, later it was shown [47] that these two transformations are special cases of more general transformations based on patch replacement considered later in Subsection 3.2.

Besides these methods, the leapfrog operation of a fullerene graph is another method that produces (bigger) fullerenes. The leapfrog operation of a fullerene graph G, $L(G)$, is usually used for construction of bigger and isolated pentagon fullerenes. The *leapfrog* graph $L(G)$ is obtained by truncating the dual of the fullerene graph G, i.e.,

$$L(G) = \mathrm{Tr}(\mathrm{Du}(G))\,,$$

where $\mathrm{Du}(G)$ is dualization, and $\mathrm{Tr}(G)$ is truncation of the graph G. At the same time leapfrog operation can be viewed as a composition of stelliation $\mathrm{St}(G)$, and dualization $\mathrm{Du}(G)$,

$$L(G) = \mathrm{Du}(\mathrm{St}(G))\,.$$

The operations stellisation, dualization and truncation for a given graph are defined as follows:

- *Stellisation*, $\mathrm{St}(G)$, adds a vertex in the center of each face of a planar graph G, and connects the new vertex with each boundary vertex of the corresponding face. Notice that this operation is also a triangulation.

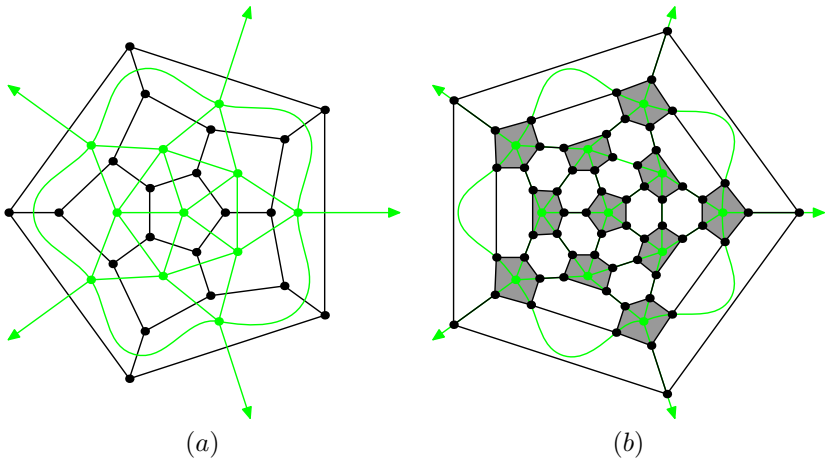

Figure 9: (a) Dodecahedron and its dual graph. (b) Buckminsterfullerene graph obtained with the leapfrog operation on the dodecahedron, truncating dodecahedron's dual.

- *Dualization* of a graph G is the operation that produces the dual of G. Recall that the dual graph of a planar graph G, $\mathrm{Du}(G)$, is a graph with vertices corresponding to each face of G. Two vertices in $\mathrm{Du}(G)$ are adjacent if the corresponding faces in G share an edge.
- *Truncation*, $\mathrm{Tr}(G)$, of a plane graph G is an operation that adds two new vertices on each edge, and then removes the vertices of G. Two vertices are adjacent if they are added to the same edge of G or they belong to two consecutive edges incident to the same vertex of G. The truncation of a polyhedron cuts off one third of each edge at each of both ends.

It is easy to see that $L(G)$ is a fullerene graph on $|2E(G)|$ vertices. Even more $L(G)$ is an isolated pentagon fullerene. The leapfrog graph of the dodecahedron C_{20} is the buckminsterfullerene C_{60}, see Figure 9.

3.1 Spiral method

A *face spiral* is an ordering of the faces of the fullerene graph such that each face in the spiral has a common edge with its predecessor and successor on the spiral (except the first and last faces). The face spiral ordering is shown in Figure 10. A *face spiral sequence* is a sequence of twelve different integers that correspond to the position of the twelve pentagons in the fullerene. The first face in the face spiral has the position 0, see Figure 10. The face spiral sequence can be also be given as a sequence of twelve fives and a number of sixes, and the position of the fives (resp. sixes) corresponds to the position of the pentagons (resp. hexagons) in the spiral ordering.

The spiral conjecture states that the surface of a fullerene polyhedron can be unwrapped as a continuous spiral strip of adjacent faces, i.e., every fullerene has a face spiral. Although each fullerene with at most 176 vertices has at least one face spiral [12] and fullerenes with icosahedral symmetry have a spiral [48], the conjecture is not true in general, since there are unspiral fullerenes with more than 380 vertices [79].

An analog to the face spiral is the vertex spiral. A spiral is a path that starts with an edge and always takes the most left (resp. right) edge not incident with a vertex that is already on the spiral. A *vertex spiral* is the numbering of the fullerene vertices in the order they appear on the spiral. Although the vertex spiral is useful for the nomenclature of the fullerene isomers, it is shown that such paths do not always exist. One such example is the $(2,1)$-icosahedral fullerene C_{80} [45].

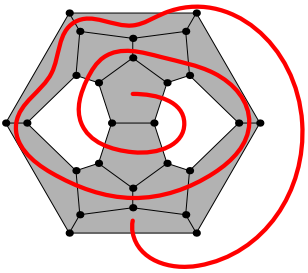

Figure 10: The fullerene on 28 vertices is spiral. The face spiral sequence is $0, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14$, or $5, 6, 5, 6, 5, 5, 5, 5, 5, 5, 5, 5, 6, 5$.

A *spiral method* is a consequence of the spiral conjecture. This method simply generates all the sequences of $\frac{n}{2} - 10$ sixes and twelve fives as a face spiral of pentagons and hexagons and tries to close them into a fullerene on n vertices. This method was the first attempt to construct all fullerenes on n vertices given by Manolopoulos and May [81]. This algorithm is incomplete, i.e., not every fullerene can be generated with it, since not all fullerenes are spiral [79].

3.2 Expansion operations

Expansion is an operation that replaces a patch from the fullerene graph with a bigger one, and the inverse operation is called a *reduction*. These operations are also known as *patch replacement* operations. The simplest patch replacement operations are Stone-Wales rearrangement and Endo-Kroto C2 insertion considered above.

According to the results of Brinkmann et al. [14], no finite set of expansion operations is sufficient to construct all fullerene graphs, starting with a smaller fullerene. Hasheminezhad et al. [62] defined an infinite set of expansions grouped in three classes: L_i for $i \geq 0$, $B_{i,j}$ for $i, j \geq 0$ and F expansion. These three expansions are defined as follows:

- L_i *expansion*. This expansion is defined for $i \geq 0$, and uses a path of length $2i + 3$ that alternate left-right at each of its vertices and connects two pentagonal faces, also known as it zig-zag path. On Figure 11 the expansion L_1 is shown. This expansion starts with a subgraph as shown on Figure $11(a)$, between the two pentagonal faces there is a *ziz-zag* path of length 5, and replaces this subgraph with a subgraph shown on Figure $11(b)$. The L_i expansion adds $i + 2$ new (hexagonal) faces, see Figure 11, i of which are between the two pentagonal faces.
- $B_{i,j}$ *expansion*. Similarly as in the case of L_i expansion, the $B_{i,j}$, $i, j \geq 0$ expansion uses a path of length $2i + 2j + 5$ between two pentagonal faces. This path alternates

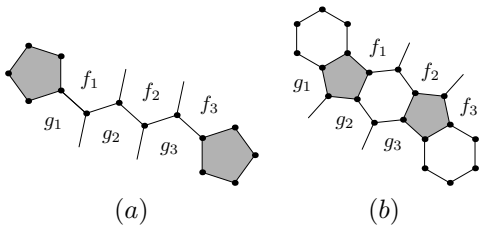

Figure 11: L_1 expansion.

left-right for all the vertices on the path except for the vertices $2i+2$ and $2i+3$, these two vertices keep the same orientation, see Figure $12(a)$. The $B_{i,j}$ expansion adds $i+j+3$ new (hexagonal) faces, $i+j+1$ of which are between the two pentagons. Figure 12 shows the expansion $B_{0,1}$, the subgraph on Figure $12(a)$ is replaced by the subgraph shown on Figure $12(b)$.

- *F expansion.* This expansion adds five hexagonal faces around a cap of a $(5,0)$-nanotube (see Figure 13) comprised only by six pentagons one of which is central. This operation is equivalent to adding an extra ring in a $(5,0)$-nanotube.

Observe that the faces drawn completely or the ones labeled by f_k or g_k are all distinct. Also, the faces that are not drawn completely can be either pentagons or hexagons.

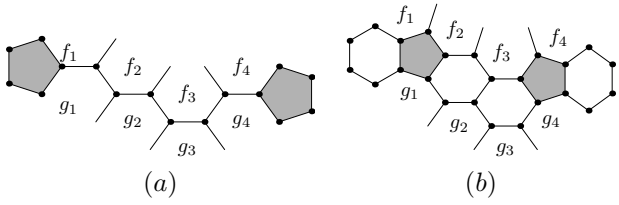

Figure 12: $B_{1,0}$ expansion.

Using this infinite class of expansions Hasheminezhad et al. showed [62] the following.

Theorem 3.1. *Every fullerene except the tetrahedral C_{28} can be constructed from the dodecahedron C_{20} using expansions $L_i, B_{i,j}$, and F. Moreover, if the fullerene is not a $(5,0)$-nanotube, it can be constructed from C_{20} using expansions L_i and $B_{i,j}$.*

Additionally, they showed that all fullerene except the tetrahedral C_{28} (see Figure 4) and a $(5,0)$-nanotube (see Figure 13) with up to 300 vertices can be constructed from the dodecahedron and L_i expansion.

4 Structural properties of fullerene graphs

As we already mentioned earlier, the distribution of the twelve pentagons determine the shape of the fullerene and its structural properties. In this section, we consider several structural properties of fullerenes, such as: cyclic-edge connectivity, diameter, bipartisation, independence number, specter, etc.

4.1 Cyclic connectivity

Fullerene graphs are 3-connected and 3-edge connected, but not 4-connected and 4-edge connected. Here we consider cyclic connectivity. Recall that an edge-cut C of G is *cyclic* if each component of $G - C$ contains a cycle. A graph is *cyclically k-edge-connected* if at least k edges must be removed to disconnect it into two components such that each contains a cycle. A cyclical edge-cut is *trivial* if it isolates a single cycle.

A graph G is *cyclically k-connected* if G can be expressed as a union of two edge disjoint subgraphs G_1 and G_2, both G_1 and G_2 containing cycles, and $|V(G_1) \cap V(G_2)| \geq k$. The *cyclic connectivity* of G is the maximum integer k (if exists) such that G is cyclically k-connected. For fullerene graphs, Došlić [28] proved the following theorem.

Theorem 4.1. *Every fullerene graph F is cyclically 5-edge-connected.*

Clearly, the result is best possible, since each pentagonal face is separated from the rest of the graph by 5 edges. We say that a cyclic 5-edge cut is *trivial*, if it separates only one pentagonal face, otherwise it is not trivial. Kardoš and Škrekovski [71], and Marušic and Kutnar [77] proved that fullerenes which have nontrivial 5-edge-cut are of unique type.

Theorem 4.2. *Nanotubes of type $(0, 5)$ are the only fullerene graphs with a nontrivial cyclic 5-edge-cut.*

A $(0, 5)$-nanotube is depicted on Figure 13. Observe that every nontrivial cyclic 5-edge-cut of a $(0, 5)$-nanotube separates the two caps (containing six pentagonal faces each) from each other.

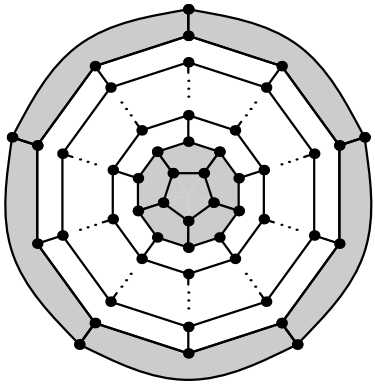

Figure 13: A $(0, 5)$-nanotube.

Similarly, for each nanotube of type (i, j) there are cyclic $(i + j)$-edge cuts separating the two caps from each other. However, the nanotubes are not the only fullerene graphs with such edge-cuts. An example of a fullerene graph, in which the twelve pentagonal faces are partitioned into four clusters containing 1, 2, 4, and 5 pentagons each, is depicted on Figure 14. It is easy to see that this graph is not a nanotube.

With the next theorem Qi and Zhang [96] determined the cyclic connectivity of fullerene graphs.

Theorem 4.3. *Every fullerene graph F is 5-cyclically connected.*

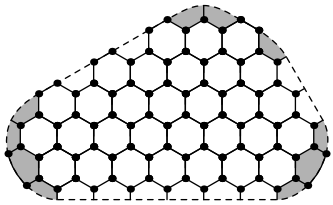

Figure 14: A half of a fullerene graph, which is not a nanotube, but it is possible to separate six pentagonal face from the other six. In order to obtain the whole graph, the depicted graph is to be glued with its mirror copy along the boundary of the outer face such that the 3-regularity is preserved.

4.2 Diameter of fullerene graphs

For large enough fullerene graphs of spherical shape, the diameter $\mathrm{diam}(F)$, the largest distance between any two vertices, is proportional to the radius of the sphere, whereas the number of vertices n is proportional to its surface. Hence, one could expect the diameter of such graphs to be of order $\Theta(\sqrt{n})$. On the other hand, for a nanotubical fullerene graph of type (i, j), the diameter $\mathrm{diam}(F)$ is proportional to the length of the cylindrical part of the graph, whereas the number of vertices n is proportional to the product of the length of the tube and its circumference $i + j$. In this case, one could expect the diameter of such graphs is of order $\Theta(n)$.

A well known result on the degree-diameter problem states that the number of vertices in a planar graph with maximum degree 3 grows at most exponentially with diameter [50]. Let G be a planar graph with maximum degree 3. Then, G has at most

$$2^{\mathrm{diam}(G)+1} - 1$$

vertices. This results gives a logarithmic lower bound on the diameter in terms of the number of vertices. The logarithmic character of the bound can be attributed to the presence of faces of large size. It would be reasonable to expect that better lower bounds exist for polyhedral graphs with bounded face size.

As mentioned above, fullerene graphs only have pentagonal and hexagonal faces, and this fact can be used to show [2] that if F is a fullerene graph on n vertices, then $\mathrm{diam}(F) \geq \sqrt{24n - 15}/6 - 1/2$.

For fullerene graphs with full icosahedral symmetry the diameter has been determined exactly in [6].

Theorem 4.4. *The diameter of a fullerene graph with n vertices is of order $\Omega(\sqrt{n})$. If F is a full icosahedral symmetry fullerene (i, j), $0 \leq i \leq j$, $0 < j$, then* $\mathrm{diam}(F) = 4j+6j-1$.

Observe that an icosahedral fullerene (i, j) has full icosahedral symmetry if $i = 0$ or $i = j$. By (2.1) we have that if $i = 0$, then $\mathrm{diam}(F) = \sqrt{9n/5} - 1$, and if $i = j$, then $\mathrm{diam}(F) = \sqrt{5n/3}-1$. As the geometrical shape of these fullerenes is "almost spherical" we believed that they have the smallest diameter, so we conjectured that the diameter of any fullerene graph on n vertices is at least $\lfloor\sqrt{5n/3}\rfloor - 1$. Nicodemos and Stehlík [84] found an infinite class of fullerene graphs of diameter at most $\sqrt{4n/3}$, where n is the number of vertices, and disproved this conjecture.

As far as the upper bound is concerned, the nanotubes of small circumference are the extremal graphs, as says the following theorem [2].

Theorem 4.5. *Let F be a fullerene graph with n vertices that is not a $(5,0)$-nanotube. Then,*

$$\operatorname{diam}(F) \leq \frac{n}{6} + \frac{5}{2}\,.$$

If F is a $(5,0)$-nanotube on $n = 30, 40$ vertices, then $\operatorname{diam}(F) = n/5$, and if $n \geq 50$, then $\operatorname{diam}(F) = n/5 - 1$.

4.3 Bipartisation of fullerenes

The *bipartite edge frustration* of a graph G, denoted by $\varphi(G)$, is the smallest cardinality of a set of edges of G that needs to be removed from G in order to obtain a bipartite spanning subgraph. Bipartite edge frustration of a fullerene graph G can be efficiently computed by finding a minimum-weight perfect matching in the pentagon-distance graph of G [35]. In the same reference it was shown that $\varphi(G) \geq 6$ for any fullerene graph G and that this bound is sharp.

If the fullerene graph satisfies the isolated pentagon rule, then $\varphi(G) \geq 12$. Furthermore, it was shown that the bipartite edge frustration of fullerene graphs with icosahedral symmetry is proportional to the square root of the number of vertices (see [35, Proposition 11 and Corollary 12]). The numerical computations suggested that it cannot behave worse than that, and prompted the authors conjecture that the independence number of a fullerene graph on n vertices is at most $\sqrt{12n/5}$.

First, Dvořák, Lidický, and Škrekovski [37] proved a theorem with a weaker multiplicative constant. Later Faria, Klein and Stehlík [43] proved the following celebrating result.

Theorem 4.6. *Let G be a fullerene graph with n vertices. Then, $\varphi(G) \leq \sqrt{\frac{12}{5}n}$. Moreover, the equality holds if and only if G is an (i,i)-icosahedral fullerene graph.*

The bipartite edge frustration is considered for a possible predictor of molecular stability: If $\varphi(G)$ is close to the upper bound, it means that there is no way to partition the 12 pentagonal faces into six pairs in such a way that the pentagons within the pairs are close to each other.

On the other side, a small value for $\varphi(G)$ does not say much about the structure of the fullerene graph and about the shape of the molecule. The smallest possible value of $\varphi(G)$ is attained for any fullerene graph where the 12 pentagonal faces can be partitioned into 6 pairs, adjacent to each other. Those pairs of pentagonal faces can be distributed in a widely varied list of possible configurations, leading to molecules of different shapes, including nanotubes of all possible types.

4.4 Independence number

Another invariant tested as a possible stability predictor is the independence number [42]. A set $I \subseteq V(G)$ is *independent* if no two vertices from I are adjacent in G. The cardinality of any largest independent set in G is called the *independence number* of G and denoted by $\alpha(G)$.

Independence number of fullerene graphs attracted attention also in the context of study of independent sets as possible models for addition of bulky segregated groups such as free radicals or halogen atoms [10]. Sharp upper bounds on the independence number of $n/2 - 2$ for general fullerenes and $n/2 - 4$ for those with isolated pentagons follow by simple counting argument [44]. Lower bounds were gradually improved from (almost) trivial $\alpha(G) \geq n/3$ valid for all 3-chromatic graphs to $\alpha(G) \geq 3n/8$ [63] valid for all triangle-free planar cubic graphs. A better lower bound of type $\alpha(G) \geq n/2 - C\sqrt{n}$, where C is some constant, was first established for icosahedral fullerenes [58].

This observation was formalized in a pair of conjectures in a recent Ph.D. thesis by Daugherty ([25, pp. 96]). The first one states that the minimum possible independence number is achieved on the icosahedral fullerenes that also figure prominently in Theorem 4.6. The second one [25, Conjecture 5.5.2] states the precise form of the conjectured lower bound, i.e., states that $\alpha(G) \geq n/2 - 3\sqrt{n/15}$. Notice that the constant $3/\sqrt{15}$ is exactly one half of the constant $\sqrt{12/5}$ from Theorem 4.6.

The first result that approaches the conjecture is due to Andova et al. [2]. They showed that $\alpha(G) \geq n/2 - 78.58\sqrt{n}$ for a graph G on n vertices. Finally, using Theorem 4.6, this conjecture was confirmed [43].

Theorem 4.7. *Let G be a fullerene graph with n vertices. Then,*

$$\alpha(G) \geq \frac{n}{2} - \sqrt{\frac{3}{5}n}\,.$$

Moreover, the equality holds if and only if G is an (i,i)-icosahedral fullerene graph.

Similarly to the bipartite edge frustration, a small value of independence number means that the corresponding polyhedron/molecule is close to being of a spherical shape. On the other hand, a value of $\alpha(G)$ close to $n/2$ does not say much about the structure or the shape of the molecule.

The relations between diameter and the independence number of fullerenes appear in Conjecture 912 of Graffiti [49]. This conjecture was first established in [2] for large fullerenes using Theorem 4.5 and the lower bound on the independence number established in [2]. Later this theorem was solved by Faria et al. [51] for all fullerenes, which confirms the following nice relation.

Theorem 4.8. *If G is a fullerene graph, then*

$$\alpha(G) \geq 2(\mathrm{diam}(G) - 1).$$

4.5 Spectra of fullerene graphs

An *eigenvalue* of a graph G is an eigenvalue of its adjacency matrix $\mathbf{A}(G)$. The set of all eigenvalues of a graph is called its *spectrum*. We denote the eigenvalues of G by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The fullerene graph G is 3-regular, and therefore the largest eigenvalue λ_1 is always equal to 3. Since the fullerene graphs are not bipartite, the smallest eigenvalue is greater than -3. In this section, we consider the bounds for the smallest eigenvalue λ_n and the second largest eigenvalue of a fullerene graph.

The fullerenes can be arranged in decreasing order by their smallest eigenvalue. This arrangement is known as *the smallest-eigenvalue order*. It should be noted that there are nonisomorphic fullerenes with the same smallest eigenvalue. Fowler et al. [51] gave the first several fullerene graphs of the smallest-eigenvalue order.

Theorem 4.9. *Amongst all fullerenes the smallest eigenvalue is maximal for the dodecahedron.*

The eigenvalues of the dodecahedron [24] are $3, \sqrt{5}, 1, 0, -2, -\sqrt{5}$ with the multiplicity, 1, 3, 5, 4, 4, 3, respectively, thus the smallest eigenvalue is $-\sqrt{5}$. Observe that there are unique fullerene graphs on 24 and 26 vertices, while there are two non-isomorphic fullerene graphs on 28 vertices, one of which is called tetrahedral fullerene. The smallest eigenvalue of these three fullerene graphs is $-1-\sqrt{2}$ with multiplicity 2, 3, and 4 respectively.

Theorem 4.10. *The smallest eigenvalue of a fullerene with at least* 28 *vertices, which is not isomorphic to the tetrahedral fullerene on* 28 *vertices is less than* $-1-\sqrt{2}$.

The smallest eigenvalue of the second non-tetrahedral fullerene on 28 vertices is ≈ -2.5247.

