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APPLICATIONS OF GRAPH SPECTRA

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PREFACE

The purpose of this volume is to draw the attention of mathematical community to rapidly growing applications of the theory of graph spectra. Besides classical and well documented applications to Chemistry and Physics, we are witnesses of the appearance of graph eigenvalues in Computer Science in various investigations. There are also applications in several other fields like Biology, Geography, Economics and Social Sciences. A monograph with a comprehensive treatment of applications of graphs spectra is missing at the present.

The present book contains five chapters: an introductory chapter with a survey of applications by representative examples and four case studies (one in Computer Science and three in Chemistry).

We quote particular chapters and indicate their contents.

Applications of Graph Spectra: An Introduction to the Literature (D. Cvetković). This introductory text provides an introduction to the theory of graph spectra and a short survey of applications of graph spectra. There are four sections: 1. Basic notions, 2. Some results, 3. A survey of applications, 4. Selected bibliographies on applications of the theory of graph spectra.

Multiprocessor Interconnection Networks (D. Cvetković, T. Davidović). Well-suited multiprocessor interconnection networks are described in terms of the graph invariant called tightness which is defined as the product of the number of distinct eigenvalues and maximum vertex degree. Load balancing problem is presented.

Selected Topics from the Theory of Graph Energy: Hypoenergetic Graphs (S. Majstorović, A. Klobučar, I. Gutman). The energy E of a graph G is the sum of the absolute values of the eigenvvalues of G. The motivation for the introduction of this invariant comes from Chemistry, where results on E were obtained already in the 1940's. The chemical background of graph energy is outlined in due detail. Then some fundamental results on E are given.

A graph G with n vertices is said to be "hypoenergetic" if $E(G) < n$. In the main part of the chapter results on graph energy, pertaining to the inequalities $E(G) < n$ and $E(G) \geq n$ are presented. Most of these were obtained in the last few years.

Nullity of Graphs (B. Borovićanin, I. Gutman). The nullity η of a graph G is the multiplicity of the number zero in the spectrum of G. In the 1970s the nullity of graphs was much studied in Chemistry, because for certain types of molecules, $\eta = 0$ is a necessary condition for chemical stability. The chemical background of this result is explained in a way understandable to mathematicians. Then the main early results on nullity are outlined.

In the last 5–10 years there is an increased interest to nullity in mathematics, and some 10 papers on this topic appeared in the mathematical literature. All these results are outlined too.

The Estrada Index (H. Deng, S. Radenković, I. Gutman). If λ_i, $i = 1, 2, \ldots, n$, are the eigenvalues of the graph G, then the Estrada index EE of G is the sum of

the terms $\exp(\lambda_i)$. This graph invariant appeared for the first time in year 2000, in a paper by Ernesto Estrada, dealing with the folding of protein molecules. Since then a remarkable number of other chemical and non-chemical applications of EE were communicated.

The mathematical studies of the Estrada index started only a few years ago. Until now a number of lower and upper bounds were obtained, and the problem of extremal EE for trees solved. Also, a number of approximations and correlations for EE were put forward, valid for chemically interesting molecular graphs.

All relevant results on the Estrada index are presented in the chapter.

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Dragoš Cvetković

APPLICATIONS OF GRAPH SPECTRA: AN INTRODUCTION TO THE LITERATURE

Abstract. We give basic definitions and some results related to the theory of graph spectra. We present a short survey of applications of this theory. In addition, selected bibliographies on applications to particular branches of science are given.

Mathematics Subject Classification (2000): 05C50, 05C90, 01A90

Keywords: graph spectra, application, bibliography, chemistry, physics, computer science

Contents

This is an introductory chapter to our book. We start with basic definitions and present some results from the theory of graph spectra. A short survey of applications of this theory is presented. Selected bibliographies on applications to particular branches of science are given in the sequel.

The plan of the chapter is as follows.

Section 1 presents basic definitions related to the theory of graph spectra. Some selected results, which will bi used in other chapters, are given in Section 2. A short survey of applications of graph eigenvalues is contained in Section 3. Section 4 contains selected bibliographies of books and papers which are related to applications of the theory of graph spectra in Chemistry, Physics, Computer Science, Engineering, Biology and Economics.

1. Basic notions

A graph $G = (V, E)$ consists of a finite non-empty set V (the vertex set of G), and a set E (of two elements subsets of V, the edge set of G). We also write $V(G)$