The above results state that the dodecahedron is the first fullerene in the smallest-eigenvalue order of fullerenes, followed by the unique fullerenes on 24 and 26 vertices and the tetrahedral fullerene on 28 vertices. In the class of isolated pentagon fullerenes the buckminsterfullerene C_{60} has the smallest eigenvalue [51].

Theorem 4.11. *The icosahedral* C_{60} *has maximum smallest eigenvalue amongst all isolated pentagon fullerenes.*

This result lead to the following result [36]

Theorem 4.12. *Among all fullerene graphs with at least* 60 *vertices, the buckminsterfullerene has the maximum smallest eigenvalue.*

Theorem 4.6 and Theorem 4.12 are connected by a result on Laplacian eigenvalues from the monograph by Godsil and Royle ([52, pp. 293]).

Theorem 4.13. *Let* G *be a graph with* n *vertices. Then* $\mathrm{bip}(G) \leq \frac{n}{4}\mu_\infty(G)$.

Here $\mathrm{bip}(G)$ denotes the maximum number of edges in a bipartite spanning subgraph of G (hence the number of edges in G minus the bipartite edge frustration), and $\mu_\infty(G)$ is the largest Laplacian eigenvalue of G.

Recall that the smallest eigenvalue $\lambda_n(G)$ of a 3-regular graph G and the largest Laplacian eigenvalue $\mu_\infty(G)$ of G are related by the following relation ([52, pp. 280]):

$$\lambda_n(G) = 3 - \mu_\infty(G).$$

By plugging this into Theorem 4.13 and noting that $\mathrm{bip}(G) = 3n/2n - \varphi(G)$ we obtain an upper bound on $\lambda_n(G)$ in terms of the bipartite edge frustration of G of the form $\lambda_n(G) \leq -3 + 4\varphi(G)/n$. By taking into account the upper bound of $\varphi(G)$ from Theorem 4.6 we immediately obtain the following upper bound on the smallest eigenvalue of a fullerene graph with n vertices [43].

Theorem 4.14. *Let* G *be a fullerene graph with* n *vertices. Then,*

$$\lambda_n(G) \leq -3 + 8\sqrt{\frac{3}{5}n}\,.$$

The difference $s(G) = 3 - \lambda_2$ is known as the *separator* of G or as a *spectral cap*. Caporossi and Stevanović [89] showed that the separator $3 - \lambda_2$ of a fullerene graph is at most 1. Even more, using the well known interlacing theorem about the spectra of a matrix, they proved that the separator of a fullerene with n vertices is at most $1 - 3/n$. These two results were conjectured by Graffiti. Related to this Došlić and Rèti [34] proved the following theorem:

Theorem 4.15. *Let G be a fullerene graph on n vertices. Then, the separator of G is at most $24/n$.*

5 Matchings

5.1 Number of perfect matchings

Since all carbon atoms are 4-valent, for every atom precisely one of the three bonds should be doubled. Such a set of double bonds is called a *Kekulé structure* in a fullerene. It corresponds to the notion of perfect matchings in fullerene graphs: a *matching* in a graph G is a set of edges of G such that no two edges in M share an end-vertex. A matching M is *perfect* if any vertex of G is incident with an edge of M.

The computation of the number of perfect matchings in typical fullerene graphs with a small number of vertices indicates that this number should grow exponentially with n [30]. The first general lower bounds for the number of perfect matchings in fullerene graphs were linear in the number of vertices [26, 27, 99]. The best of them asserts that a fullerene graph with n vertices has at least $\lceil 3(n+2)/4 \rceil$ different perfect matchings [99]. The number of perfect matchings was proved to be exponential for several special classes of fullerene graphs: $(0, 5)$-nanotubes [77], icosahedral fullerenes [30] or those who are obtained using specific operations [32], before the following general result from [69].

Theorem 5.1. *Let G be a fullerene graph with n vertices that has no non-trivial cyclic 5-edge-cut. The number of perfect matchings of G is at least $2^{\frac{n-380}{61}}$.*

The idea of the proof is to find a perfect matching with $(n - 380)/61$ non-adjacent resonant hexagons. For such a perfect matching, any subset of the set of resonant hexagons can be switched to obtain a different perfect matching. The bound from Theorem 5.1 is not optimal. Doslić [33] studied the number of perfect matchings in leapfrog fullerene graphs, and found the following.

Theorem 5.2. *Let G be a leapfrog fullerene on n vertices. If n is divisible by 4, then the number of perfect matchings is at least $F_{n/4+1} + n/2$, otherwise the number of perfect matchings is at least $F_{\lceil n/4 \rceil+1} + 1$, where F_n denotes the n-th Fibonacci number.*

A little is known about the relationship between the number of perfect matchings of a fullerene graph and the shape of the corresponding molecule.

5.2 Resonance in fullerene graphs

Let M be a perfect matching in a fullerene graph G. A hexagonal face is *resonant* if it is incident with three edges in M. A set of disjoint resonant hexagons of G is called *resonant pattern* (also known as *sextet pattern*). A fullerene graph is *k-resonant* if any i, $0 < i \leq k$, disjoint hexagons form a resonant pattern.

Ye et al. [94] showed that every fullerene graph is 1-resonant. Even more, they proved that every fullerene leapfrog graph is 2-resonant. Since every leapfrog fullerene graph is IPR fullerene, they naturally ask if all IPR fullerenes are 2-resonant. Kaiser et al. [67] answered this question.

Theorem 5.3. *Every IPR fullerene graph is 2-resonant.*

The fullerene graphs in general are not 3-resonant, i.e., only "small" fullerenes are 3-resonant [94].

Theorem 5.4. *If a fullerene graph G is 3-resonant, then $|V(G)| \leq 60$.*

The maximum size of a set of resonant hexagons in G is called the *Clar number* of G, and denoted by $c(G)$. Zhang and Ye [98] showed the following.

Theorem 5.5. *A Clar number on fullerene graph with n vertices is at most* $\left\lfloor \dfrac{n-12}{6} \right\rfloor$.

They also showed that there are infinitely many fullerene graphs that attain this upper bound; among all 1812 fullerenes on 60 vertices there are exactly 18 whose Clar number is 8 (including the buckminsterfullerene). This upper bound is achieved for C_{70}, and for infinitely many armchair and zig-zag nanotubes.

The *sextet polynomial* is defined in [64, 85] as $B_G(x) = \sum_{k=0}^{m} r(G,k)x^k$, where $r(G,k)$ is the number of resonant patterns of G of size k, and m is the Clar number of G. Sereni and Stehlík [88] proved a conjecture made by Zhang and He [97] that for every fullerene graph the value $B_G(1)$ is smaller than the number of perfect matchings in the graph.

A k-regular spanning subgraph of a graph G is called k-factor of G. A fullerene that has a 2-factor form by the boundaries of it faces is called fullerene of *Clar type*. It is known that if a fullerene is of Clar type, then it has isolated pentagons, i.e., it is a IPR fullerene, see Pisanski [86]. It also holds that the number of fullerenes with n vertices is equal to the number of Clar type fullerenes with $3n$ vertices.

5.3 Saturation number

The last invariant considered here, the saturation number, is also related to matchings. The existence of perfect (and hence maximum) matchings in fullerene graphs has been established long time ago, and there are many papers concerned with their structural and enumerative properties [27, 69, 72]. Another class of matchings, the maximal matchings, have received much less attention so far, in spite of being potentially useful as mathematical models of dimer absorption. A matching M is *maximal* if it cannot be extended to a larger matching of G. The *saturation number* of G, denoted by $s(G)$, is the cardinality of any smallest maximal matching of G. The saturation number of fullerene graphs was studied in [27, 36]. Using the lower bound on the diameter the bounds on the saturation number were improved in [2]. Still that was not the best possible bound of the saturation number of the fullerene graphs. In [3] we prove that the saturation number for fullerenes on n vertices is essentially $n/3$.

Theorem 5.6. *Let F be a fullerene graph on n vertices. Then,*

$$\frac{n}{3} - 2 \leq s(F) \leq \frac{n}{3} + O(\sqrt{n})\,.$$

In order to prove the lower bound of this theorem we used the discharging method. For the upper bound we first used Theorem 4.6, and obtained a bipartite graph F'. Later, we established that F' is an induced subgraph of a hexagonal lattice, or an induced subgraph of a hexagonal tube (defined as on Figure 6). Then we defined a maximal matching on F' such that from each hexagon precisely four vertices are covered by the matching.

6 Hamiltonicity of fullerene graphs

A cycle C of a graph G is *hamiltonian* if C passes through every vertex of G. Tait [91] in 1884 conjectured that every 3-connected planar cubic graph has a Hamiltonian cycle. Later Tutte [92] showed that this conjecture is false. Back in 1974, Grünbaum and Zaks [60] asked whether 3-connected planar graphs with faces of size p and q, $q > p$ are Hamiltonian for any p and q. It was shown that cubic polyhedral graphs with faces of sizes 3 and 6, or faces of size 4 and 6 are hamiltonian [55, 56].

However, Tait's Conjecture still remained open for fullerene graphs. Barnette [9] made a more general conjecture, he conjectured that all cubic polyhedral graphs with maximum face size at most six having no triangles and no two adjacent quadrangles are hamiltonian. He reduced the conjecture to the case of cubic polyhedral graphs with maximum face size at most six with no triangles nor two adjacent quadrangles, are also known as *Barnette graphs*. In order to attack the hamiltonicity conjecture for fullerene graphs, long cycles in fullerenes were studied [40, 66, 74, 39]. Marušič [82] showed that for every fullerene graph, its leapfrog fullerene contains a hamiltonian path. Kardoš [68] on the other side worked on the more general conjecture, Barnette's Conjecture, and proved the following.

Theorem 6.1. *Let G be a 3-connected planar cubic graph with faces of size at most 6. Then G is hamiltonian.*

This theorem directly implies implies Taits's Conjecture on fullerene graphs. For the proof of this theorem a more general definition of a 2-factor was introduced, in this case a 2-*factor* is any spanning subgraph F of a Barnette graph G such that each component of F is a connected regular graph of degree 1 or 2, i.e., an isolated edge (considered here as a 2-cycle) or a cycle. The proof has several major steps. First a 2-factor with many resonant hexagons is found. Then the 2-factor is modified in order to have an odd number of cycles if needed. Finally the resonant hexagons are used to glue all the cycles into a single cycle, i.e., to construct a Hamiltonian cycle. In order to achieve this, a computer program was used.

7 Fullerene graphs and topological indices

Topological indices or *molecular descriptors* are graph invariants than can correlate with a physical or chemical property of a molecule presented as a graph. The first topological index was introduced by Harry Wiener [93], back in 1947, and afterwards a list of descriptors were introduced such as: the Randić index, the Hosoya index, the Estrada index, the Zagreb Indices, the Szeged index, the Balaban index, etc.

Let G be a graph and $u \in V(G)$. Then the *distance* of u is defined as $W_G(u) = \sum_{v \in V(G)} d_G(u, v)$, where $d(u, v)$ denotes the distance between the vertices u and v. The *Wiener* index [93] of a graph G, $W(G)$, is the sum of all the distances in G, i.e., $W(G) = \sum_{u,v \in V(G)} d(u, v) = \frac{1}{2} \sum_{u \in V(G)} W_G(u)$. Hua et al. [65] considered a Wiener

dimension of one type of $(0,6)$-nanotubes, and based on the results they made the following conjecture.

Conjecture 7.1. *Let G be a fullerene with n vertices. Then, the Wiener index of G, $W(G)$, is of order $\Theta(n^3)$.*

The bound of the Wiener index for nanotubical fullerenes are determined in [4]. Suppose that $\{W_G(u) \mid u \in V(G)\} = \{d_1, d_2, \ldots, d_k\}$. Assume in addition that G contains t_i pairs of vertices on distance d_i, $1 \leq i \leq k$. We say that the *Wiener dimension* $\dim_{\mathrm{W}}(G)$ of G is k. Alizadeh et al. [1] have shown that the $(0,5)$-nanotubical fullerene graph on $10k$ ($k \geq 3$) vertices has the Wiener dimension k. As a consequence the Wiener index of these fullerenes was obtained. This result confirms Conjecture 7.1 for $(0,5)$-nanotubes.

Another topological index based on the distance is the *Balaban* index. This index for a graph G is defined [7] as

$$\mathrm{J}(G) = \frac{m}{m-n+2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}},$$

where n and m are the number of vertices and edges, respectively.

Knor et al. [73] studied the Balaban index for cubic graphs, and determined that the Balaban index tends to zero as the number of vertices increases. More precisely, they showed the following.

Theorem 7.2. *Let G be a a fullerene graph on n vertices, $n \geq 60$. Then $\mathrm{J}(G) \leq 25/\sqrt{n}$.*

The last result means that Balaban index does not distinguish well the fullerene graphs when they are sufficiently large. Determining the distances on an infinite hexagonal tube [5] the authors [4] show that this approach is much faster for nanotubes.

Let G be a fullerene graph and $e = uv$ an edge in G. Let $n_v(e)$ be the number of edges closer to v than to the vertex u. Similarly, let $n_0(e)$ be the number of equidistant vertices form u and v. The following indices are base on these invariants. The PI index is defined by $\mathrm{PI}(G) = \sum_{e=uv}[n_v(e) + n_u(e)]$. The *Szeged* index is topological index introduced by Gutman [61], defined as $\mathrm{Sz}(G) = \sum_{e=uv} n_v(e)n_u(e)$. Randić [87] modified this topological index in order to find better applications in chemistry, and the new index was named *revised Szeged* index. This index is defined by $\mathrm{Sz}^*(G) = \sum_{e=uv}[n_v(e) + n_0(e)/2] \cdot [n_u(e) + n_0(e)/2]$. Mottaaghi and Mehranian [83] studied PI, Szeged and revised Szeged index for a nanotubical IPR fullerenes on $60 + 12n$, $n \in \mathbb{N}$, vertices, and found that these indices are of order $\Theta(n^2)$, $\Theta(n^3)$ and $\Theta(n^3)$, respectively.

8 Fullerene generating programs

There are several programs available that can generate fullerenes. *Buckygen* is a program by Brinkmann, McKay and Goedgebeur for the efficient generation of all nonisomorphic fullerenes. It generates triangulations where all vertices have degree 5 or 6, or its dual representation-fullerene graphs. This program can also be used to generate isolated pentagon rule (IPR) fullerenes. *SaGe* generates fullerene graphs using the Buckygen generator. The algorithms used in the Buckygen generator are described in [16, 53]. Programs for generation of certain types of graphs are *Plantri* and *Fullgen*, both created by Brinkmann and McKay. These programs are based on the papers [17, 19, 20]. *GaGe* [18] is an Open

Source program implemented in C and Java, that generates graphs of different types. This program allows to view selected graphs in various ways or save them in several formats. *House of Graphs* provides a count lists of fullerene, fullerenes without a spiral starting at pentagon, and fullerenes without a spiral. These fullerenes are generated with Buckygen and Fullgen.

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On maximum signless Laplacian Estrada index of graphs with given parameters

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Abstract

For a simple graph G on n vertices, the signless Laplacian Estrada index is defined as $SLEE(G) = \sum_{i=1}^{n} e^{q_i}$, where $q_1, q_2, \ldots, q_n$ are the eigenvalues of the signless Laplacian matrix of G. In this paper, the unique graph on n vertices with maximum signless Laplacian Estrada index is determined among graphs with given number of cut edges, pendent vertices, (vertex) connectivity and edge connectivity, respectively.

Keywords: Signless Laplacian Estrada index, semi-edge walk, cut edge, vertex connectivity, edge connectivity.

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1 Introduction

Throughout this paper, each graph, say G, is simple with its vertex and edge sets $V(G)$ and $E(G)$, respectively. If $|V(G)| = n$, then G is considered as an n-*vertex* graph. Let u and v be two vertices of G. We say that u is a *neighbor* of v, if they are joined together in G. The

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number of neighbors of v in G is called the *degree* of v, and denoted by $d_G(v)$. The vertex v of G is referred to as a *pendent vertex* if it has only one neighbor (i.e. $d_G(v) = 1$). A *cut edge* of a (connected) graph G is an edge whose deletion disconnects G. The *vertex* (resp. *edge*) *connectivity* of G is the minimum number of vertices (resp. edges) which need to be removed to disconnect G or convert it to a single vertex.

Let $\mathbf{A}(G)$ be the adjacency matrix of G and $\mathbf{D}(G) = [d_{ij}]_{n\times n}$ be the diagonal matrix, where the element d_{ij} is equal to $d_G(v_i)$ if $i = j$, and 0 otherwise. The *Laplacian matrix* and *signless Laplacian matrix* of G are denoted by $\mathbf{L}(G)$ and $\mathbf{Q}(G)$, respectively, where $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ and $\mathbf{Q}(G) = \mathbf{D}(G) + \mathbf{A}(G)$ (see [7,22]). We represent the eigenvalues of $\mathbf{A}(G)$, $\mathbf{L}(G)$ and $\mathbf{Q}(G)$ by $\lambda_1, \lambda_2, \ldots, \lambda_n$; $\mu_1, \mu_2, \ldots, \mu_n$; and $q_1, q_2, \ldots, q_n$, respectively.

Estrada [11,12], for the first time, defined a graph-spectrum-based invariant and named it *Estrada index*, which is as follows:

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

Fath-Tabar et al. [13] proposed the *Laplacian Estrada index* (after here LEE), in full analogy with Estrada index as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

Estrada and Laplacian Estrada indices have been studied in a large variety of problems. In the mathematical literature, there are two types of problems in almost all papers researching on such indices: finding bounds for the index (e.g. [1, 4, 16, 20, 24]), and determining extremal graphs with respect to the index (e.g. [10,21,23,25]).

Ayyaswamy et al. [2] defined the *signless Laplacian Estrada index* ($SLEE$) as

$$SLEE(G) = \sum_{i=1}^{n} e^{q_i}.$$

They also established lower and upper bounds for $SLEE$ in terms of the number of vertices and edges. They showed that for any graph G on n vertices and m edges,

$$\sqrt{n + 4\,m + n\,(n-1)\,e^{\frac{4\,m}{n}}} \leq SLEE(G) \leq n - 1 + e^{\sqrt{(n^2-n+2\,m)m}}$$

with equality on both sides if and only if G is empty. In the same sense, Binthiya et al. [5] established upper bound for $SLEE$ in terms of the vertex connectivity of graph and the specific corresponding extremal graph. They find that [5, Theorem 3.1.] for each (n, m)-graph G with vertex connectivity κ,

$$SLEE(G) \leq \kappa\, e^{n-2} + (n - \kappa - 2)\, e^{n-3} + e^{2\,n+\kappa-4}.$$

It is well-known that the Laplacian and signless Laplacian spectra of bipartite graphs coincide (see [14,15]). Thus, for a bipartite graph G, $SLEE(G) = LEE(G)$. Chemically, since the vast majority of molecular graphs are bipartite, we can use the provided statements in $SLEE$ for LEE, and vice versa. However, the interesting case occurs when $SLEE$

and LEE differ, namely, in fullerenes, fluoranthenes and other non-alternant conjugated species [3, 9, 17–19].

Moreover, Cvetković et al. [8] gathered many reasons about advantage of studying $\mathbf{Q}$-spectra. They found that the signless Laplacian spectra perform better in comparison to spectra of other commonly used graph matrices, say the Laplacian, or the Seidel matrix. Also, they expressed that among generalized adjacency matrices, i.e. matrices which are a linear combination of $\mathbf{A}(G)$, $\mathbf{J}$ (the all-ones matrix) and $\mathbf{I}$ (the identity matrix) with a non-zero coefficient for $\mathbf{A}(G)$, the signless Laplacian seems to be the most convenient for use in studying graph properties.

The goal of this paper is to find the unique extremal graph with maximum $SLEE$ among all n-vertex graphs with given number of cut edges, pendent vertices, (vertex) connectivity, or edge connectivity.

Our main results are the following two theorems:

Theorem 1.1. *Let $0 \leq p < n$, and $G_{n,p}$ be the graph obtained by attaching p pendent vertices to one vertex of complete graph K_{n-p} (see Figure 1). Then, up to isomorphism, we have:*

1. *Among the set of all n-vertex graphs having p cut edges, $G_{n,p}$ is the unique graph with maximum $SLEE$.*
2. *Among the set of all n-vertex graphs having p pendent vertices, $G_{n,p}$ is the unique graph with maximum $SLEE$.*

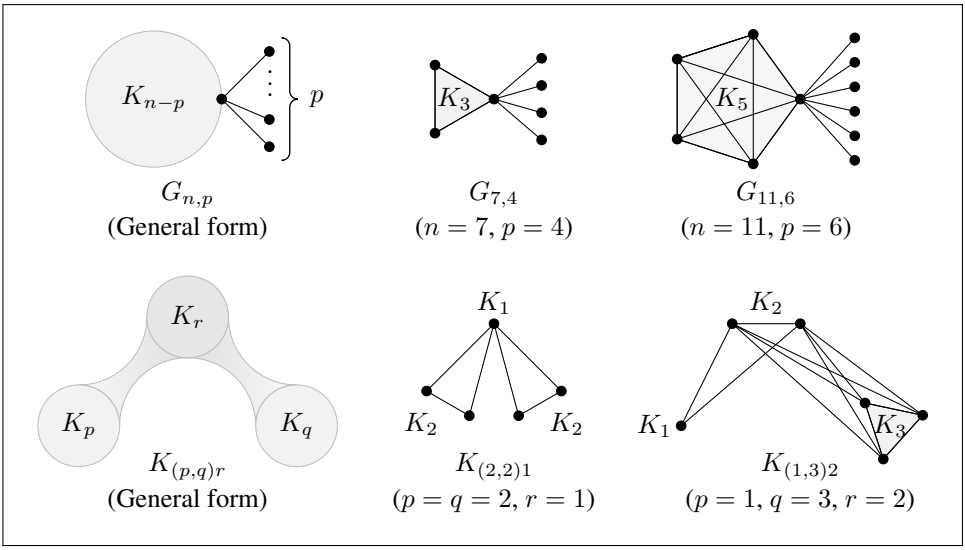

Figure 1: An illustration of the general forms of $G_{n,p}$ and $K_{(p,q)r}$, with some examples.

Theorem 1.2. *Let p, q and r be three non-negative integers, and let $K_{(p,q)r}$ be the graph obtained from three vertex-disjoint complete graphs K_p, K_q and K_r, by attaching any vertex of K_r to all vertices of both K_p and K_q (see Figure 1). Then, up to isomorphism, we have:*

1. *Among the set of all n-vertex graphs with vertex connectivity κ, where $0 \leq \kappa \leq n-1$, $K_{(n-1-\kappa,1)\kappa}$ is the unique graph with maximum $SLEE$.*
2. *Among the set of all n-vertex graphs with edge connectivity κ', where $0 \leq \kappa' \leq n-1$, $K_{(n-1-\kappa',1)\kappa'}$ is the unique graph with maximum $SLEE$.*

2 Preliminaries and lemmas

Before proving our main theorems, we shall provide some fundamental definitions and propositions. In this section, we first declare some basic and useful notations, definitions and a proved theorem; afterward, we propose three effective lemmas to prove Theorems 1.1 and 1.2.

Denote by $T_k(G)$ the k-th signless Laplacian spectral moment of the graph G, i.e., $T_k(G) = \sum_{i=1}^{n} q_i^k$. By applying the Taylor expansion to the function e^x, we have:

$$SLEE(G) = \sum_{k \geq 0} \frac{T_k(G)}{k!}. \tag{2.1}$$

Moreover, by the following definition and theorem, we can easily compare the $SLEE$'s of some graphs.

Definition 2.1. [8] A *semi-edge walk* of length k in a graph G is an alternating sequence $W = v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$ of vertices $v_1, v_2, \ldots, v_k, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ such that the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of the edge e_i, for any $i = 1, 2, \ldots, k$. If $v_1 = v_{k+1}$, then W is said to be a *closed semi-edge walk*.

Theorem 2.2. *[8] The signless Laplacian spectral moment T_k is equal to the number of closed semi-edge walks of length k.*

Let G and G' be two graphs, and $x, y \in V(G)$, and $x', y' \in V(G')$. Denoting by $SW_k(G; x, y)$, the set of all semi-edge walks of length k in G, each of which starts at vertex x and ends at vertex y. Note that $|SW_k(G; x, y)| = |SW_k(G; y, x)|$ for any $x, y \in V(G)$. For convenience, we may denote $SW_k(G; x, x)$ by $SW_k(G; x)$. The notation $SW_k(G)$ will be used as the set of all closed semi-edge walks of length k in G, i.e. $SW_k(G) = \bigcup_{x \in V(G)} SW_k(G; x)$. We will use the notation $(G; x, y) \preceq_s (G'; x', y')$ when for any $k \geq 0$, $|SW_k(G; x, y)| \leq |SW_k(G'; x', y')|$. Moreover, if $(G; x, y) \preceq_s (G'; x', y')$, and there exists some k_0 where $|SW_{k_0}(G; x, y)| < |SW_{k_0}(G'; x', y')|$, then we will write $(G; x, y) \prec_s (G'; x', y')$. We abbreviate $(G; x, x) \preceq_s (G'; x', x')$ as $(G; x) \preceq_s (G'; x')$, and $(G; x, x) \prec_s (G'; x', x')$ as $(G; x) \prec_s (G'; x')$.

Indeed, by using the above notations, we can restate the Theorem 2.2 as:

$$T_k(G) = |SW_k(G; x)| = |\bigcup_{x \in V(G)} SW_k(G; x)| = \sum_{x \in V(G)} |SW_k(G; x)|. \tag{2.2}$$

Let G be a graph and E be a set of edges. If $E \subseteq E(G)$, then we write $G - E$ for the graph obtained from G by removing all of its edges in E. Also, if $E \subseteq E(\overline{G})$, then we denote by $G + E$ the graph obtained from G by adding all of edges in E to the graph. For convenience, we set $G + e$ for $G + \{e\}$. The next result immediately follows from equations (2.1) and (2.2).

Lemma 2.3. *Let G be a graph. If e is an edge such that $e \notin E(G)$, then $SLEE(G) < SLEE(G+e)$.*

Under the terms of the following lemma, we may call the vertices $w_1, \ldots, w_r$ as *transferred neighbors*, and the graph G as *transfer route* graph. Also, we may say that G_u *is obtained from G_v by transferring some neighbors of v to the set of neighbors of u.*

Lemma 2.4. *Let G be a graph and $v, u, w_1, w_2, \ldots, w_r \in V(G)$. Suppose that $E_v = \{e_1 = vw_1, \ldots, e_r = vw_r\}$ and $E_u = \{\overline{e}_1 = uw_1, \ldots, \overline{e}_r = uw_r\}$ are subsets of edges, that are not in G (i.e. $e_i, \overline{e}_i \notin E(G)$, for $i = 1, 2, \ldots, r$). Let $G_u \cong G + E_u$ and $G_v \cong G + E_v$. If $(G; v) \prec_s (G; u)$, and $(G; w_i, v) \preceq_s (G; w_i, u)$ for each $i = 1, 2, \ldots, r$, then $SLEE(G_v) < SLEE(G_u)$, where G_u and G_v are shown in Figure 2.*

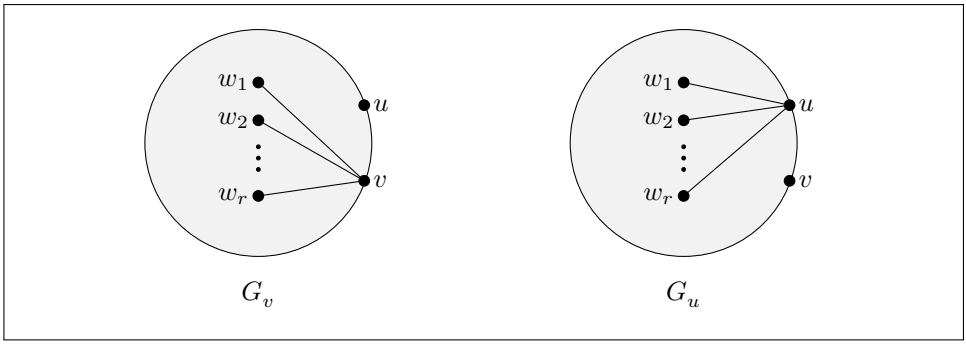

Figure 2: An illustration of the graphs G_v and G_u in Lemma 2.4.

Proof. Since $(G; v) \prec_s (G; u)$, there exists an injection

$$f_k : SW_k(G; v) \to SW_k(G; u)$$

for each $k \geq 0$. Similarly, $(G; w_i, v) \preceq_s (G; w_i, u)$ implies that there exist following injections for each $i = 1, 2, \ldots, r$, and $k \geq 0$:

$$f_k^i : SW_k(G; w_i, v) \to SW_k(G; w_i, u)$$

$$g_k^i : SW_k(G; v, w_i) \to SW_k(G; u, w_i)$$

For any $W \in SW_k(G; x, y)$ where $x, y \in \{v, w_1, \ldots, w_r\}$, let $\overline{W}$ be as follows:

1) If $k = 0$ and $W = w_t$, where $t \in \{1, \ldots, r\}$, then $\overline{W} = W$.
2) If $W \in SW_k(G; v)$, then $\overline{W} = f_k(W)$.
3) If $W \in SW_k(G; w_t, v)$, then $\overline{W} = f_k^t(W)$.
4) If $W \in SW_k(G; v, w_t)$, then $\overline{W} = g_k^t(W)$.
5) If $W \in SW_k(G; w_t, w_j)$, where $t, j \in \{1, \ldots, r\}$, then $\overline{W} = W$.

To prove the statement, it is enough to show that $T_k(G_v) \leq T_k(G_u)$, and there exists k_0 such that inequality is strict.

If $W \in SW_k(G_v)$, then W can be decomposed uniquely to $s+1$ sections as $W = W_1e_{j_1}W_2e_{j_2}W_3\cdots W_se_{j_s}W_{s+1}$, where $e_{j_1},\ldots,e_{j_s} \in E_v$, and for each $i \in \{2,3,\ldots,s\}$, there are $x_i, y_i \in \{v, w_1, \ldots, w_r\}$ such that $W_i \in SW_{k_i}(G; x_i, y_i)$. Moreover, since W is closed, for some $x', y' \in \{v, w_1, \ldots, w_r\}$, $W' = W_{s+1}W_1 \in SW_{k'}(G; x', y')$ where $k' = k_1 + k_{s+1}$. Therefore, we can uniquely decompose $\overline{W'}$ to $\overline{W}_{s+1}\,\overline{W}_1$, where $\overline{W}_{s+1}$ is a semi-edge walk of length k_{s+1} in G, starting at x and ending at z, and $\overline{W}_1$ is a semi-edge walk of length k_1 in G, starting at z and ending at y, for some $z \in V(G)$ and $x, y \in \{u, w_1, \ldots, w_r\}$.

Now, one can show that the map $h_k : SW_k(G_v) \to SW_k(G_u)$ defined by the rule

$$\begin{aligned} h_k(W) &= h_k(W_1e_{j_1}W_2e_{j_2}W_3\cdots W_se_{j_s}W_{s+1}) \\ &= \overline{W}_1\overline{e}_{j_1}\overline{W}_2\overline{e}_{j_2}\overline{W}_3\cdots\overline{W}_s\overline{e}_{j_s}\overline{W}_{s+1} \end{aligned}$$

is injective, for each $k \geq 0$. Thus, $T_k(G_v) \leq T_k(G_u)$, for any $k \geq 0$.
Moreover, for some k_0, f_{k_0} is not surjective, and $|SW_{k_0}(G, v)| < |SW_{k_0}(G, u)|$, i.e. $T_{k_0}(G_v) < T_{k_0}(G_u)$. Hence $SLEE(G_v) < SLEE(G_u)$. □

The following lemma enables us to provide the necessary conditions in Lemma 2.4, and to use it to compare $SLEE$'s of some particular graphs.

Lemma 2.5. *Let G be a graph and $u, v \in V(G)$. If v is a pendent vertex attached to u, then $(G; v) \preceq_s (G; u)$, with equality if and only if $d_G(u) = d_G(v) = 1$. Moreover, $(G; w, v) \preceq_s (G; w, u)$ for each $w \in V(G) \setminus \{v\}$.*

Proof. The case $k = 0$ is trivial. Let $k > 1$ and $W = veW'ev \in SW_k(G; v)$, where W' is a semi-edge walk of length $k-2$ in G. We may construct an injection $f_k : SW_k(G; v) \to SW_k(G; u)$, by the rule $f_k(W) = ueW'eu$. Thus $|SW_k(G; v)| \leq |SW_k(G; u)|$, for any $k \geq 2$. Moreover, if $d_G(u) > 1$, then we have $|SW_1(G; v)| = d_G(v) = 1 < d_G(u) = |SW_1(G; u)|$. Recall that if $d_G(u) = 1$, then G has an automorphism, interchanges u and v and fixes the other vertices.

In a similar way, by changing the end of each member of $SW_k(G; w, v)$ from v to u, we find that $(G; w, v) \preceq_s (G; w, u)$ for each $w \in V(G) \setminus \{v\}$. Note that for $k = 0$, $|SW_0(G; v, v)| = 1 > 0 = |SW_0(G; v, u)|$. □

3 The proof of Theorem 1.1

At the end of this section, we prove our first main theorem which determines the unique extremal graph with maximum $SLEE$ among the set of all n-vertex graphs with given number of cut edges or pendent vertices. However, we should bring forth another lemma to this purpose.
Let us denote by $\mathcal{G}(n, p)$, the set of all graphs obtained by attaching p pendent vertices to some vertices of a complete graph K_{n-p} , for $0 \leq p < n$.

Lemma 3.1. *Suppose that $1 \leq p \leq n-3$, and $G \in \mathcal{G}(n, p)$. If u and v are two distinct non-pendent vertices of G, such that $d_G(v) = n - p - 1 < d_G(u)$, then $(G; v) \prec_s (G; u)$.*

Proof. Obviously, u has at least one pendent neighbor and each neighbor of v is u itself or one of its neighbors. Thus, for each $k > 1$, the map $f_k : SW_k(G; v) \to SW_k(G; u)$ defined by the rule $f_k(ve_1We_kv) = ue'_1We'_ku$ is well-defined and injective, where $e_i = vw_i$ and $e'_i = uw_i$, for some neighbors w_i of v and $i \in \{1, k\}$. Therefore, $|SW_k(G; v)| \leq |SW_k(G; u)|$, for any $k > 1$. Moreover, $|SW_1(G; v)| = d_G(v) = n - p - 1 < d_G(u) = |SW_1(G; u)|$ implies $(G; v) \prec_s (G; u)$. □

Proof of Theorem 1.1. To prove the first part, let G be an extremal n-vertex graph with maximum $SLEE$, having p cut edges. We shall show that $G \cong G_{n,p}$.

If $p = 0$, then by Lemma 2.3, $G \cong K_n \cong G_{n,0}$. Moreover, if $n = 1$ or 2, then $p = n - 1$, and $G \cong K_n \cong G_{n,n-1}$. Therefore, suppose that $n \geq 3$ and $p \geq 1$.

If E is the set of all cut edges in G, then by Lemma 2.3, all of $p + 1$ connected components of $G-E$ are complete. Suppose that there exists one edge e of E, attaching vertices u and v in G, where $d_G(u), d_G(v) \geq 2$. Let G' be the graph obtained from G by transferring all neighbors of v except u to the set of neighbors of u, and H be the transfer route graph. By Lemma 2.5, $(H; v) \prec_s (H; u)$. Thus, Lemma 2.4 results in $SLEE(G) < SLEE(G')$. This is a contradiction, because both graphs G and G' have the same number of cut edges. Therefore, each cut edge incidents to a pendent vertex.

Let V_p be a set of vertices of G, each of which is a pendent vertex of a cut edge such that there is no cut edge with both ends in V_p. By Lemma 2.3, $G - V_p$ is a complete graph on $n - p$ vertices. Thus G is a graph obtained from K_{n-p}, by attaching p pendent vertices to some vertices of K_{n-p}, which means $G \in \mathcal{G}(n, p)$.

If $G \ncong G_{n,p}$, then there are at least two non-pendent vertices, say u and v, such that each of them has at least one pendent neighbor. Now, by Lemmas 2.4 and 3.1 and transferring pendent neighbors of v to the set of neighbors of u, we may get a graph with higher $SLEE$ than G in $\mathcal{G}(n, p)$, which is a contradiction again. Therefore, $G \cong G_{n,p}$.

Now, to prove the second part, suppose that G is an extremal n-vertex graph with maximum $SLEE$, having p pendent vertices. If H is the graph obtained from G, by removing all of its p pendent vertices, then by Lemma 2.3, H is a complete graph on $n - p$ vertices. Thus $G \in \mathcal{G}(n, p)$. Finally, the proof of this part is accomplished by using the same argument mentioned in the above paragraph. □

4 The proof of Theorem 1.2

In this section, we are going to prove Theorem 1.2, which determines the unique extremal graph with maximum $SLEE$ among the set of all n-vertex graphs with given (vertex) connectivity or edge connectivity.

We start with the following lemma:

Lemma 4.1. *If $2 \leq q \leq p$, and $r \geq 0$, then*

$$SLEE(K_{(p,q)r}) < SLEE(K_{(p+q-1,1)r}).$$

Proof. Suppose that $V(K_p) = \{x_1, x_2, \ldots, x_p\}$, and $V(K_q) = \{y_1, y_2, \ldots, y_q\}$, and $V(K_r) = \{z_1, z_2, \ldots, z_r\}$. Let G be the graph obtained from $K_{(p,q)r}$ by transferring neighbors $y_2, \ldots, y_q$ of y_1 to the set of neighbors of x_1, and H be the transfer route graph.

If $r = 0$, then obviously $(H; y_1) \prec_s (H; x_1)$. If $r > 0$, then, since any neighbor of y_1 in H is a neighbor of x_1, by a similar method used in the proof of Lemma 3.1, we can also show that $(H; y_1) \prec_s (H; x_1)$ and $(H; y_i, y_1) \preceq_s (H; y_i, x_1)$, for each $i \in \{2, \ldots, q\}$.

Therefore, Lemma 2.4 implies $SLEE(K_{(p,q)r}) < SLEE(G)$. Note that, since $p \geq 2$, G is a proper subgraph of $K_{(p+q-1,1)r}$. Thus, by Lemma 2.3,

$$SLEE(K_{(p,q)r}) < SLEE(G) < SLEE(K_{(p+q-1,1)r}).$$

□

Proof of Theorem 1.2. Note that the case $\kappa = n - 1$ is trivial, because $K_{(0,1)\kappa} \cong K_n$ is (up to isomorphism) the unique graph with vertex connectivity $n - 1$.

Let G be an extremal graph with maximum $SLEE$, among n-vertex graphs with connectivity κ. Suppose that S is a subset of $V(G)$, where $G-S$ is disconnected, and $|S| = \kappa$. By Lemma 2.3, there exist integers p and q, such that $1 \leq q \leq p$, $p + q = n - \kappa$, and $G - S$ is the union of two complete components K_q and K_p. Again, by Lemma 2.3, each vertex in S is attached to another one and also to vertices of both K_q and K_p. It means that $G \cong K_{(p,q)\kappa}$. If $q \geq 2$, then Lemma 4.1 implies $SLEE(G) < SLEE(K_{(p+q-1,1)\kappa})$, which is a contradiction. Hence, $q = 1$, and therefore $G \cong K_{(n-1-\kappa,1)\kappa}$. This proves the first part of the theorem.

To prove the second part, we note that if G is a graph with vertex and edge connectivity κ and κ', respectively, then $\kappa \leq \kappa'$ (see [6]). If $\kappa = \kappa'$, then by previous part of the proof we have $SLEE(G) \leq SLEE(K_{(n-1-\kappa',1)\kappa'})$, and equality holds if and only if $G \cong K_{(n-1-\kappa',1)\kappa'}$. Moreover, if $\kappa < \kappa'$ then $K_{(n-1-\kappa,1)\kappa}$ is a proper subgraph of $K_{(n-1-\kappa',1)\kappa'}$. In this case, Lemma 2.3 and the above arguments show that

$$SLEE(G) \leq SLEE(K_{(n-1-\kappa,1)\kappa}) < SLEE(K_{(n-1-\kappa',1)\kappa'}).$$

This completes the proof. □

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Nontrivial nuciferous graphs exist

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Abstract

A nuciferous graph is a simple graph with a non-singular 0-1 adjacency matrix A such that all the diagonal entries of A^{-1} are zero and all the off-diagonal entries of A^{-1} are non-zero. Sciriha *et al.* conjectured that except K_2, no nuciferous graph exists. We disprove this conjecture. Moreover, we conjecture that there are infinitely many nuciferous Cayley graphs.

Keywords: Nuciferous graph, Cayley graph.

Math. Subj. Class.: 05C50

1 Introduction

Let G be a simple graph with non-singular 0-1 adjacency matrix A. If all the diagonal entries of A^{-1} are zero and all the off-diagonal entries of A^{-1} are non-zero, then G is called a *nuciferous graph*. The concept of nuciferous graphs has arisen in the context of the quantum mechanical theory of the conductivity of non-singular carbon molecules in the Source and Sink Potential model [2]. According to Sciriha [4]:

> "In the graph-theoretical Source and Sink Potential model, a molecule is either an insulator or a conductor for electrons with energy zero. Of particular interest are two classes of graphs with analogous vertex pairs, i.e., the same behavior for any two- vertex connection. These are uniform-core (insulating for all two-vertex connections) and nuciferous graphs, which conduct for all two-vertex connections. A graph G in the first class reaches the minimum possible nullity when any two distinct connecting vertices are deleted. In the second class, the nullity reaches one, the maximum possible, when any vertex is deleted."

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To date, the only nuciferous graph known is K_2 which we call it the trivial one. In [5] it was conjectured that there are no others. We disprove this conjecture.

We remark that in [1] weighted graphs that have an adjacency matrix with the required structure in the inverse as in nuciferous graphs were found.

2 Nuciferous Cayley graphs

Making use of the database of vertex-transitive graphs by Gordon Royle [3] and an exhaustive computer search, we found several nuciferous graphs. In fact among vertex-transitive graphs with at most 31 vertices, there are 21 nuciferous graphs. All the 21 nuciferous graphs we found are Cayley graphs: 6 on 24, 3 on 28 and 12 on 30 vertices. Recall that a Cayley graph $\mathrm{Cay}(\Gamma, S)$ for a given group Γ and connection set $S \subset \Gamma$ is the graph with vertex set Γ and with u connected to v if and only if $vu^{-1} \in S$. Table 1 shows the list of nuciferous Cayley graphs up to 31vertices according to their groups in which C_n and D_n denote cyclic and dihedral groups of order n, respectively, and Sym_k and Alt_k denote the symmetric and alternative groups on k elements, respectively. We notice that in Table 1 the

Order	Group	Degree	# of nuciferous
24	$D_{12} \times C_2$	15	1
24	$\mathrm{Alt}_4 \times C_2$	7	2
24	$\mathrm{Sym}_3 \times C_4$	15	1
24	D_{24}	15	1
24	Sym_4	7	2
24	Sym_4	15	1
28	D_{28}	13	1
28	D_{28}	15	2
30	C_{30}	11	1
30	C_{30}	15	1
30	$D_{10} \times C_3$	11	1
30	$D_{10} \times C_3$	22	1
30	$D_6 \times C_5$	11	1
30	D_{30}	11	1
30	D_{30}	15	10

Table 1: Number of nuciferous Cayley graphs with at most 31 vertices according to their group

two degree 7 graphs on $\mathrm{Alt}_4 \times C_2$ are isomorphic to the two degree 7 graphs on Sym_4; all the degree 11 graphs are isomorphic; and the degree 15 graph on C_{30} is isomorphic to one of the degree 15 graphs on D_{30}.

Tables 2 and 3 depict the adjacency matrix A and the inverse A^{-1} of one of the two nuciferous Cayley graphs with 24 vertices on the group $\mathrm{Alt}_4 \times C_2$.

Based on our findings on nuciferous Cayley graphs we pose the following:

Conjecture 2.1. *There exist infinitely many nuciferous Cayley graphs.*

$$A = \left[\begin{array}{cccccccccccccccccccccccc}
0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0
\end{array}\right]$$

Table 2: The adjacency matrix of a nuciferous graph with 24 vertices

$$A^{-1} = \frac{1}{21}\begin{bmatrix}
0 & 1 & 5 & 5 & 4 & 4 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -4 & -4 & 4 & 4 & -2 & -2 & -4 & -4 & -6 & 2 \\
1 & 0 & 5 & 5 & -4 & -4 & -1 & -1 & -2 & -2 & -4 & -4 & 1 & 1 & 1 & 1 & 4 & 4 & -1 & -1 & 4 & 4 & 2 & -6 \\
5 & 5 & 0 & 1 & -4 & 1 & -2 & -1 & 1 & -1 & 4 & -4 & -1 & -2 & 4 & -4 & 2 & -6 & 1 & -1 & 1 & -4 & 4 & 4 \\
5 & 5 & 1 & 0 & 1 & -4 & -1 & -2 & -1 & 1 & -4 & 4 & -2 & -1 & -4 & 4 & -6 & 2 & -1 & 1 & -4 & 1 & 4 & 4 \\
4 & -4 & -4 & 1 & 0 & 4 & -1 & 4 & 4 & 1 & -4 & 5 & -1 & -6 & 1 & -4 & -1 & 1 & -2 & 2 & 5 & 1 & -1 & -2 \\
4 & -4 & 1 & -4 & 4 & 0 & 4 & -1 & 1 & 4 & 5 & -4 & -6 & -1 & -4 & 1 & 1 & -1 & 2 & -2 & 1 & 5 & -1 & -2 \\
1 & -1 & -2 & -1 & -1 & 4 & 0 & 1 & -4 & 1 & 2 & 1 & 5 & 4 & -2 & 4 & 4 & -4 & 5 & -4 & -1 & -6 & -4 & 1 \\
1 & -1 & -1 & -2 & 4 & -1 & 1 & 0 & 1 & -4 & 1 & 2 & 4 & 5 & 4 & -2 & -4 & 4 & -4 & 5 & -6 & -1 & -4 & 1 \\
-1 & -2 & 1 & -1 & 4 & 1 & -4 & 1 & 0 & 4 & -1 & -6 & -4 & 5 & 4 & -1 & 1 & -4 & 1 & 5 & 2 & -2 & 4 & -4 \\
-1 & -2 & -1 & 1 & 1 & 4 & 1 & -4 & 4 & 0 & -6 & -1 & 5 & -4 & -1 & 4 & -4 & 1 & 5 & 1 & -2 & 2 & 4 & -4 \\
1 & -4 & 4 & -4 & -4 & 5 & 2 & 1 & -1 & -6 & 0 & 1 & 4 & -2 & 4 & 5 & -2 & -1 & 4 & -1 & -4 & 1 & -1 & 1 \\
1 & -4 & -4 & 4 & 5 & -4 & 1 & 2 & -6 & -1 & 1 & 0 & -2 & 4 & 5 & 4 & -1 & -2 & -1 & 4 & 1 & -4 & -1 & 1 \\
-1 & 1 & -1 & -2 & -1 & -6 & 5 & 4 & -4 & 5 & 4 & -2 & 0 & 1 & 1 & 2 & -4 & 4 & 1 & -4 & -1 & 4 & 1 & -4 \\
-1 & 1 & -2 & -1 & -6 & -1 & 4 & 5 & 5 & -4 & -2 & 4 & 1 & 0 & 2 & 1 & 4 & -4 & -4 & 1 & 4 & -1 & 1 & -4 \\
-4 & 1 & 4 & -4 & 1 & -4 & -2 & 4 & 4 & -1 & 4 & 5 & 1 & 2 & 0 & 1 & -2 & -1 & -1 & -6 & 5 & -4 & 1 & -1 \\
-4 & 1 & -4 & 4 & -4 & 1 & 4 & -2 & -1 & 4 & 5 & 4 & 2 & 1 & 1 & 0 & -1 & -2 & -6 & -1 & -4 & 5 & 1 & -1 \\
4 & 4 & 2 & -6 & -1 & 1 & 4 & -4 & 1 & -4 & -2 & -1 & -4 & 4 & -2 & -1 & 0 & 1 & 1 & -4 & 1 & -1 & 5 & 5 \\
4 & 4 & -6 & 2 & 1 & -1 & -4 & 4 & -4 & 1 & -1 & -2 & 4 & -4 & -1 & -2 & 1 & 0 & -4 & 1 & -1 & 1 & 5 & 5 \\
-2 & -1 & 1 & -1 & -2 & 2 & 5 & -4 & 1 & 5 & 4 & -1 & 1 & -4 & -1 & -6 & 1 & -4 & 0 & 4 & 1 & 4 & -4 & 4 \\
-2 & -1 & -1 & 1 & 2 & -2 & -4 & 5 & 5 & 1 & -1 & 4 & -4 & 1 & -6 & -1 & -4 & 1 & 4 & 0 & 4 & 1 & -4 & 4 \\
-4 & 4 & 1 & -4 & 5 & 1 & -1 & -6 & 2 & -2 & -4 & 1 & -1 & 4 & 5 & -4 & 1 & -1 & 1 & 4 & 0 & 4 & -2 & -1 \\
-4 & 4 & -4 & 1 & 1 & 5 & -6 & -1 & -2 & 2 & 1 & -4 & 4 & -1 & -4 & 5 & -1 & 1 & 4 & 1 & 4 & 0 & -2 & -1 \\
-6 & 2 & 4 & 4 & -1 & -1 & -4 & -4 & 4 & 4 & -1 & -1 & 1 & 1 & 1 & 1 & 5 & 5 & -4 & -4 & -2 & -2 & 0 & 1 \\
2 & -6 & 4 & 4 & -2 & -2 & 1 & 1 & -4 & -4 & 1 & 1 & -4 & -4 & -1 & -1 & 5 & 5 & 4 & 4 & -1 & -1 & 1 & 0
\end{bmatrix}$$

Table 3: The inverse of the adjacency matrix given in Table 2 of a nuciferous graph with 24 vertices

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No chemical graph on more than two vertices is nuciferous

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Abstract

A simple graph is nuciferous if its 0–1 adjacency matrix is nonsingular and if its inverse has zero entries on its main diagonal and a non–zero entry at each off–diagonal position. A nuciferous graph is a molecular graph that represents an ipso omni–insulating but distinct omni–conducting molecule. It has been conjectured in 2012 that only K_2, the complete graph on two vertices, is nuciferous. We show that this conjecture is true for chemical graphs, that is, graphs whose vertex degree is at most three.

Keywords: Nuficerous graph, chemical graph, NSSD, non-singular graph, molecular conductivity.

Math. Subj. Class.: 05C50, 05B20

1 Introduction

A *molecular graph* is a simple graph whose vertices represent the atoms of some molecule and whose edges represent the bonds between the atoms in the molecule. The subclass of molecular graphs that are connected and represent conjugated systems of unsaturated carbon atoms forms the class of *chemical graphs*, whose vertices represent the carbon atoms and whose edges represent the σ–bonds between them [3]. Since the atoms are unsaturated, the degree of each vertex in a chemical graph is one, two or three.

The graph $G - v$ is obtained from a graph G by removing the vertex v and all the edges incident to it. If v and w are vertices in G distinct from u, then we represent the graph $(G - u) - v$ as $G - u - v$ and the graph $((G - u) - v) - w$ as $G - u - v - w$. The *deck* of a graph G is the set $\{G - 1, G - 2, \ldots, G - n\}$ of its vertex–deleted subgraphs.

A $n \times n$ real symmetric matrix A with zero diagonal is the adjacency matrix of an edge–weighted graph G (without loops) on n vertices if a non–zero entry corresponds to an edge and a zero entry to a non–edge. An adjacency matrix of a simple graph G, referred to as a 0–1 adjacency matrix, has zero diagonal and each non–zero entry is 1.

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The *characteristic polynomial* $\phi(G,\lambda)$ of a matrix $\mathbf{M}$ is the determinant $|x\mathbf{I}-\mathbf{M}|$, where $\mathbf{I}$ is the identity matrix. The *eigenvalues* of $\mathbf{M}$ are the roots of its characteristic polynomial. The *nullity* $\eta(\mathbf{M})$ of $\mathbf{M}$ is the multiplicity of the zero root of the characteristic polynomial of $\mathbf{M}$. The matrix $\mathbf{M}$ is *singular* if $\eta(\mathbf{M})>0$ and is *nonsingular* if $\eta(\mathbf{M})=0$.

If $\mathbf{A}$ is the adjacency matrix of a molecular graph G, then the characteristic polynomial, eigenvalues and nullity of G are the same as those of $\mathbf{A}$. A graph is singular if its adjacency matrix is singular and non–singular otherwise. The nullity $\eta(G)$ of a molecular graph G corresponds to the number of non–bonding orbitals (zero energy level) of the molecule represented by G.

The electron orbital energies given by the Hückel approximation of Schrödinger's equation on the quantum theory of molecules correspond to the eigenvalues of the 0–1 adjacency matrix. According to the Source and Sink Potential quantum mechanical model for molecular conduction in a chemical graph G [4, 6], electron transmission $T(E)$, at the energy E, is determined in terms of the characteristic polynomials of $\phi(G,E)$, $\phi(G-v,E)$, $\phi(G-w,E)$ and $\phi(G-v-w,E)$, where the carbon atoms v and w are in contact with wires in a circuit containing the molecule G [3, 7]. At the Fermi energy ($E=0$), with a small bias voltage across the molecule, electron transmission or insulation was found to depend critically on the nullity of the adjacency matrices of the three aforementioned subgraphs of G relative to the nullity of the parent graph G [7].

In [3, Theorems 4.1 and 4.4], it was proved that for a nonsingular molecular graph G with adjacency matrix $\mathbf{A}$, conduction between carbon atoms i and j at the Fermi energy occurs if and only if the ij^{th} entry of $\mathbf{A}^{-1}$ is non–zero. This is true even if $i=j$, in which case the connection is said to be *ipso*. It is thus theoretically possible that, at the Fermi energy ($E=0$), conduction occurs for all connecting vertex pairs $i\neq j$, but insulation occurs for all $i=j$. Such a molecule is called a *distinct omni–conducting but ipso omni–insulating molecule* in [3], and corresponds to a nonsingular molecular graph G whose 0–1 adjacency matrix $\mathbf{A}$, with zero diagonal, has an inverse having zero entries on its diagonal and non–zero entries off its diagonal. In [7], such graphs are referred to as *nuciferous*.

Definition 1.1 ([7, Definition 7.8])**.** Let G be a nonsingular simple graph with the off–diagonal entries of the inverse $\mathbf{A}^{-1}$ of its 0–1 adjacency matrix $\mathbf{A}$ being nonzero and real, and all the diagonal entries of $\mathbf{A}^{-1}$ being zero. Then G is said to be a *nuciferous graph*.

The *complete graph* K_n has n vertices and every pair of distinct vertices is connected by an edge. The complete graph K_2 is nuciferous, since its adjacency matrix $\mathbf{K}=\begin{pmatrix}0&1\\1&0\end{pmatrix}$ is an involution ($\mathbf{K}^2=\mathbf{I}$). In [7], it was conjectured that there are no other nuciferous graphs.

Conjecture 1.2 ([7, Conjecture 7.11])**.** *The graph K_2 is the only nuciferous graph.*

The purpose of this paper is to prove Conjecture 1.2 for the subclass of chemical graphs, whose vertex degree is at most three. In order to do this, we use the class of NSSDs (Non–Singular graphs with a Singular Deck) defined in [1], which is a superclass of that of nuciferous graphs.

Definition 1.3. A graph is a *NSSD* if both the real symmetric matrices $\mathbf{A}$ and $\mathbf{A}^{-1}$ have zero diagonal.

In this paper we use only *simple NSSDs*, that is NSSDs for which $\mathbf{A}$ is a 0–1 adjacency matrix. Simple NSSDs correspond to molecular graphs that represent ipso omni–insulating

carbon molecules. An *ipso omni–insulator* is a molecule that, at the Fermi energy, does not conduct when $i = j$, but may, or may not, conduct when $i \neq j$, for wires connecting at i and j [3].

We provide the following characterization of a nuciferous graph in relation to a NSSD.

Theorem 1.4. *A graph G with 0–1 adjacency matrix $\mathbf{A}$ is nuciferous if and only if G is a simple NSSD and each off–diagonal entry of $\mathbf{A}^{-1}$ is non–zero.*

The paper is organised as follows. Section 2 contains further notation used in this paper, together with preliminary results that lead to the main result. The nullity of subgraphs of NSSDs used for the proof of the main result are determined in Section 3. In Section 4, Conjecture 1.2 is proved to hold true for chemical graphs.

2 Preliminaries

We shall use a result by Fiedler and Markham [2] that relates the nullity of the blocks of a partitioned nonsingular matrix with those of its inverse.

Theorem 2.1 ([2, Theorem 2])**.** *If $\mathbf{M}$ is a nonsingular matrix such that $\mathbf{M}$ and $\mathbf{M}^{-1}$ are partitioned as*

$$\mathbf{M}\mathbf{M}^{-1} = \begin{pmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}_{21} & \mathbf{M}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{N}_{11} & \mathbf{N}_{12} \\ \mathbf{N}_{21} & \mathbf{N}_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

for some conformable partitioning of $\mathbf{M}$ and $\mathbf{M}^{-1}$, then $\eta(\mathbf{M}_{11}) = \eta(\mathbf{N}_{22})$.

In Theorem 2.1, the block matrices $\mathbf{M}_{11}$ and $\mathbf{N}_{22}$ are called *complementary block submatrices* of each other. Theorem 2.1 can be extended to any submatrix of $\mathbf{M}$ as follows.

Theorem 2.2. *If $\mathbf{M}$ is a $n \times n$ nonsingular matrix, then the nullity of any $p \times q$ submatrix $\mathbf{R}$ of $\mathbf{M}$ is equal to the nullity of the $(n-q) \times (n-p)$ complementary block submatrix of $\mathbf{R}$ in $\mathbf{M}^{-1}$.*

We shall also make use of the following elementary lemma.

Lemma 2.3. *The rank of a non–zero real and symmetric matrix, with diagonal entries equal to zero, cannot be equal to* 1.

If $\mathbf{A}$ is a non–singular symmetric matrix and has the integer entries 0 and 1, then $\mathbf{A}^{-1}$ is symmetric and has rational entries. Thus, we can associate a graph G^{-1} with $\mathbf{A}^{-1}$; such a graph would be a weighted, undirected graph and with rational edge weights. We call G^{-1} the *inverse* of G.

We now show that the zero diagonal entries of the inverse of the adjacency matrix of an ipso omni–insulator determine the nullity of the vertex–deleted subgraphs of G. By Theorem 2.1, the nullity of any $(n-1) \times (n-1)$ principal submatrix of $\mathbf{A}$ has nullity equal to that of its 1×1 complementary block submatrix $\begin{pmatrix} 0 \end{pmatrix}$ in $\mathbf{A}^{-1}$, that is, it has nullity one. Since each diagonal entry of $\mathbf{A}^{-1}$ is zero, it follows that each of the vertex–deleted subgraphs $G-1, G-2, \ldots, G-n$ of an ipso omni–insulator (a simple NSSD) is singular [1].

Theorem 2.4. *The following statements are equivalent for a molecular graph G:*

1. *G is an ipso omni–insulator;*

2. *G is a simple NSSD;*

3. *G is a simple, nonsingular graph G on n vertices whose vertex–deleted subgraphs $G-1, G-2, \ldots, G-n$ are singular;*

4. *G is a nonsingular simple graph whose inverse is an undirected weighted graph with no loops.*

From Theorems 1.4 and 2.4, we have:

Theorem 2.5. *A nuciferous graph is a simple NSSD whose inverse is a complete graph with rational edge weights and no loops.*

3 The nullity of vertex–deleted subgraphs of simple NSSDs

We now make use of Theorem 2.1 again to obtain the nullity of vertex–deleted subgraphs of simple NSSDs after the removal of up to three of their vertices. In order to do so, we first require the following result, which follows directly from Lemma 2.3.

Proposition 3.1. *For a simple NSSD, no $q \times q$ principal submatrix of the adjacency matrix $\mathbf{A}$ or of its inverse $\mathbf{A}^{-1}$ has nullity $(q-1)$.*

Proof. Since a principal submatrix of $\mathbf{A}$ is a 0–1 symmetric matrix with zero diagonal, by Lemma 2.3, its rank cannot be one. By definition of a simple NSSD, $\mathbf{A}^{-1}$ exists and its diagonal is also zero. Furthermore, the entries of $\mathbf{A}^{-1}$ are rational. Thus, the result holds true for $\mathbf{A}^{-1}$ as well. □

Together with the fact that only the zero $q \times q$ matrix has nullity q, we now show that the nullity of vertex–deleted subgraphs of simple NSSDs may be inferred from those of the complementary block submatrix in $\mathbf{A}^{-1}$ using Theorem 2.1 and Proposition 3.1.

3.1 Nullity of $G - u$

We have already proved, in the paragraph prior to Theorem 2.4, that the nullity of all the one–vertex–deleted subgraphs of any NSSD is one.

Theorem 3.2 ([1])**.** *If G is a simple NSSD, then $G - u$ has nullity one for any vertex u of G.*

3.2 Nullity of $G - u - v$

The nullity of two–vertex–deleted subgraphs of NSSDs may be one of two values, as shown in Theorem 3.3 below. This result was proved in [1] for NSSDs which are not necessarily simple.

Theorem 3.3 ([1])**.** *If G is a simple NSSD, then $G - u - v$ has nullity zero if $\{u, v\}$ is an edge of G^{-1} and has nullity two otherwise.*

Thus, if G is a NSSD, then for $i \neq j$, the ij^{th} entry of $\mathbf{A}^{-1}$ is zero if $G-i-j$ is singular and is nonzero if $G - i - j$ is nonsingular. This provides an interesting interpretation for the zero–nonzero pattern of the inverse of a simple NSSD.

3.3 Nullity of $G - u - v - w$

The nullity of three–vertex–deleted subgraphs of simple NSSDs relates to triangles (circuits of size three) present in their inverse.

Theorem 3.4. *If G is a simple NSSD, then $G - u - v - w$ has nullity*

a) zero, if the edges $\{u, v\}$, $\{u, w\}$ and $\{v, w\}$ form a triangle in G^{-1};

b) three, if none of $\{u, v\}$, $\{u, w\}$ or $\{v, w\}$ is an edge in G^{-1};

c) one, otherwise.

Proof. Let u, v, w be any three distinct vertices of the NSSD G. By Theorem 2.1, the nullity of $G-u-v-w$ is equal to the nullity of the 3×3 complementary block submatrix $\mathbf{V}$ in $\mathbf{A}^{-1}$. By Proposition 3.1, the nullity of $G - u - v - w$ must be 0, 1 or 3. The nullity is three if and only if $\mathbf{V} = \mathbf{0}$, which is equivalent to saying that none of $\{u, v\}$, $\{u, w\}$ or $\{v, w\}$ is an edge of G^{-1}. Since the matrix $\mathbf{V}$ is of the form $\begin{pmatrix} 0 & c_1 & c_2 \\ c_1 & 0 & c_3 \\ c_2 & c_3 & 0 \end{pmatrix}$ for some real numbers c_1, c_2, c_3 and $|\mathbf{V}| = 2c_1c_2c_3$, $\eta(\mathbf{V}) = 0$ if and only if none of c_1, c_2 or c_3 is zero. In such a case, the edges $\{u, v\}$, $\{u, w\}$ and $\{v, w\}$ are all edges of G^{-1} and thus form a triangle in G^{-1}. In any other case, $\eta(\mathbf{V}) > 0$ and the result is established. □

4 Nuciferous chemical graphs

In this section we prove Conjecture 1.2 for chemical graphs, that is, for graphs whose degree is at most three.

Theorem 4.1. *The only nuciferous chemical graph is K_2.*

Proof. The 0–1 adjacency matrix $\mathbf{K}$ of an undirected graph K_2 with no loops satisfies $\mathbf{K} = \mathbf{K}^{-1}$ and can be readily verified to be a nuciferous chemical graph. Thus, let G be any simple graph different from K_2. The trivial graph on a single vertex is not a simple NSSD, since it is singular, while the other graph on two vertices is disconnected, and hence singular. Graphs on three vertices are either singular or complete. Each vertex–deleted subgraph of K_3 is K_2 which is not singular. Hence G must have at least four vertices in order to be a simple NSSD. By Theorem 1.4, this is a necessary condition for G to be nuciferous. We now show that the vertex degrees of G must all be greater than three for G to be nuciferous.

Choose any arbitrary vertex v from among the vertices of G. If v is of degree one, then the adjacency matrix $\mathbf{A}$ of G can be partitioned into $\begin{pmatrix} \mathbf{H} & \mathbf{r} & \mathbf{0} \\ \mathbf{r}^\mathsf{T} & 0 & 1 \\ \mathbf{0}^\mathsf{T} & 1 & 0 \end{pmatrix}$, where the last column portrays the adjacency of v. Since $\mathbf{A}$ is nonsingular, there exists $\mathbf{A}^{-1}$ with conformal partition $\begin{pmatrix} \mathbf{L} & \mathbf{y} & \mathbf{v} \\ \mathbf{y}^\mathsf{T} & 0 & \beta \\ \mathbf{v}^\mathsf{T} & \beta & 0 \end{pmatrix}$. Consider

$$\begin{pmatrix} \mathbf{H} & \mathbf{r} & \mathbf{0} \\ \mathbf{r}^\mathsf{T} & 0 & 1 \\ \mathbf{0}^\mathsf{T} & 1 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{L} & \mathbf{y} & \mathbf{v} \\ \mathbf{y}^\mathsf{T} & 0 & \beta \\ \mathbf{v}^\mathsf{T} & \beta & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^\mathsf{T} & 1 & 0 \\ \mathbf{0}^\mathsf{T} & 0 & 1 \end{pmatrix}.$$

By multiplying the last row of $\mathbf{A}$ by the first column of $\mathbf{A}^{-1}$, we obtain $\mathbf{y}^{\mathsf{T}} = \mathbf{0}^{\mathsf{T}}$, and hence $\mathbf{y} = \mathbf{0}$. Thus, not all of the off–diagonal entries of $\mathbf{A}^{-1}$ are nonzero. By Definition 1.1, $\mathbf{A}$ is not a nuciferous graph.

If v is of degree two and is adjacent to vertices u and w in G, then in the graph $G-u-w$, v is an isolated vertex. Thus $G - u - w$ is singular. By Theorem 3.3, it must have nullity two, which implies that $\{u, w\}$ is not an edge in G^{-1}. Thus, there exists an off–diagonal entry of $\mathbf{A}^{-1}$ equal to zero, so G is not a nuciferous graph.

Now let the degree of v be three and let the three neighbours of v be u, w and z. Since v is again an isolated vertex of $G - u - w - z$, this vertex–deleted subgraph is singular. By Theorem 3.4, the nullity of $G - u - w - z$ is either one or three, and in either case, at least one of $\{u, w\}$, $\{u, z\}$ or $\{w, z\}$ is not an edge in G^{-1}. Again, this means that $\mathbf{A}^{-1}$ has a zero entry off its diagonal; thus G is not a nuciferous graph.

Hence the degree of all the vertices of a nuciferous graph G on at least four vertices must be greater than three. Consequently, the only nuciferous chemical graph is K_2. □

Remark 4.2. After this work was completed, the authors were informed of the existence of the article by Ghorbani [5] in which examples of non–chemical nuciferous graphs were presented. This shows that Theorem 4.1 proved here cannot be strengthened to cover general graphs.

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New bounds for the sum of powers of normalized Laplacian eigenvalues of graphs*

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Abstract

For a simple and connected graph, a new graph invariant $s^*_\alpha(G)$, defined as the sum of α powers of the eigenvalues of the normalized Laplacian matrix, has been introduced by Bozkurt and Bozkurt (2012). Lower and upper bounds for this index have been proposed by the authors. In this paper, we localize the eigenvalues of the normalized Laplacian matrix by adapting a theoretical method, proposed in Bianchi and Torriero (2000), based on majorization techniques. Through this approach we derive upper and lower bounds of $s^*_\alpha(G)$. Some numerical examples show how sharper results can be obtained with respect to those existing in literature.

Keywords: Graphs, majorization, topological indices, bounds.

Math. Subj. Class.: 05C35, 05C05, 05C50

1 Introduction

Among the various indices in Mathematical Chemistry, a whole new family of descriptors $s^*_\alpha(G)$, defined as the sum of α powers of the eigenvalues of the normalized Laplacian matrix, has been proposed by Bozkurt and Bozkurt in [7]. These authors found a number of bounds for arbitrary α and particularly for $\alpha = -1$, which is the case of the degree Kirchhoff Index. Recently, Bianchi et al. proposed a variety of lower and upper bounds for $s^*_\alpha(G)$ in [1] and for the Kirchhoff Index in [2] derived via majorization techniques. In particular, the authors showed that it is possible to obtain tighter results taking into account additional information on the localization of the eigenvalues of proper matrices associated to the graph. From a theoretical point of view, some well–known inequalities on the localization of real eigenvalues have been provided in literature and they can be used to compute

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the above mentioned bounds.
Alternative inequalities involving the localization of some eigenvalues of the transition matrix of the graph have been numerically computed in [9] and [10] by applying a theoretical methodology proposed in Bianchi and Torriero [5] based on nonlinear global optimization problems solved through majorization techniques. By means of these results, tighter lower bounds for the Kirchhoff Index for some classes of graphs have been derived in [9].
The original contribution of this paper is to exploit this fruitful theoretical method (see [5]) with the aim to provide some formulae that allow us to compute lower bounds for the first and the second eigenvalues of the normalized Laplacian matrix in a fairly straightforward way. These limitations on the eigenvalues are then used to assess bounds for $s^*_\alpha(G)$ proposed in [1]. We then obtain new bounds for $s^*_\alpha(G)$ considering both non-bipartite and bipartite graphs.

In Section 2 some preliminaries on graph theory are given. Furthermore, the definition of $s^*_\alpha(G)$ and the existing bounds on this index are presented. In Section 3 we describe the nonlinear optimization problem based on majorization techniques. This methodology, useful for our analysis, allows us to localize the first and second eigenvalues of the normalized Laplacian matrix. Lower bounds of these normalized Laplacian eigenvalues have been obtained in Section 4. We prove that our limitation on the first normalized Laplacian eigenvalue is always sharper than the existing one for non-complete graph. By means of this result, we provide bounds on $s^*_\alpha(G)$ tighter than those given in [7]. Finally, in Section 5 a numerical comparison for bipartite and non-bipartite graphs is reported.

2 Notations and preliminaries

In this section we first recall some basic notions on graph theory. For more details refer to [17].
Let $G = (V, E)$ be a simple, connected, undirected graph where $V = \{1, 2, \ldots, n\}$ is the set of vertices and $E \subseteq V \times V$ the set of edges, $|E| = m$.
The degree sequence of G is denoted by $\pi = (d_1, d_2, .., d_n)$ and it is arranged in non-increasing order $d_1 \geq d_2 \geq \cdots \geq d_n$, where d_i is the degree of vertex i. It is well known that $\sum_{i=1}^{n} d_i = 2m$ and that if G is a tree, i.e. a connected graph without cycles, $m = n - 1$. Let $A(G)$ be the adjacency matrix of G and $D(G)$ be the diagonal matrix of vertex degrees. The matrix $L(G) = D(G) - A(G)$ is called Laplacian matrix of G, while $\mathcal{L}(G) = D(G)^{-1/2} L(G) D(G)^{-1/2}$ is known as normalized Laplacian matrix. Let $\mu_1 \geq \mu_2 \geq ... \geq \mu_n$ be the (real) eigenvalues of $L(G)$ and $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ be the (real) eigenvalues of $\mathcal{L}(G)$. The following properties of spectra of $L(G)$ and $\mathcal{L}(G)$ hold:

$$\sum_{i=1}^{n} \mu_i = \mathrm{tr}(L(G)) = 2m; \;\; \mu_1 \geq 1 + d_1 \geq \frac{2m}{n}; \;\; \mu_n = 0, \; \mu_{n-1} > 0.$$

$$\sum_{i=1}^{n} \lambda_i = \mathrm{tr}(\mathcal{L}(G)) = n; \;\; \sum_{i=1}^{n} \lambda_i^2 = \mathrm{tr}(\mathcal{L}^2(G)) = n + 2 \sum_{(i,j)\in E} \frac{1}{d_i d_j}; \;\; \lambda_n = 0; \lambda_1 \leq 2.$$

Our aim is the analysis of a particular topological index, $s^*_\alpha(G)$. In particular, Zhou (see [18]) proposed the index:

$$s_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha, \alpha \neq 0, 1,$$

defined as the sum of the α-th power of the non-zero Laplacian eigenvalues of a graph G.

Over the last years this index and its bounds have been intensely studied: Zhou (see [18]) established some properties of $s_\alpha(G)$ and some improvements have been provided in [14], [16], [19] and [20]. In [3], taking into account the Schur-convexity or Schur-concavity of the functions $s_\alpha(G)$ for $\alpha > 1$ and $\alpha < 0$ or $0 < \alpha < 1$ respectively, the same bounds as in [18] have been derived. Furthermore, considering additional information on the localization of the eigenvalues, the authors provide also sharper bounds.

Bozkurt and Bozkurt in [7] introduced parallely to [18] the following new graph invariant:

$$s^*_\alpha(G) = \sum_{i=1}^{n-1} \lambda_i^\alpha, \alpha \neq 0, 1,$$

characterized as the sum of the α-th power of the non-zero normalized Laplacian eigenvalues of a graph. Several properties of this index have been proposed in [7] and some lower and upper bounds for a connected graph have been derived.

In [1], considering the Schur-convexity or Schur-concavity of the functions $s^*_\alpha(G)$ and using additional information on the localization of the eigenvalues, the following Theorems, which generalize Theorem 3.3 in [7], have been proved.

Theorem 2.1. *Let G be a simple connected graph with $n \geq 3$ vertices and $\lambda_1 \geq \theta$:*

1. *if $\alpha < 0$ or $\alpha > 1$ then*
$$s^*_\alpha(G) \geq \theta^\alpha + \frac{(n-\theta)^\alpha}{(n-2)^{\alpha-1}} \tag{2.1}$$
2. *if $0 < \alpha < 1$ then*
$$s^*_\alpha(G) \leq \theta^\alpha + \frac{(n-\theta)^\alpha}{(n-2)^{\alpha-1}}. \tag{2.2}$$

Theorem 2.2. *Let G be a simple connected graph with $n \geq 4$ vertices which is not complete and $\lambda_1 \geq \theta$, $\lambda_2 \geq \beta$ with $\theta \geq \beta$ and $\theta + \beta(n-2) > n$.*

1. *if $\alpha < 0$ or $\alpha > 1$ then*
$$s^*_\alpha(G) \geq \theta^\alpha + \beta^\alpha + \frac{(n-\theta-\beta)^\alpha}{(n-3)^{\alpha-1}} \tag{2.3}$$
2. *if $0 < \alpha < 1$ then*
$$s^*_\alpha(G) \leq \theta^\alpha + \beta^\alpha + \frac{(n-\theta-\beta)^\alpha}{(n-3)^{\alpha-1}}. \tag{2.4}$$

It is noteworthy to state that the results in Theorem 2.2 are tighter than those in Theorem 2.1 (for more details see [3] and [4]).

In [7], the bounds in Theorem 2.1 have been previously proved identifying θ as

$$P = 1 + \sqrt{\frac{2}{n(n-1)} \sum_{(i,j \in E)} \frac{1}{d_i d_j}}. \tag{2.5}$$

In Section 4, by applying some results proved in [5], we provide lower bounds of λ_1 and λ_2 that enable us to assess tighter bounds of $s^*_\alpha(G)$ than in [7]. In particular, we obtain an alternative value of θ than (2.5) (referred as Q) and a specific value of β (referred as R).

3 A nonlinear optimization problem to bound eigenvalues

We now recall a methodology based on majorization techniques (see [5] and [15]) that allows us to find a suitable localization of λ_1 and λ_2.
At this regard, we define the set

$$S_b^{\lambda} = \{\boldsymbol{\lambda} \in \mathbb{R}_+^{n-1} : \lambda_1 \geq \lambda_2 \geq ... \geq \lambda_{n-1} \geq 0, \sum_{i=1}^{n-1} \lambda_i = n, g(\boldsymbol{\lambda}) = \sum_{i=1}^{n-1} \lambda_i^p = b\},$$

where p is an integer greater than 1, $b \in \mathbb{R}$ and g is a continuous function, homogeneous of degree p, real and strictly Schur-Convex (see [15]).
The following fundamental lemma holds (see Lemma 2.1 in [5]):

Lemma 3.1. *Fix $b \in \mathbb{R}$ and consider the set S_b^{λ}. Then either $b = \frac{n^p}{(n-1)^{p-1}}$ or there exists a unique integer $1 \leq h^* < (n-1)$ such that:*

$$\frac{n^p}{(h^*+1)^{p-1}} < b \leq \frac{n^p}{(h^*)^{p-1}}, \tag{3.1}$$

where $h^* = \left\lfloor \sqrt[p-1]{\frac{n^p}{b}} \right\rfloor$.

A lower bound for λ_h $(h = 1, ..., n-1)$ can be obtained by solving the following optimization problem $P^*(h)$:

$$\min\ (\lambda_h)\ \text{ subject to } \boldsymbol{\lambda} \in S_b^{\lambda} \qquad\qquad P^*(h)$$

The solution of the nonlinear optimization problem $P^*(h)$ is given in the following Theorem that we recall from Theorem 3.2 in [5] (for detailed proof see [5]).

Theorem 3.2. *The solution of the optimization problem $P^*(h)$ is $(\frac{n}{n-1})$ if $b = \frac{n^p}{(n-1)^{p-1}}$.*

If $b \neq \frac{n^p}{(n-1)^{p-1}}$, the solution of the optimization problem $P^*(h)$ is δ^* where

1. *for $h = 1$, δ^* is the unique root of the equation*

$$f(\delta, p) = h^*\delta^p + (n - h^*\delta)^p - b = 0 \tag{3.2}$$

   in $I = \left(\frac{n}{h^*+1}, \frac{n}{h^*}\right]$;
2. *for $1 < h \leq (h^*+1)$, δ^* is the unique root of the equation*

$$f(\delta, p) = (n-h)\delta^p + (h-1)\frac{(n-(n-h)\delta)^p}{(h-1)^p} - b = 0 \tag{3.3}$$

   in $I = (0, \frac{n}{n-1}]$;
3. *for $h > (h^*+1)$, δ^* is zero.*

It is noteworthy that we use this Theorem in the next Section to obtain lower bounds for λ_1 and λ_2.

4 New bounds for normalized Laplacian eigenvalues and $s^*_\alpha(G)$

We now present a schematic framework of the main steps we follow in order to provide new limitations for λ_1 and λ_2 useful to get new bounds for the descriptor $s^*_\alpha(G)$.

1. **A new lower bound Q for λ_1**
   At this regard, we consider Theorem 3.2 limiting[1] the analysis when $p = 2$: in this case we know indeed that $b = n + 2\sum_{(i,j)\in E} \frac{1}{d_i dj}$. For Lemma 3.1, when $b = \frac{n^2}{(n-1)}$ the solution of optimization problem $P^*(h)$ is $\left(\frac{n}{n-1}\right)$. This is the case of the complete graph K_n. Instead, when $b \neq \frac{n^2}{(n-1)}$, $h^* = \left\lfloor \frac{n^2}{b} \right\rfloor$.
   Considering non-complete graphs, to get a lower bound for λ_1 we solve Equation (3.2) being $h = 1$. By some basic algebra, the acceptable solution in the interval I is equal to $\delta^* = \frac{\left(n+\sqrt{\frac{b(h^*+1)-n^2}{h^*}}\right)}{(1+h^*)}$ and we refer to this value as Q.
2. **New bounds for $s^*_\alpha(G)$ based on Q**
   Considering Theorem 2.1 we obtain new bounds for $s^*_\alpha(G)$ by replacing the generic limitation θ with Q in (2.1) and (2.2).
3. **Comparison between Q and P**
   The value of Q can be compared to P (see Equation (2.5)) in order to show how bounds (2.1) and (2.2), computed by assuming $\theta = Q$, perform better than those with $\theta = P$ (as proposed in [7]). It is well known that, for every connected graph of order n (see [2]), we have:

$$\frac{1}{n-1} \leq \frac{2}{n} \sum_{(i,j)\in E} \frac{1}{d_i d_j} < 1, \tag{4.1}$$

   and the left inequality is attained for the complete graph $G = K_n$.
   Figure 1 reports patterns of P and Q, varying the quantity $t = 2 \cdot \sum_{(i,j)\in E} \frac{1}{d_i d_j}$ in the proper interval $\left(\frac{n}{n-1}, n\right)$ (see Equation (4.1)) for alternative values of number of vertices n. Being $P = 1 + \sqrt{\frac{t}{n(n-1)}}$, it is easy to see that P has a monotonic behaviour with respect to t. $P \in \left(\frac{n}{n-1}, 1 + \sqrt{\frac{1}{n-1}}\right)$, while $Q \in (\frac{n}{n-1}, 2)$. Furthermore, Figure 1 shows that Q increases faster than P when $t \in \left(\frac{n}{n-1}, n\right)$.

[1] For values of $p \neq 2$, b depends on the graph's structure and topology. So the procedure can be only numerically applied: we need to compute the eigenvalues of normalized Laplacian matrix, but this information allows to directly obtain $s^*_\alpha(G)$. In this case, the evaluation of bounds is useless.

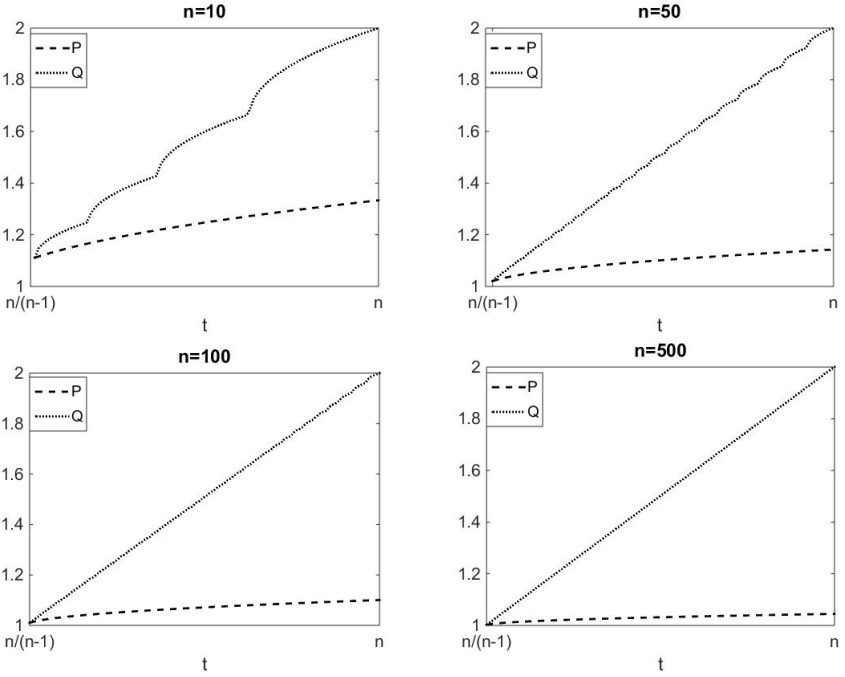

Figure 1: Q and P according to different values of $t \in \left(\frac{n}{n-1}, n\right)$ and several number of vertices.

Going deeply into the analysis, we now analytically prove that our bound Q on λ_1 is always better than bound P provided in [7]

Main Result. The limitation Q is strictly greater than P for non-complete graphs.

Proof. We start considering:

$$f(t) = Q - P = \frac{\left(n + \sqrt{\frac{(n+t)(h^*+1)-n^2}{h^*}}\right)}{(1+h^*)} - 1 - \sqrt{\frac{t}{n(n-1)}}, \tag{4.2}$$

where $f(t) \in \left(0, 1 - \sqrt{\frac{t}{n(n-1)}}\right)$, $h^* = \left\lfloor \frac{n^2}{n+t} \right\rfloor$ and $h^* \in \left(\left\lfloor \frac{n}{2} \right\rfloor, n-1\right)$.

Furthermore, when

$$t = \frac{n(n-x)}{n+x} \text{ with } x = \begin{cases} 0, 2, 4, ..., (n-2) & \text{if} \quad n \quad \text{is even} \\ 1, 3, 5, ..., (n-2) & \text{if} \quad n \quad \text{is odd} \end{cases} \tag{4.3}$$

$\frac{n^2}{n+t}$ is an integer (i.e. $h^* = \frac{n^2}{n+t}$).

We can now distinguish two cases:

- when (4.3) holds, $\frac{n^2}{n+t}$ is an integer. Doing some algebra, we have $f(t) = \frac{t}{n} - \sqrt{\frac{t}{n(n-1)}}$. It is immediate to see that $f(t) > 0$, with $f(t) = 0$ only for complete graphs (being in that case $t = \frac{n}{n-1}$);

- otherwise, $\frac{n^2}{n+t}$ is not an integer. Being $f(t) \geq 0$ at the boundaries of its domain and $f(t) > 0$ for values of t so that h^* is an integer, by proving that $f(t)$ is strictly increasing on its remaining domain, we have $f(t) > 0$. Since $f(t)$ is required to be strictly increasing, we compute
$f'(t) = \frac{1}{2h^*\sqrt{\frac{(n+t)(h^*+1)-n^2}{h^*}}} - \frac{1}{2n(n-1)}\frac{1}{\sqrt{\frac{t}{n(n-1)}}}$ (defined in $t \neq \frac{n(n-x)}{n+x}$).
In order to show that $f'(t) > 0$, by simple algebra we get:
$t\,(n(n-1) - h^*(h^*+1)) + nh^*\,(n - (h^*+1)) > 0$.
Being $h^* < n-1$ for non-complete graphs, we have $f'(t) > 0$.

It follows that $Q > P$ for non-complete graphs.

□

Now, $\lambda_1 \geq Q \geq P$ entails that bounds (2.1) and (2.2) with $\theta = Q$ perform better than those in [7] (see [3] and [4] for more theoretical details).

4. **A new lower bound R for λ_2**
With the aim to improve previous results, we can now derive additional information on λ_2. We still apply Theorem 3.2, considering the case $h = 2$. Since $h \leq (h^* + 1)$, we solve the Equation (3.3) finding in the interval I the acceptable solution:

$$R = \delta^* = \frac{n - \sqrt{\frac{b(n-1)-n^2}{n-2}}}{n-1}.$$

5. **New bounds for $s^*_\alpha(G)$ based on Q and R**
Considering Theorem 2.2, it is possible to obtain new bounds for $s^*_\alpha(G)$ by replacing the generic limitations θ and β with Q and R respectively in (2.3) and (2.4). In order to assess these bounds, both conditions of Theorem 2.2 must be satisfied.

   In this case, the leftmost inequality of (4.1) implies $b \geq \frac{n^2}{n-1}$. By plugging this information in the value of R, we easily obtain $R \leq \frac{n}{n-1}$ that fulfills the condition $R \leq Q$ of Theorem 2.2. The other condition, $Q + R(n-2) > n$, required by Theorem 2.2 will be numerically checked in the next Section.

In case of bipartite graphs it is well known that $\lambda_1 = 2$. If we set $\theta = 2$ in Theorem 2.1, we derive the same results found in [1]. Furthermore, by placing $\theta = 2$ and $\beta = R$ in bounds (2.3) and (2.4), we also provide limitations for bipartite graphs.

5 Some numerical results

The proposed bounds have been evaluated on different graphs. We now focus only on non-bipartite graphs and we provide a comparison with literature (see [7]).
In order to assure a robust analysis, graphs have been randomly generated following the Erdös-Rényi (ER) model $G_{ER}(n, q)$ (see [6], [8], [11] and [12]). Graphs have been obtained by using a MatLab code that gives back only connected graph based on the ER model (see [9] and [10]). In this fashion, the graph is constructed by connecting nodes randomly such that edges are included with probability independent from every other edge. The results are based on a classic assumption of a probability of existence of edges q equal to 0.5. We obtain indeed that the generated graphs have a number of edges not far from the half of its maximum value as proved in the literature (see for example [13]).

At this regard, in Table 1, $s^*_\alpha(G)$ has been computed for several graphs by fixing α equal to 0.5. We report values of upper bound (2.2) evaluated by using $\theta = Q$ or $\theta = P$ (as proposed in [7]).

We refer to these bounds as (2.2Q) and (2.2P). Likewise bound (2.4QR) identifies bound (2.4) evaluated when $\theta = Q$ and $\beta = R$, where the results has been provided assuring that assumptions of Theorem 2.2 are satisfied. Relative errors r measures the absolute value of the difference between the upper bounds and $s^*_\alpha(G)$ divided by the value of $s^*_\alpha(G)$. We observe an improvement with respect to existing bounds according to all the analyzed graphs and the improvement appears reduced for very large graphs. However, for large graphs the formula provided in [7] already gives a very low relative error.

n	d_1	m	$s^*_\alpha(G)$	bound (2.2Q)	bound (2.4QR)	bound (2.2P)	r(2.2Q)	r(2.4QR)	r(2.2P)
4	2	3	3.35	3.44	3.43	3.46	2.86%	2.55%	3.47%
5	4	9	4.46	4.47	4.47	4.47	0.23%	0.21%	0.25%
6	3	6	5.30	5.47	5.46	5.48	3.13%	3.00%	3.27%
7	5	14	6.43	6.48	6.48	6.48	0.83%	0.81%	0.86%
8	5	13	7.33	7.48	7.48	7.48	2.02%	1.98%	2.06%
9	6	16	8.31	8.48	8.48	8.48	2.04%	2.01%	2.07%
10	8	25	9.39	9.51	9.48	9.52	1.36%	1.04%	1.37%
20	15	95	19.37	19.51	19.49	19.51	0.71%	0.62%	0.72%
30	19	209	29.36	29.50	29.50	29.50	0.49%	0.46%	0.49%
50	33	604	49.37	49.50	49.50	49.50	0.27%	0.26%	0.27%
100	60	2459	99.37	99.50	99.50	99.50	0.13%	0.12%	0.13%
200	116	10001	199.38	199.50	199.50	199.50	0.06%	0.05%	0.06%
300	179	22437	299.37	299.50	299.50	299.50	0.04%	0.04%	0.04%
500	279	62456	499.38	499.50	499.50	499.50	0.03%	0.02%	0.03%

Table 1: Upper bounds for $s^*_\alpha(G)$ for $\alpha = 0.5$ and relative errors.

The comparison has been extended in order to test the behaviour of the upper bounds on alternative graphs. First of all, in the ER model used to generate graphs, the parameter q can be thought of as a weighting function. As q increases from 0 to 1, the model becomes more and more likely to include graphs with more edges and less and less likely to include graphs with fewer edges. In this regard, we assign several values of q moving from the default value of 0.5. For sake of simplicity we report only the relative errors derived for graphs generated by using respectively $q = 0.1$ and $q = 0.9$ (see Figure 2). In all cases bound (2.4QR) assures the best approximation to $s^*_\alpha(G)$ for $\alpha = 0.5$. We observe a best behaviour of all bounds when $q = 0.9$ because we are moving towards the complete graph. We have indeed that the density of the graphs increases as long as greater probabilities are considered.

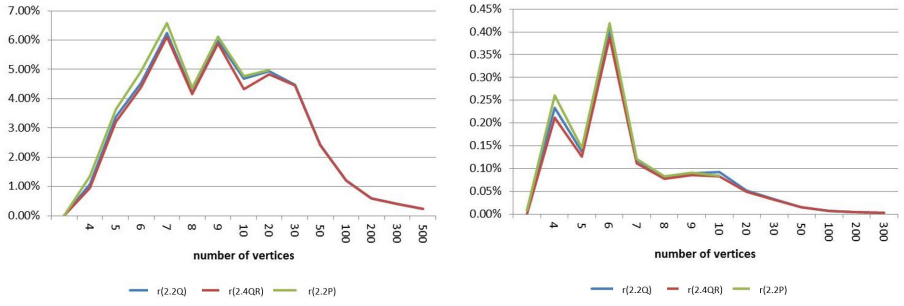

Figure 2: Relative errors of upper bounds of $s^*_{0.5}(G)$ for graphs $ER(n, 0.1)$ and $ER(n, 0.9)$ respectively.

Finally, for the same index $s^*_{0.5}(G)$, upper bounds have been evaluated for trees[2]. Table 2 depicts slighter differences for larger graphs in this case too. However it could be noticed how the relative improvement of bounds respect to other bounds is greater than in case of non-bipartite graphs. Despite greater relative errors are observed, bound (2.4QR) is confirmed as the tighter bound also in this case.

	Trees			
n	$s^*_\alpha(G)$	r(2.2Q)	r(2.4QR)	r(2.2P)
4	3.35	2.04%	1.95%	3.47%
5	4.32	2.17%	2.14%	3.48%
6	5.23	3.56%	3.51%	4.73%
7	6.19	3.62%	3.59%	4.67%
8	7.15	3.67%	3.64%	4.61%
9	8.22	2.35%	2.34%	3.20%
10	8.85	6.35%	6.32%	7.15%
20	18.07	7.45%	7.44%	7.88%
30	27.63	6.47%	6.47%	6.77%
50	45.73	8.07%	8.06%	8.25%
100	91.23	8.97%	8.97%	9.06%
200	182.72	9.14%	9.14%	9.18%
300	274.71	8.99%	8.99%	9.02%
500	457.71	9.11%	9.11%	9.13%

Table 2: $s^*_{0.5}(G)$ and relative errors for Trees T.

The analysis has been further developed considering a value of α equal to 1.5. Generating a similar sample of graphs, both $s^*_{1.5}(G)$ and the relative bounds have been derived. For sake of simplicity we report only the results for $ER(n, 0.5)$ observing that the additional information on the localization of λ_1 and λ_2 lead to the tighter lower bound (2.3QR). Analogous results have been obtained by considering both ER graphs with alternative values of q and bipartite graphs.

n	d_1	m	$s^*_\alpha(G)$	bound (2.1Q)	bound (2.3QR)	bound (2.1P)	r(2.1Q)	r(2.3QR)	r(2.1P)
4	3	4	4.79	4.66	4.67	4.62	2.69%	2.39%	3.49%
5	2	4	6.22	5.65	5.69	5.60	9.07%	8.51%	9.95%
6	4	9	6.85	6.59	6.60	6.57	3.78%	3.63%	4.00%
7	6	13	7.77	7.57	7.57	7.56	2.56%	2.49%	2.65%
8	7	18	8.75	8.56	8.56	8.55	2.15%	2.10%	2.20%
9	4	12	10.28	9.58	9.59	9.55	6.88%	6.79%	7.15%
10	7	26	10.83	10.52	10.55	10.51	2.90%	2.60%	2.94%
20	13	98	20.88	20.50	20.52	20.50	1.81%	1.71%	1.81%
30	19	222	30.88	30.50	30.51	30.50	1.21%	1.18%	1.21%
50	31	644	50.85	50.50	50.51	50.50	0.68%	0.67%	0.68%
100	62	2512	100.87	100.50	100.50	100.50	0.37%	0.36%	0.37%
200	117	9918	200.88	200.50	200.50	200.50	0.19%	0.19%	0.19%
300	179	22540	300.87	300.50	300.50	300.50	0.12%	0.12%	0.12%
500	279	62063	500.88	500.50	500.50	500.50	0.08%	0.08%	0.08%

Table 3: Lower bounds for $s^*_{1.5}(G)$ and absolute value of relative errors.

6 Conclusions

In this paper we provide tighter bounds for the sum of the α-power of the non-zero normalized Laplacian eigenvalues taking into account additional information on the localization of the eigenvalues of the normalized Laplacian matrix of the graph, $\mathcal{L}(G)$. To this aim lower bounds of the eigenvalues are derived by means of the solution of a class of suitable non-linear optimization problems based on majorization techniques. We provide indeed closed

[2]Tree has been generated by using Prüfer code. The Prüfer sequence of a labeled tree is a unique sequence associated to the tree. The sequence for a tree on n vertices has length $n-2$ and it can be generated by a simple iterative algorithm. It is a way to map bijectively trees on n vertices into $n-2$ long sequences of integers drawn from n.

formulae that allow to compute upper and lower bounds of $s^*_\alpha(G)$ by using the additional information on the first and the second eigenvalue of $\mathcal{L}(G)$. It is noteworthy that even only considering the limitation on the first normalized Laplacian eigenvalue we improve existing bounds of $s^*_\alpha(G)$ for non-complete graphs. Numerical comparisons confirm how bounds based also on the second normalized Laplacian eigenvalue are former than those presented in literature. In particular, the analysis has been developed randomly generating both bipartite and non-bipartite graphs with a different number of vertices.

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On ± 1 eigenvectors of graphs

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Dedicated to the memory of Ante Graovac

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Abstract

While discussing his spectral bound on the independence number of a graph, Herbert Wilf asked back in 1986 what kind of a graph admits an eigenvector consisting solely of ± 1 entries? We prove that Wilf's problem is NP-complete, but also that the set of graphs having a ± 1 eigenvector is quite rich, being closed under a number of different graph compositions.

Keywords: Eigenvector, adjacency matrix, Wilf's problem.

Math. Subj. Class.: 05C50

1 Introduction

Chemical graphs, defined as simple, connected, unweighted graphs with the maximum vertex degree at most three, correspond to carbon skeletons of known and potential π-conjugated hydrocarbon molecules, and their adjacency spectra provide models for energies of the π-molecular orbitals of such systems within the simple Hückel approach (see, e.g., [10]). Restriction on the maximum vertex degree confines the eigenvalues of a chemical graph to the interval $[-3, +3]$. Jerry Ray Dias [6] noted that the examples of chemical graphs with adjacency eigenvalues 1, $\sqrt{2}$, $\sqrt{3}$, 2, $\sqrt{5}$, $\sqrt{6}$, $\sqrt{7}$ and 3 are all readily found, and he discussed structural factors associated with the presence of each of these eigenvalues. However, he could not find any chemical graph with eigenvalue $\sqrt{8}$ and made an intriguing conjecture [6, §6] that no such graph exists. Together with Patrick Fowler and

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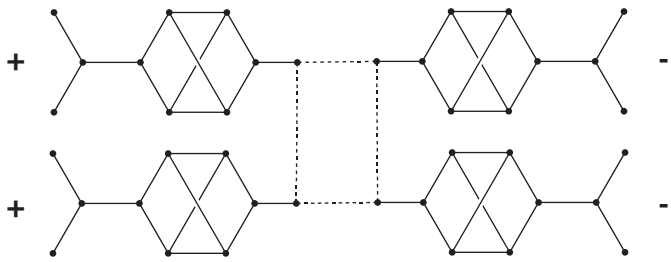

Figure 1: *Construction of a graph with the maximum degree three and eigenvalue* $\sqrt{8}$ *from* $4k$ *copies of smaller such graph containing a leaf. Copies of the local eigenvector corresponding to the eigenvalue* $\sqrt{8}$ *are taken with the signs* $+, +, -, -, +, +, -, -, \ldots$ *to give an eigenvector corresponding to the eigenvalue* $\sqrt{8}$ *in the larger graph. (Reprinted from [7].)*

Marko Milošević, the present author disproved Dias' conjecture by giving a number of constructions of chemical graphs with the eigenvalue $\sqrt{8}$ in [7]. One particular construction, showcased in Fig. 1, stands out as it relies on a curious property of cycles with $4k$ vertices—that its vertices can be partitioned into two sets such that the neighbors of each vertex are equinumerously divided among both sets. This property is easily seen to be equivalent to the existence of a ± 1 eigenvector corresponding to the adjacency eigenvalue 0.

Quite some time later, while meticulously preparing his research monograph on the spectral radius of graphs [14], the first author found out that Herbert Wilf had asked already in 1986 what kind of a graph admits an eigenvector consisting solely of ± 1 entries? In Wilf's case, the question arised in the discussion of his spectral bound on the independence number of regular graphs [16]. Although the question explicitly asks just for a ± 1 eigenvector of a graph, it is implicitly assumed in [16] that such an eigenvector corresponds to the smallest eigenvalue of a regular graph. This implicit assumption renders the question nearly impossible to answer in a simple manner, as there exist strongly regular graphs with the same parameter set such that some of them have and the others do not have a ± 1 eigenvector corresponding to the smallest eigenvalue. We will, therefore, treat Wilf's question in its more general form and consider the problem of the existence of a ± 1 eigenvector corresponding to any eigenvalue of a graph.

The paper is organized as follows. In the rest of this section we list necessary definitions and preliminaries. In Section 2 we prove that this problem is polynomially reducible to the problem of the existence of a ± 1 eigenvector corresponding to the eigenvalue 0, and that the latter problem is NP-complete. In Section 3 we give a simple and straightforward algorithm for solving both problems, and use it to show that the three Chang graphs all have a ± 1 eigenvector corresponding to the smallest eigenvalue, while $L(K_8)$, the fourth $(28, 12, 6, 4)$-strongly regular graph, does not have such an eigenvector. Nevertheless, we show in Section 4 that the set of graphs with a ± 1 eigenvector corresponding to the eigenvalue 0 has rich structure, being closed under a number of different graph compositions.

Cartesian product of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the graph $G_1 + G_2$ with the vertex set $V_1 \times V_2$ such that two vertices (u_1, u_2) and (v_1, v_2) are adjacent in $G_1 + G_2$ if either $u_1 = v_1$, $(u_2, v_2) \in E_2$ or $(u_1, v_1) \in E_1$, $u_2 = v_2$. Cartesian product of graphs is a special case of a more general graph composition, called the NEPS of graphs.

Let $\mathcal{B}$ be a set of nonzero binary n-tuples, i.e., $\mathcal{B} \subseteq \{0,1\}^n \setminus \{(0,\ldots,0\}$, such that for every $i = 1,\ldots,n$ there exists $\beta \in \mathcal{B}$ with $\beta_i = 1$. The *non-complete extended p-sum* of graphs $G_1 = (V_1, E_1), \ldots, G_n = (V_n, E_n)$ with the basis $\mathcal{B}$, denoted by $\mathrm{NEPS}(G_1, \ldots, G_n; \mathcal{B})$, is the graph with the vertex set $V_1 \times \cdots \times V_n$ in which two vertices $u = (u_1, \ldots, u_n)$ and $v = (v_1, \ldots, v_n)$ are adjacent if and only if there exists $\beta \in \mathcal{B}$ such that for $i = 1, \ldots, n$ holds $u_i = v_i$ if $\beta_i = 0$ and $(u_i, v_i) \in E_i$ if $\beta_i = 1$. The *Kronecker product* $A \otimes B$ of matrices $A = (a_{ij})_{m,n}$ and $B = (b_{ij})_{p,q}$ is the $mp \times nq$ matrix obtained from A by replacing each entry a_{ij} by the block $a_{ij}B$. It is well known (see, e.g., [13]) that the Kronecker product is distributive with respect to the standard product of matrices:

$$(AB) \otimes (CD) = (A \otimes C)(B \otimes D). \tag{1.1}$$

2 NP-completeness of the existence of ±1-eigenvectors

We start by showing that in order to be able to decide if the adjacency matrix of a graph has a ± 1 eigenvector associated to an arbitrary eigenvalue, it is sufficient to know how to decide if the adjacency matrix has a ± 1-eigenvector corresponding to the eigenvalue 0.

PMEIG problem. Given a simple graph G with an adjacency matrix A, find an eigenvector of A all of whose entries are equal to either $+1$ or -1, if it exists.

PMEIG0 problem. Given a simple graph G with an adjacency matrix A, find an eigenvector of A corresponding to the eigenvalue 0, all of whose entries are equal to either $+1$ or -1, if it exists.

Theorem 2.1. ***PMEIG*** *is polynomially reducible to* ***PMEIG0****.*

Proof. Let G be an n-vertex simple graph with an adjacency matrix A. If G has a ± 1 eigenvector x corresponding to some eigenvalue λ of A, then from

$$Ax = \lambda x$$

and the fact that the entries of Ax and x are integers, we conclude that λ must be an integer itself. (λ cannot be a rational number as it is a root of the monic polynomial $\det(\lambda I - A)$ with integer coefficients.) The value $|\lambda|$ is bounded from above by the spectral radius $\lambda_1(A)$ by the Perron-Frobenius theorem, which is further bounded from above by the maximum vertex degree Δ by the Rayleigh quotient (see, e.g., [14, pp. 8–11] for the discussion of the Perron-Frobenius theorem and the Rayleigh quotient). Thus,

$$\lambda \in \{-\Delta, \ldots, \Delta\}. \tag{2.1}$$

Recall that the adjacency spectrum of the Cartesian product $G + H$ of two graphs G and H is fully described by the adjacency spectra of G and H (see, e.g., [4, pp. 30–32]): if λ is an eigenvalue of G with an eigenvector x and μ is an eigenvalue of H with an eigenvector y, then $\lambda + \mu$ is the eigenvalue of $G + H$ with the eigenvector $x \otimes y$, where $\otimes$ denotes the Kronecker product of matrices. Moreover, all eigenvalues and eigenvectors of $G + H$ are representable in this form.

It is well-known that the adjacency spectrum of the complete bipartite graph $K_{m,m}$ consists of the simple eigenvalue m with the all-one eigenvector j^+, the simple eigenvalue $-m$ with the eigenvector j^- whose entries are equal to 1 in one part and to -1 in the other part of the bipartition, and the eigenvalue 0 of multiplicity $2m - 2$.

Thus, if G has an integer eigenvalue λ with a ± 1 eigenvector x, then $G + K_{|\lambda|,|\lambda|}$ has an eigenvalue 0 with the corresponding ± 1 eigenvector equal to either $x \otimes j^+$ or $x \otimes j^-$. We see that, due to (2.1), to solve **PMEIG** it is enough to solve **PMEIG0** for the $\Delta+1 \leq n$ graphs

$$G, \quad G + K_{1,1}, \quad G + K_{2,2}, \quad \ldots, \quad G + K_{\Delta,\Delta}.$$

Since these graphs have n, $2n$, $4n$, $\ldots$, $2\Delta n$ vertices, respectively, this represents a polynomial-time Turing reduction from **PMEIG** to **PMEIG0**. □

Next, observe that each ± 1 eigenvector x of A corresponding to the eigenvalue 0 determines the partition $V = V_x^+ \cup V_x^-$ of the vertex set V of G:

$$\begin{aligned} V_x^+ &= \{u \in V : x_u = 1\}, \\ V_x^- &= \{u \in V : x_u = -1\}. \end{aligned}$$

Due to

$$Ax = 0$$

and the fact that for each $u \in V$

$$(Ax)_u = \sum_{v \sim u} x_v, \tag{2.2}$$

we see that the partition $V^+ = V_x^+$, $V^- = V_x^-$ satisfies:

$$\begin{gathered} \textit{For each vertex } u \in V \textit{ the number of its neighbors in } V^+ \\ \textit{is equal to the number of its neighbors in } V^-. \end{gathered} \tag{2.3}$$

We will say that a graph G with the vertex set V is *eigenpartite* if there exists a partition $V = V^+ \cup V^-$, $V^+ \cap V^- = \emptyset$, satisfying the property (2.3). From (2.2) it is obvious that if G is eigenpartite, then G has a ± 1 eigenvector x corresponding to the eigenvalue 0, obtained by setting its components to $+1$ for vertices in V^+ and to -1 for vertices in V^-. Hence **PMEIG0** is equivalent to the problem of eigenpartiteness of G.

The proof of the following theorem was communicated to the author by Brendan McKay and László Lovász.

Theorem 2.2. ***PMEIG0*** *is NP-complete.*

Proof. We prove this theorem by reducing a known NP-complete problem to **PMEIG0**. For an integer $k \geq 2$, a *k-uniform hypergraph* H is an ordered pair $H = (V, E)$, where the set of vertices V is a finite nonempty set, and the set of edges E is a family of distinct k-subsets of V. A hypegraph $H = (V, E)$ is *2-colorable* if it admits a partition of its vertex set V into two color classes so that no edge in E is monochromatic. It was shown in [12] that deciding 2-colorability of k-uniform hypergraphs is NP-complete for every fixed $k \geq 3$. Even more, deciding 2-colorability of a 4-uniform hypergraph so that each edge has two vertices of each color is also NP-complete.

Take an instance $H = (V, E)$ of the latter hypergraph problem. Construct a simple graph G with the vertex set $V \cup E' \cup E''$, where E' and E'' are two copies of E:

$$E' = \{e' : e \in E\}, \qquad E'' = \{e'' : e \in E\}.$$

For each edge $e' = e'' = \{w, x, y, z\}$ of H, G contains the edges

$$\{e'w, e'x, e'y, e'z, e''w, e''x, e''y, e''z\}.$$

If the hypergraph H has a 2-coloring so that each edge has two vertices of each color, then the graph G is eigenpartite: partition V as $V' \cup V''$ according to the 2-coloring of H, put all of E' in one part and all of E'' in the other part. The neighbors of each vertex u in V of G are those elements of E' and E'' that correspond to the edges of E in H incident to u, so that u satisfies (2.3). The neighbors of each vertex e' in E' of G are those vertices of V that are incident to the corresponding edge e in H, of which two are in V' and the other two are in V'', so that e' satisfies (2.3) as well.

Conversely, if the graph G is eigenpartite, then the hypergraph H is 2-colorable with each edge having two vertices of each color: just color the vertices of V according to the eigenpartition. □

3 An exhaustive search algorithm for PMEIG0

The eigenspace $\mathcal{E}_0$ of the eigenvalue 0 of A, as a kernel of A, consists of vectors whose entries are coefficients of linear combinations of the columns of A with value equal to 0. To compute the basis of $\mathcal{E}_0$ it thus suffices to compute the column echelon form $\begin{bmatrix} B \\ C \end{bmatrix}$ of the row augmented matrix $\begin{bmatrix} A \\ I \end{bmatrix}$. During the computation of the column echelon form of A, the identity matrix in $\begin{bmatrix} A \\ I \end{bmatrix}$ serves to keep track of the coefficients of linear combinations of columns of A which yield the columns of B. Thus, the basis of $\mathcal{E}_0$ consists of those (nonzero) columns of C for which the corresponding column of B is a zero column. Since the entries of A and I are integers, the column echelon form can be computed in integer arithmetic by Bareiss algorithm [1].

INPUT: An $n \times n$ adjacency matrix A
OUTPUT: A ± 1-eigenvector x of the eigenvalue 0 of A, if it exists

Use Bareiss algorithm to compute the column echelon form $\begin{bmatrix} B \\ C \end{bmatrix}$ of $\begin{bmatrix} A \\ I \end{bmatrix}$

$D \leftarrow$ the nonzero columns of C such that the corresponding column of B is 0
if D is empty **then**
    return "there is no such eigenvector"
end if
$k \leftarrow$ the number of columns of D
$U \leftarrow$ the set of row indices of D yielding a submatrix E of rank k
for each $z \in \{-1, +1\}^U$ **do**
    solve the linear system $Ey = z$
    $x \leftarrow Dy$
    if x is a ± 1 vector **then**
        return x
    end if
end for
return "there is no such eigenvector"

The second part of the algorithm then exhaustively searches the set of all ± 1 vectors over U for their potential extensions to the full ± 1 eigenvector of the eigenvalue 0: any $z \in \{-1, +1\}^U$ can be uniquely written as $z = Ey$, since E has the full rank, and then

$x = Dy$ is the unique eigenvector of 0 that coincides with z over U.

Since Bareiss algorithm has polynomial running time, the time complexity of the above algorithm is controlled by multiplicity of the eigenvalue 0. Although it is believed that almost all graphs have simple eigenvalues only (which is supported by a recent proof of Tao and Vu [15] of Babai's conjecture that the Erdös-Rényi random graph $G(n, \frac{1}{2})$ has all simple eigenvalues with probability $1 - o(1)$), the problem with the above algorithm, as expected, is that most of the interesting graphs, to which we would like to apply it, do have high multiplicity of the eigenvalue 0. For example, the graph constructed in Theorem 2.2 in the reduction from the problem of 2-coloring 4-uniform hypergraph $H = (V, E)$ to **PMEIG0**, is bipartite with the bipartition $(V, E' \cup E'')$. Multiplicity of its eigenvalue 0 is then, according to [5], at least the difference $2|E| - |V|$ in sizes of its bipartition, so that the above algorithm then has running time complexity not less than $2^{2|E|-|V|}$.

The above algorithm can be used to test existence of a ± 1 eigenvector for any other fixed eigenvalue λ of the adjacency matrix A simply by supplying $A - \lambda I$ instead of A to it. We have run this algorithm on the triangular graph $L(K_8)$ and the three Chang graphs cospectral to it. Recall that the triangular graph is the line graph $L(K_m)$, defined on the pairs of an n-set, with two pairs adjacent if they have an element in common. It is a strongly regular graph with the parameters $(\nu, k, \lambda, \mu) = (m(m-1)/2, 2(m-2), m-2, 4)$. Chang [2, 3] and Hoffman [11] proved that if G is a strongly regular graph with these parameters, then for $m \neq 8$, $m \geq 4$, G is isomorphic to the triangular graph $L(K_m)$, while for $m = 8$, G is isomorphic either to $L(K_8)$ or to one of three Chang graphs. For $m = 8$, all four of these graphs have the adjacency spectrum $[12, 4^{(7)}, -2^{(20)}]$, with exponents denoting multiplicities. Interestingly, the above algorithm reports that each of the three Chang graphs has a ± 1 eigenvector corresponding to the least eigenvalue -2, while the triangular graph $L(K_8)$ does not have such eigenvector. Since these four graphs share the same local neighborhood structure, it becomes apparent that one could hardly hope to find a simple answer to Wilf's implicit question of existence of a ± 1 eigenvector corresponding to the smallest eigenvalue of a regular graph.

4 Constructions of eigenpartite graphs

Although it is NP-complete to check whether a given graph is eigenpartite, sheer simplicity of its defining condition 2.3 makes it easy to construct new eigenpartite graphs.

Probably the simplest way to construct an eigenpartite graph from an arbitrary graph G is by taking two copies of it and adding edges between different copies in accordance to G: an edge is added between two vertices in different copies whenever these vertices are adjacent in G. V^+ is then formed by the vertices in one copy, and V^- by the vertices of the other copy of G. A few more constructions are variations on this theme:

- (Suggested by Brendan McKay.) Suppose that G and H are graphs with degree sequences S and T, respectively, such that (S, T) is also degree sequence of a bipartite graph K with the bipartition (U, V). An eigenpartite graph is obtained by superimposing G on the vertices of U in accordance to S, and by superimposing H on the vertices of V in accordance to T. (U, V) then represents the eigenpartition of this new graph.
- (Suggested by Ross Kang.) Let G be an eigenpartite graph with an eigenpartition (V^+, V^-). Replace each vertex of G with an independent set of k vertices. Between two distinct independent k-sets corresponding to adjacent vertices in G, superimpose

an arbitrary j-regular bipartite graph on $k+k$ vertices. One part of the eigenpartition of the new graph is then formed by the k-sets corresponding to the vertices in V^+, and the other part by the k-sets corresponding to the vertices in V^-.

- (Suggested by Ross Kang.) Let G be a $2s$-regular eigenpartite graph with an eigenpartition (V^+, V^-). Choose positive integers m, n, p, q, r such that $sp + m = sq = sr + n$. Replace each vertex of V^+ by an m-regular graph, and replace each vertex of V^- by an n-regular graph. Between the subgraphs corresponding to two neighbouring vertices of V^+ superimpose a bipartite p-regular graph; between the subgraphs corresponding to two neighbouring vertices of V^- superimpose a bipartite r-regular graph; between the subgraphs corresponding to a vertex of V^+ adjacent to a vertex of V^- superimpose a bipartite q-regular graph. Similarly, one part of the eigenpartition of the new graph is then formed by the subgraphs corresponding to the vertices in V^+, and the other part by the subgraphs corresponding to the vertices in V^-.

The set of eigenpartite graphs is, in addition, closed to taking arbitrary NEPS. Important property of $\mathrm{NEPS}(G_1, \ldots, G_n; \mathcal{B})$ is that its spectrum can be represented by the spectra of $G_1, \ldots, G_n$ [4, Theorem 2.3.4]: if λ_i is an eigenvalue of G_i with the corresponding eigenvector x_i, for $i = 1, \ldots, n$, then

$$\Lambda = \sum_{\beta \in \mathcal{B}} \lambda_1^{\beta_1} \cdots \lambda_n^{\beta_n}$$

is the eigenvalue of $\mathrm{NEPS}(G_1, \ldots, G_n; \mathcal{B})$ with the corresponding eigenvector

$$x = x_1 \otimes \cdots \otimes x_n,$$

where $\otimes$ denotes the Kronecker product of matrices. Thus, if each x_i is a ± 1 eigenvector corresponding to the eigenvalue 0 of G_i, then $x = x_1 \otimes \cdots \otimes x_n$ is a ± 1 eigenvector corresponding to the eigenvalue 0 of $\mathrm{NEPS}(G_1, \ldots, G_n; \mathcal{B})$.

Many standard graph products are instances of NEPS: the Cartesian product of two graphs is obtained for the basis $\mathcal{B} = \{(1,0), (0,1)\}$, the direct product for $\mathcal{B} = \{(1,1)\}$, and the strong product for $\mathcal{B} = \{(1,1), (1,0), (0,1)\}$.

The last construction we present here relies on partial Cartesian product of graphs [9]. Let $G = (V, E)$ and $H = (W, F)$ be two graphs. For $S \subseteq V$, the *partial Cartesian product* of G and H with respect to S is the graph $G +_S H$ with the vertex set $V \times W$, with two vertices (v_1, w_1) and (v_2, w_2) adjacent if and only if either $v_1 = v_2 \in S$ and $(w_1, w_2) \in F$ or $(v_1, v_2) \in E$ and $w_1 = w_2$. If $S = V$ then $G +_S H$ is just the standard Cartesian product $G + H$, while if $S = \{v\}$ is a singleton, then $G +_{\{v\}} H$ is a particular case of the rooted product of graphs [8].

If A_G and A_H are adjacency matrices of G and H, respectively, then the adjacency matrix A of $G +_S H$ is given by

$$A = I_S \otimes A_H + A_G \otimes I,$$

where I_S is the diagonal matrix defined as

$$(I_S)_{u,v} = \begin{cases} 1, & \text{if } u = v \in S, \\ 0, & \text{otherwise,} \end{cases}$$

and I is the standard unit matrix. If x is an eigenvector corresponding to the eigenvalue λ of G and y is an eigenvector corresponding to the eigenvalue 0 of H, then from (1.1)

$$A(x \otimes y) = (I_S x) \otimes (A_H y) + (A_G x) \otimes (Iy) = \lambda x \otimes y$$

due to $A_H y = 0$. Hence

Lemma 4.1. *If H has an eigenvalue 0, then the spectrum of G is contained in the spectrum of $G +_S H$ for each $S \subseteq V(G)$.*

In addition, if x and y are ± 1 vectors, then $x \otimes y$ is also a ± 1 vector, so that

Corollary 4.2. *If G and H are eigenpartite graphs, then $G +_S H$ is an eigenpartite graph for each $S \subseteq V(G)$.*

Note that the construction showcased in Fig. 1 is a partial Cartesian product of a graph G with the eigenvalue $\sqrt{8}$, with S consisting of one of its leaves, and a cycle C_{4k}, which has eigenvalue 0. Hence by Lemma 4.1, the resulting partial Cartesian product has maximum degree three and the eigenvalue $\sqrt{8}$ for each $k \geq 1$.

5 Conclusion

We have studied here Wilf's question of what kind of a graph admits an eigenvector consisting solely of ± 1 entries [16]? Under Wilf's implicit assumption that the ± 1 eigenvector should correspond to the smallest eigenvalue of a regular graph, the question hardly has a simple answer, due to the difference in behavior between the triangular graph $L(K_8)$ and the three Chang graphs, all four being nonisomorphic strongly regular graphs with the same parameters $(28, 12, 6, 4)$.

Without this assumption, it turns out that to answer whether a graph has a ± 1 eigenvector corresponding to any of its eigenvalues, it is enough to be able just to answer whether a graph has a ± 1 eigenvector corresponding to the eigenvalue 0. This, unfortunately, does not make the situation any easier, as the latter problem turns out to be NP complete.

Regardless of these negative results, the set of graphs having a ± 1 eigenvector corresponding to the eigenvalue 0 turns out to be quite rich: it is closed under taking arbitrary NEPS and partial Cartesian products of its elements, and for an arbitrary graph G it contains a graph having G as its induced subgraph.

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Resonance graphs of fullerenes*

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Abstract

A fullerene G is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The resonance graph $R(G)$ of G reflects the structure of its perfect matchings. The Zhang-Zhang polynomial of a fullerene is a counting polynomial of resonant structures called Clar covers. The cube polynomial is a counting polynomial of induced hypercubes in a graph.

In the present paper we show that the resonance graph of every fullerene is bipartite and each connected component has girth 4 or is a path. Also, the equivalence of the Zhang-Zhang polynomial of a fullerene and the cube polynomial of its resonance graph is established. Furthermore, it is shown that every subgraph of the resonance graph isomorphic to a hypercube is an induced subgraph in the resonance graph. For benzenoid systems and tubulenes each connected component of the resonance graph is the covering graph of a distributive lattice; for fullerenes this is not true, as we show with an example.

Keywords: Fullerene, resonance graph, Zhang-Zhang polynomial, cube polynomial, Kekulé structure, perfect matching, distributive lattice, median graph.

Math. Subj. Class.: 92E10, 05C31, 05C70, 06D99

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1 Introduction

A fullerene is a molecule of carbon in the form of a hollow sphere, ellipsoid, tube, or many other shapes. The first fullerene molecule was discovered 30 years ago. In graph theory, a fullerene is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. Kekulé structures of an unsaturated hydrocarbon represent the possible positions of double bonds in the molecule, which corresponds to a perfect matching of a molecular graph. In recent years, a lot of research has been done on the symmetries of fullerenes and their Kekulé structure counts. The concept of the resonance graph of a fullerene was introduced in [9]. The resonance graph of a hydrocarbon reflects the structure of its perfect matchings. There are many results on resonance graphs of benzenoid systems [14] and open-ended carbon nanotubes (tubulenes) [11, 19], but nothing has been done on resonance graphs of fullerenes.

In the present paper we investigate basic properties of resonance graphs of fullerenes. It is shown that the resonance graph of every fullerene is bipartite and each connected component has girth 4 or is a path. Further, the equivalence of Zhang-Zhang polynomial of a fullerene and the cube polynomial of its resonance graph is established. The corresponding results are already known for benzenoid systems and tubulenes (see [14, 12, 11, 17, 3]). Moreover, we prove that every subgraph of the resonance graph of a fullerene that is isomorphic to a hypercube is actually an induced subgraph. We also give an example of a fullerene such that one of the connected components of its resonance graph is not the covering graph of a distributive lattice. This is surprising since all such components are covering graphs of distributive lattices in the case of benzenoid systems and tubulenes (see [15, 13]).

2 Preliminaries

A *fullerene* G is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. By Euler's formula it follows that the number of pentagonal faces is exactly 12 in every fullerene.

A *1-factor* of a fullerene G is a spanning subgraph of G such that every vertex has degree one. Edges of the 1-factor form an independent set of edges i.e. a *perfect matching* of G (in the chemical literature these are known as Kekulé structures; for more details see [5]). Petersen's theorem states that in a bridgeless 3-regular graph, there is always a perfect matching [8]. Therefore, a fullerene always has at least one perfect matching.

Let M be a perfect matching of G. A hexagon h of G is *M-alternating* if the edges of h appear alternately in and out the perfect matching M. Such a hexagon h is also called a *sextet*.

The *resonance graph* $R(G)$ of a fullerene G is the graph whose vertices are the perfect matchings of G, and two perfect matchings M_1 and M_2 are adjacent whenever their symmetric difference $M_1 \oplus M_2$ forms a set of edges of exactly one hexagon of G.

Let G be a fullerene. A *Clar cover* is a spanning subgraph of G such that every component of it is either a hexagon or an edge. The set of hexagons in a Clar cover is a *resonant set* of G. A resonant set with the maximum number of hexagons is a *Clar formula* of G. The number of hexagons in the Clar formula is a *Clar number* $Cl(G)$ of G. The *Zhang-Zhang polynomial* of G (also called the Clar covering polynomial, see [18]) is defined in

the following way:

$$ZZ(G,x) = \sum_{k=0}^{Cl(G)} z(G,k)x^k,$$

where $z(G,k)$ is the number of Clar covers of G with k hexagons. Note that for a fullerene G number $z(G,0)$ equals the number of vertices of $R(G)$ and $z(G,1)$ equals the number of edges of $R(G)$.

The *n-dimensional hypercube* Q_n is the graph whose vertices are all binary strings of length n and two vertices are adjacent if and only if their strings differ exactly in one position. A *Lucas cube* Λ_n is the graph whose vertex set is the set of all binary strings of length n without consecutive 1's and also without 1 in the first and the last bit. The edges are defined analogously as for the hypercube.

Let H be a graph. The *Cube polynomial* of H is defined as follows:

$$C(H,x) = \sum_{i\geq 0} \alpha_i(H)x^i,$$

where $\alpha_i(H)$ denotes the number of induced subgraphs of H that are isomorphic to the i-dimensional hypercube.

The *Cartesian product* $G\Box H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$ and $(a,x)(b,y) \in E(G\Box H)$ whenever $ab \in E(G)$ and $x = y$, or, if $a = b$ and $xy \in E(H)$.

Let $\mathbf{P} = (P, \leq)$ be a poset, i.e. $\leq$ is a binary relation on P, which is reflexive, antisymmetric and transitive. For $x, y \in P$, a *lower bound* of x and y is an element $z \in P$ such that $z \leq x$ and $z \leq y$. A lower bound z of x and y is said to be the *greatest lower bound* (if it exists) if $z' \leq x$ and $z' \leq y$, $z' \in P$, imply that $z' \leq z$. If x and y have a greatest lower bound, then it is unique and denoted by $x \wedge y$. Similarly we can define the least upper bound $x \vee y$ whenever it exists. A *lattice* is a poset in which every pair of elements have the least upper bound and the greatest lower bound. Further, when operations $\wedge$ and $\vee$ of a lattice admit distributive laws we call it a *distributive lattice*. By $x < y$ we mean that $x \leq y$ and $x \neq y$. We say that y *covers* x if $x < y$ and $x < a \leq y$ imply $a = y$. The *covering graph* $\mathcal{C}(\mathbf{P})$ of a poset $\mathbf{P}$ is a graph whose vertices are elements of P and $x, y \in P$ are adjacent in $\mathcal{C}(\mathbf{P})$ if and only if x covers y or y covers x.

Let G be a graph. A *median* of a triple of vertices u, v, w of G is a vertex z that lies on a shortest u, v-path, on a shortest u, w-path and on a shortest v, w-path. Note that z can be one of the vertices u, v, w. A graph is a *median graph* if every triple of its vertices has a unique median. These graphs were first introduced in [1] by Avann. Median graphs arise naturally in the study of ordered sets and distributive lattices. It is known that trees and grid graphs are examples of median graphs.

A graph H is a *retract* of G if there are homomorphisms (edge–preserving functions) $f : V(H) \to V(G)$ and $g : V(G) \to V(H)$ such that $g(f(a)) = a$ for every $a \in V(H)$. Note that if H is a retract of G it is convenient to take H as a subgraph of G and f to be an inclusion map. It is known that median graphs can be characterized as retracts of hypercubes [2].

3 Some results about resonance graphs of fullerenes

In this section we will prove some basic properties of resonance graphs of fullerenes. The first theorem claims that the resonance graph of every fullerene is a bipartite graph. In the proof we use the concept of the dual graph G^*, which has a vertex for each face of G. The dual graph has an edge whenever two faces of G are separated from each other by an edge.

Theorem 3.1. *Let G be a fullerene. Then its resonance graph $R(G)$ is bipartite.*

Proof. It is known that $R(G)$ is bipartite if and only if $R(G)$ does not contain an odd cycle. Let $C = M_0M_1 \dots M_t$ be a cycle in $R(G)$, where $M_0 = M_t$. Hence there exists a sequence of hexagons $h_1, h_2, \dots, h_t$ such that $E(h_i) = M_{i-1} \oplus M_i$ for every $i \in \{1, 2, \dots, t\}$. For every hexagon h of a fullerene G we define $\delta(h)$ to be the number of times h appears in the sequence $h_1, h_2, \dots, h_t$. We will show that $\delta(h)$ is an even number for every hexagon h of G. We consider two options:

(i) Let h be a hexagon with an edge e lying on some pentagon of G. We know that $M_0 = M_0 \oplus E(h_1) \oplus E(h_2) \oplus \dots \oplus E(h_t)$, hence there must be an even number of terms in the sequence $h_1, h_2, \dots, h_t$ containing the edge e. Since h is the only hexagon of G that contains e, $\delta(h)$ must be even.

(ii) Now suppose that no edge of h lies on a pentagon. Let G^* be the dual graph of some planar drawing of G and let p_0 be a pentagon of G such that $d_{G^*}(h, p_0) = \min\{d(h, p) \mid p \text{ pentagon of } G\}$. Furthermore, let $h, h_1, \dots, h_n, p_0$ be a shortest path from h to p_0 in G^*. Let e be the common edge of h and h_1. Similar as in (i) we can see that $\delta(h) + \delta(h_1)$ is even. Assume that $\delta(h)$ is odd. Then $\delta(h_1)$ must be odd. Let e' be the common edge of h_1 and h_2 – see Figure 1. But $\delta(h_2)$ is odd too since $\delta(h_1) + \delta(h_2)$ is even. If we repeat this discussion we obtain that $\delta(h_n)$ is odd. But the hexagon h_n contains an edge lying on pentagon p_0 and therefore, by (i), $\delta(h_n)$ must be even. This contradiction shows that $\delta(h)$ is even.

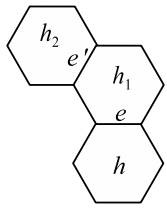

Figure 1: Hexagons h, h_1 and h_2.

We have proved that $\delta(h)$ is an even number for every hexagon h of G. Hence $t = \sum_{h \in T} \delta(h)$ is even, i.e. C is an even cycle. □

Next we show that every connected component (different from a path) of the resonance graph of a fullerene has girth 4. We begin with the following lemma.

Lemma 3.2. *Let G be a fullerene and H a connected component of the resonance graph $R(G)$ such that H is not a path. If $V_1(H)$ is the set of all vertices in H that have degree one and $M \in V(H) - V_1(H)$, then we can find in a fullerene G at least two disjoint hexagons which are M-alternating cycles.*

Proof. The proof is the same as the proof of Lemma 3.1 in [11]. □

With Lemma 3.2 the following theorem is almost obvious.

Theorem 3.3. *Let G be a fullerene and H a connected component of the resonance graph $R(G)$. Then H is either a path or a graph of girth 4.*

Proof. Suppose that H is not a path. The set of all vertices in $V(H)$ which have degree one will be denoted by $V_1(H)$. If the set $V(H) - V_1(H)$ is empty it follows that H is the path P_2, which is a contradiction since H is not a path. Hence, let $M \in V(H) - V_1(H)$.

By Lemma 3.2, in a fullerene G there are two disjoint hexagons h_1 and h_2 which are M-alternating cycles. Thus, M lies in a 4-cycle $MM_1M_2M_3$ where $M_1 = M \oplus E(h_1)$, $M_2 = M_1 \oplus E(h_2)$ and $M_3 = M_2 \oplus E(h_1)$. By Theorem 3.1 the resonance graph $R(G)$ is bipartite, therefore, H is bipartite too. Hence, there is no 3-cycle in H. Since every vertex lies in some 4-cycle, the girth of H is 4 and the proof is completed. □

4 Equivalence of Zhang-Zhang polynomial and cube polynomial for fullerenes

In this section we prove that the Zhang-Zhang polynomial of every fullerene equals the cube polynomial of its resonance graph. The same result was proved in [17] for benzenoid systems and in [3] for tubulenes. However, the proof in [17] cannot be applied in our case, since it is based on directed resonance graph (which is not defined for fullerenes, since fullerenes are not bipartite). Therefore, we combine ideas from [10], [17] and [3] to prove the following theorem:

Theorem 4.1. *Let G be a fullerene. Then the Zhang-Zhang polynomial of G equals the cube polynomial of its resonance graph $R(G)$ i.e.*

$$ZZ(G, x) = C(R(G), x)\,.$$

Proof. Let k be a nonnegative integer. For a fullerene G we denote by $\mathbb{Z}(G, k)$ the set of all Clar covers of G with exactly k hexagons. On the other hand, consider a graph H; the set of induced subgraphs of H that are isomorphic to a k-dimensional hypercube is denoted by $\mathbb{Q}_k(H)$. Let us define a mapping f_k from the set of Clar covers of a fullerene G with k hexagons to the set of induced subgraphs of the resonance graph $R(G)$ isomorphic to the k-dimensional hypercube

$$f_k : \mathbb{Z}(G, k) \longrightarrow \mathbb{Q}_k(R(G))$$

in the following way: for a Clar cover $C \in \mathbb{Z}(G, k)$ consider those perfect matchings M_1, M_2, ..., M_i of G that each hexagon in C is M_j-alternating and each isolated edge of C is in M_j, for all $j = 1, 2, \ldots, i$. Assign $f_k(C)$ as an induced subgraph of $R(G)$ with vertices $M_1, M_2, \ldots, M_i$.

Note first that in case when $k = 0$ Clar covers are without hexagons, i.e. Clar covers are perfect matchings of a fullerene and if C is such a Clar cover then $f_k(C)$ is a vertex of the resonance graph and the mapping is obviously bijective. So from now on k will be a positive integer.

First show that f_k is a well-defined mapping.

Lemma 4.2. *For each Clar cover $C \in \mathbb{Z}(G,k)$ we have $f_k(C) \in \mathbb{Q}_k(R(G))$.*

Proof. The proof in [17] is based on proper and improper alternating cycles, which are not well defined in our case. But we can apply the same proof as in [3]:
It is sufficient to show that $f_k(C)$ is isomorphic to the k-dimensional hypercube Q_k. Let $h_1, h_2, \ldots, h_k$ be hexagons of C. Obviously, every hexagon of C has two possible perfect matchings. Let us call these "possibility 0" and "possibility 1". For any vertex M of $f_k(C)$ let $b(M) = (b_1, b_2, \ldots, b_k)$, where $b_i = 1$ if on h_i possibility 1 is selected, and $b_i = 0$ otherwise, $i = 1, 2, \ldots, k$. It is obvious that $b : V(f_k(C)) \to V(Q_k)$ is a bijection. For $M' \in V(f_k(C))$, let $b(M') = (b'_1, b'_2, \ldots, b'_k)$. If M and M' are adjacent in $f_k(C)$ then $M \oplus M' = E(h_i)$ for some $i, 1 \leq i \leq k$. Therefore, $b_j = b'_j$ for each $j \neq i$ and $b_i \neq b'_i$, which implies $(b_1, b_2, \ldots, b_k)$ and $(b'_1, b'_2, \ldots, b'_k)$ are adjacent in Q_k. Conversely, if $(b_1, b_2, \ldots, b_k)$ and $(b'_1, b'_2, \ldots, b'_k)$ are adjacent in Q_k, it follows that M and M' are adjacent in $f_k(C)$. Hence b is an isomorphism between $f_k(C)$ and Q_k.

□

The following lemma shows that f_k is an injective mapping. For the proof see [17, 3].

Lemma 4.3. *The mapping $f_k : \mathbb{Z}(G,k) \longrightarrow \mathbb{Q}_k(R(G))$ is injective for each positive integer k.*

The next lemma was proved in [17] for benzenoid systems. Here we extend it to fullerenes.

Lemma 4.4. *Let G be a fullerene. If the resonance graph $R(G)$ contains a 4-cycle $M_1M_2M_3M_4$, then $h = M_1 \oplus M_2$ and $h' = M_1 \oplus M_4$ are disjoint hexagons. Also, we have $h = M_3 \oplus M_4$ and $h' = M_2 \oplus M_3$.*

Proof. We can apply the proof of Lemma 2.4 in [17]. □

To prove that the mapping f_k is surjective, we apply a similar proof as in [3], but to prove Claim 1 and Claim 2 in the proof, we use Lemma 4.4 (which is shorter). We give the whole proof since notation from it is then used in the proof of Proposition 4.8.

Lemma 4.5. *The mapping $f_k : \mathbb{Z}(G,k) \longrightarrow \mathbb{Q}_k(R(G))$ is surjective for each positive integer k.*

Proof. Let k be a positive integer and $Q \in \mathbb{Q}_k(R(G))$. Since Q is a subgraph of $R(G)$ isomorphic to a k-dimensional hypercube, vertices of Q can be identified with binary strings $(u_1, u_2, \ldots, u_k)$, so that two vertices of Q are adjacent in Q if and only if their binary strings differ in precisely one position. Consider the following vertices of Q: $M = (0,0,0,\ldots,0)$, $N^1 = (1,0,0,\ldots,0)$, $N^2 = (0,1,0,\ldots,0)$, …, $N^k = (0,0,0,\ldots,1)$. It is obvious that MN^i is an edge of $R(G)$ for every $i, 1 \leq i \leq k$. By definition of $R(G)$, the symmetric difference of perfect matchings M and N^i is the edge set of a hexagon of G. We denote this hexagon by h_i and we obtain the set of hexagons $\{h_1, \ldots, h_k\}$ of fullerene G. If two of these hexagons were the same, for example if $h_i = h_j$ for $i, j \in \{1, \ldots, k\}$ and $i \neq j$, then $N^1 = N^2$ - a contradiction. Hence, we have the set of k distinct hexagons. In the next claim we show that these hexagons are pairwise disjoint.

Claim 4.6. *The hexagons h_i, $1 \leq i \leq k$, are pairwise disjoint.*

Proof. Let $i, j \in \{1, \ldots, k\}$ and $i \neq j$. Let W be a vertex of Q having exactly two 1's and these are in the ith and jth position. Obviously, MN^1WN^2 is a 4-cycle and therefore, by Lemma 4.4, h_i and h_j are disjoint hexagons. □

Claim 4.7. *Let XY be an edge of Q. If the binary representations of X and Y differ at the j-th place, then the symmetric difference $X \oplus Y$ is the edge set of the hexagon h_j.*

Proof. We can apply the same proof as in [10]:
Without loss of generality assume that $j = 1$. Let $X = (0, \ldots)$ and $Y = (1, \ldots)$. Let s be the number of 1's in X. Consider the path $X^0, X^1, \ldots, X^s$ in Q, where X^i has exactly i 1's and these are in the same position as the first i 1's in X. Furthermore, consider the path $Y^0, Y^1, \ldots, Y^s$ in Q, where Y^i differ from X^i in precisely the first position. Obviously, X^i and Y^i are adjacent in Q and we also notice that $X^0 = M, Y^0 = N^1, X^s = X, Y^s = Y$. We use induction to prove that the symmetric difference of X^i and Y^i is the hexagon h_1. If $i = 0$, this follows from the definition of the hexagon h_1. Now suppose that the statement holds for $i = r$, i.e. the symmetric difference of X^r and Y^r is the hexagon h_1. Consider the cycle $X^rX^{r+1}Y^{r+1}Y^r$. By the inductive assumption and Lemma 4.4 it follows that the symmetric difference of X^{r+1} and Y^{r+1} is the hexagon h_1. Therefore, the symmetric difference of $X^s = X$ and $Y^s = Y$ is the hexagon h_1. □

We notice that $M^0 = M = (0, 0, 0, \ldots, 0)$, $M^1 = N^1 = (1, 0, 0, \ldots, 0)$, $M^2 = (1, 1, 0, \ldots, 0)$, …, $M^k = (1, 1, 1, \ldots, 1)$ is the path in Q and by Claim 2, the edge M^iM^{i+1} corresponds to the hexagon h_{i+1} for every $i, 0 \leq i \leq k-1$. So going from M^0 to M^k the perfect matchings only change in pair-wise disjoint hexagons $h_1, \ldots, h_k$, hence the perfect matching M^k contains a sextet of each hexagon in $\{h_1, \ldots, h_k\}$. Since Q is connected graph it follows that every vertex of Q contains a sextet of each hexagon from $\{h_1, \ldots, h_k\}$ and also vertices of Q differ only on edges of exactly these same hexagons.

Let C be a subgraph of G, induced with edges in the set $M^k \cup E(h_1) \cup \ldots \cup E(h_k)$. It is easy to see that C is a Clar cover with k hexagons and $V(f_k(C)) = V(Q)$. Since both Q and $f_k(C)$ are induced subgraphs of the resonance graph, it follows $f_k(C) = Q$. □

Lemma 4.2, Lemma 4.3 and Lemma 4.5 together imply Theorem 4.1. □

In the proof of Theorem 4.1 we considered just induced subgraphs of the resonance graph that are isomorphic to a hypercube. It is natural to ask what happens if we consider all subgraphs that are isomorphic to a hypercube. In the next proposition we show that every subgraph of the resonance graph of a fullerene that is isomorphic to a hypercube is actually an induced subgraph. The same can be shown for benzenoid systems and tubulenes.

Proposition 4.8. *Let G be a fullerene. Then every subgraph of $R(G)$, isomorphic to a hypercube, is induced subgraph in $R(G)$.*

Proof. Let Q be a subgraph of the resonance graph, isomorphic to the k-dimensional hypercube. If $k = 0$, the proposition is obvious. So let $k \geq 1$. Let F and F' be two distinct vertices in Q such that they are not adjacent in Q. It suffices to prove that F and F' are not adjacent in $R(G)$. Let all notation be the same as in the proof of Lemma 4.5. Since F and F' are not adjacent in Q, their binary representations differ in more than one coordinate. Since every coordinate represents position of double bonds of one of the hexagons $h_1, \ldots, h_k$, F and F' differ in double bonds of more than one hexagon. Hence, they are not adjacent in the resonance graph $R(G)$. □

5 Example

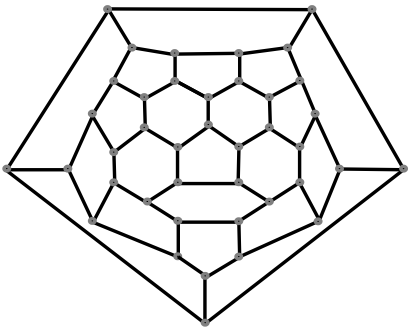

Figure 2: A fullerene G with two rings consisting of $5 + 5$ hexagons.

In Figure 2 we can see an example of a fullerene G with 10 hexagon faces, forming two disjoint rings, each having 5 hexagons. A subgraph of fullerene G induced on one of those two rings is a graph called cyclic fibonacene which resonance graph is isomorphic to a Lucas cube Λ_5 (see [20]). Since the two rings of hexagons are disjoint and the union of their vertex sets is the vertex set of G, one of the components of the resonance graph of G is isomorphic to the Cartesian product of two 5-dimensional Lucas cubes, $\Lambda_5 \Box \Lambda_5 = H$, see Figure 3. The Clar number of fullerene G is obviously 4, since there is no resonant set of size 5 in G. Since a Clar cover with k hexagons induces a k-dimensional hypercube in the corresponding resonance graph, the largest induced hypercubes in H are of size 4. It is easy to see that every perfect matching with 4 sextets is a vertex of H. It is also not difficult to check that there is no maximal resonant set with 3 hexagons in G. Therefore all components of the resonance graph of G different from H contain at most 2-dimensional hypercubes (due to their large number only the component H of the resonance graph $R(G)$ is drawn in Figure 3).

To conclude the example, we calculate the first two coefficients of Zhang-Zhang polynomial using cube polynomial of a fullerene from Figure 2. Since we already know that graph H from Figure 3 includes all 3-dimensional and 4-dimensional hypercubes of resonance graph $R(G)$, it suffices to count them in H. The number of 4-dimensional hypercubes in H is 25 and the number of 3-dimensional hypercubes in H is 75 (see Figure 3) therefore, the number of Clar covers with 4 and 3 hexagons is 25 and 75, respectively.

6 Distributive lattice structure and median graphs

We have already mentioned that the resonance graph (or each connected component of the resonance graph) of every benzenoid graph or tubulene is the covering graph of some distributive lattice. For the details see [6, 15, 13]. Therefore it is interesting that this result is no longer true (in general) for resonance graphs of fullerenes. Here we give an example of a fullerene such that a connected component of its resonance graph is not the covering graph of a distributive lattice.

In Figure 3 we can see the largest connected component H of the resonance graph of fullerene G from Figure 2. It is obvious that the diameter of H, $diam(H)$ is 8, since the

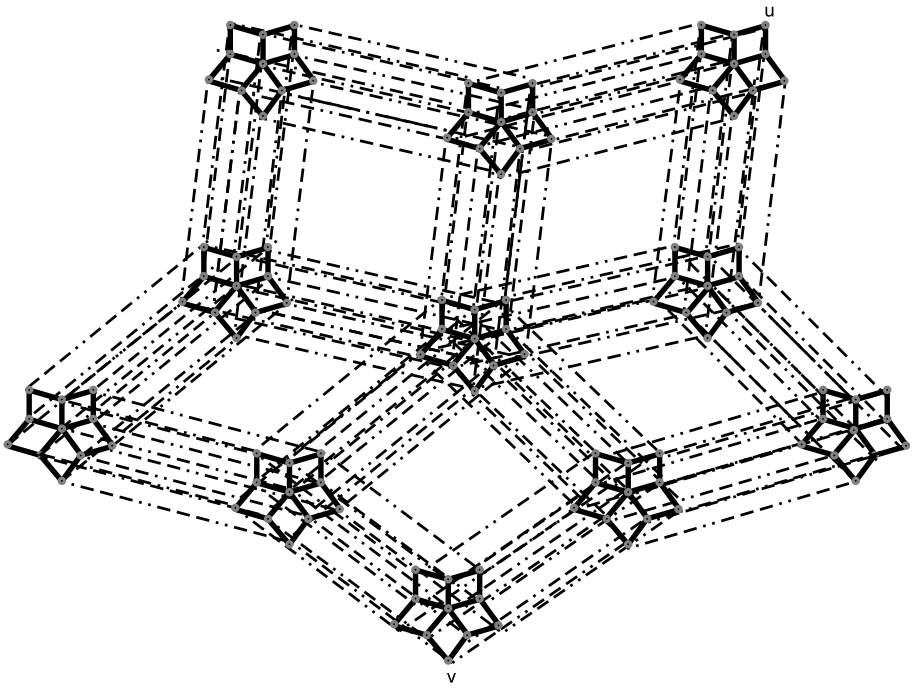

Figure 3: The largest connected component H of the resonance graph of fullerene G.

distance between vertices u and v from Figure 3 is 8. To show that graph H is not the covering graph of any distributive lattice, we use Theorem 6.1. Before stating the theorem, we introduce some notation.

Let $\mathbf{2}^n$ denote the distributive lattice of all subsets of an n-element set. Then the covering graph $\mathcal{C}(\mathbf{2}^n)$ is an n-dimensional hypercube. Also, if $(L, \leq)$ is a lattice, then a linearly ordered set $C \subseteq L$ is called a *chain*. For a chain C of L we define its *length* by $l(C) = |C| - 1$. Then the *length* $l(L)$ of L is the maximum of the lengths of the chains in L. Now the following result can be stated.

Theorem 6.1. *[4] A finite graph G is the covering graph of a distributive lattice of length n if and only if G is a retract of $\mathcal{C}(\mathbf{2}^n)$ and $diam(G) = n$.*

It follows from Theorem 6.1 that if H is the covering graph of some distributive lattice, then H is a retract of a 8-dimensional hypercube Q_8. But it is obvious from Figure 3 that the degree of the vertex in the center of H is 10 and, therefore, H cannot be a subgraph of Q_8, since all the vertices in Q_8 have degree 8. Hence, H is not the covering graph of any distributive lattice.

Next we consider the relationship between resonance graphs of fullerenes and median graphs. It was shown that the resonance graph (or its connected component) of a benzenoid graph or a tubulene is always a median graph (see [16, 13]). Both proofs rely on a distributive lattice structure for resonance graphs, which cannot be established for fullerenes. Since covering graphs of distributive lattices and median graphs are closely connected [4], it is

natural to ask if resonance graphs of fullerenes are not (in general) median graphs. However, we can easily show that graph H in Figure 3 is a median graph. To this end, let us introduce the following procedure.

Let G be a graph. Suppose $V(G) = V_1 \cup V_2$, where $V_1 \cap V_2 \neq \emptyset$, each $\langle V_i \rangle$ (an induced subgraph of G with vertices V_i) is an isometric subgraph of G, and no edge of G joins $V_1 \setminus V_2$ to $V_2 \setminus V_1$. An *expansion* of G with respect to V_1 and V_2 is a graph H obtained from G by the following steps.

i) Replace each $v \in V_1 \cap V_2$ by vertices v_1 and v_2, and insert the edge v_1v_2.

ii) Insert edges between v_1 and all neighbours of v in $V_1 \setminus V_2$; insert edges between v_2 and all neighbours of v in $V_2 \setminus V_1$.

iii) Insert the edges v_1u_1 and v_2u_2 if $v, u \in V_1 \cap V_2$ are adjacent in G.

An expansion is *convex* if $\langle V_1 \cap V_2 \rangle$ is a convex subgraph of G. Now we can state the following well-known theorem, which is called Mulder's Convex Expansion Theorem.

Theorem 6.2. *[7] A graph is a median graph if and only if it can be obtained from the one-vertex graph by a convex expansion procedure.*

It is easy to check that the Lucas cube Λ_5 can be obtained from a one-vertex graph by a convex expansion procedure (see Figure 4), therefore, Λ_5 is a median graph.

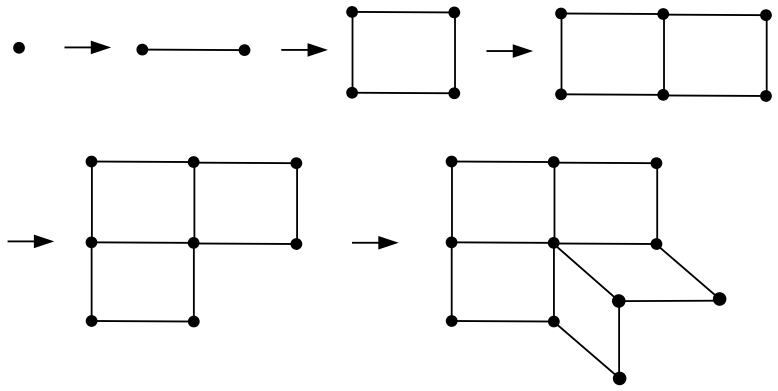

Figure 4: A convex expansion procedure for Λ_5.

Since the Cartesian product of median graphs is another median graph, graph H from Figure 3 is median. Since we do not know any example of a fullerene such that some connected component of its resonance graph is not a median graph, we propose the following conjecture.

Conjecture 6.3. *Let G be a fullerene. Then every connected component of the resonance graph $R(G)$ is a median graph.*

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Wilfried Imrich's 75th Birthday Colloquium

Wilfried Imrich was born on May 25th, 1941 in Vienna. On June 17th, 2016, a colloquium was organized at the Graz University of Technology to celebrate his 75th birthday. The colloquium started with a laudatio by Peter Kirschenhofer (Leoben). In the central part of the event the following talks were presented:

(i) Ultrametric spaces, trees, and random walks (Wolfgang Woess, Graz),
(ii) Automorphism groups of one-ended graphs (Florian Lehner, Hamburg),
(iii) Extending Wiener index to arbitrary partitions (Sandi Klavar, Ljubljana), and
(iv) From chaos on trees to symmetry breaking (Rafa Kalinowski, Krakw).

We do not intend to summarize Wilfried's outstanding career here (see [1]), but will just mention that he is the world's leading expert on graph products and that, because of his co-authorships with Lszl Babai, Lszl Lovsz, and Jaroslav Neetil, Wilfried has Erds number 2 in at least three ways. We do wish, however, to emphasize his deep connections with the Slovene graph theory school and his lasting impact on it. Wilfried was an important figure in the development of graph theory in Slovenia from its very beginning. Together with Tomo Pisanski he was a co-founder of the Ljubljana-Leoben graph theory seminar and had 3 Ph.D. students from Slovenia. He has also published several dozen joint papers with more than a dozen Slovenian co-authors, as well as three books on graph products that have become classic references for the field.

It is a pleasure to conclude this short report on Wilfried Imrich's 75th Birthday Colloquium by pointing to Wilfried's impressive mathematical achievements obtained in the last years. Hence, we are looking forward to future beautiful theorems from him!

Sandi Klavar

Associate Editor

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Norbert Seifter is 60!

Norbert Seifter (left) Participants of the LL2016 Graph Theory Seminar in Judenburg (right).

In 2016, the traditional Ljubljana-Leoben Graph Theory Seminar took place in Judenburg, Austria, the home town of Norbert Seifter. See the page of LL2016: `https://www.math.tugraz.at/mathc/ll2016/`. Judenburg was chosen in order to honour Norbert's 60-th birthday, with a special session dedicated to Bojan Mohar who also turned 60 this year.

From the first meeting in Ljubljana in 1981, Austrian and Slovenian graph theorists established a sound and fruitful collaboration: frequent research visits, bilateral projects, exchange of students, and organising workshops – all this resulted in numerous joint publications.

Norbert has been an active participant and organizer of many of these events ever since he started, upon completing his PhD in 1981, his professional career at the Department of Applied Mathematics at Montanuniversitaet Leoben, where to this day holds regular courses on programming, optimisation, operations research, numerical analysis, information systems, neural networks, fuzzy-sets and fuzzy-logic. Fields of his research interest include matrix theory, automorphism groups of undirected and directed graphs, highly arc transitive digraphs, growth of graphs and groups, combinatorial group theory, dominating sets in undirected and directed graphs, and several other topics in discrete applied mathematics.

Happy birthday, Norbert! And remain so enthusiastic about the structure of infinite graphs still for many years to come.

Aleksander Malnič

Editor

Bojan Mohar's 60th Birthday

In the frame of the Leoben-Ljubljana Graph Theory Seminar 2016 (Judenburg, Austria, September 25-28, 2016) a special session was organized to celebrate Bojan Mohar's 60th birthday.

Bojan Mohar is an outstanding representative of the Slovenian graph theory school. In 1985 he obtained his PhD under the guidance of Toma Pisanski. Since 2005 he has been holder of a Canada Research Chair in Graph Theory at Simon Fraser University, Vancouver, Canada. He continues to be deeply involved in research at the Faculty of Mathematics and Physics, University of Ljubljana, Slovenia, and at the Institute of Mathematics, Physics and Mechanics, also in Ljubljana.

Bojan Mohar is a world recognized mathematician who works in the area of graph theory. This year he was awarded the Euler Medal for the year 2010. Let us quote a part of the citation for this award: "Bojan Mohars outstanding research and leadership over a period of thirty years place him as one of todays foremost discrete mathematicians worldwide. His deep and important contributions have dramatically improved our understanding of the structural properties of graphs. His research spans many areas, including topological graph theory, graph minors, infinite graphs, spectral graph theory, algebraic graph theory, and computational geometry." To this citation we add a couple of specific achievements of Bojan. His monograph "Graphs on Surfaces" (Johns Hopkins University Press, 2001), written jointly with Carsten Thomassen, is the central contemporary work on topological graph theory. Among numerous editorial duties Bojan Mohar serves as one of the two Editors-in-Chief of the renowned Journal of Combinatorial Theory Series B. He is also a recipient of Slovenian national awards; in particular, in 2009 he became an "Ambassador of Science of the Republic of Slovenia".

Happy Birthday, Bojan!

Sandi Klavžar
Associate Editor

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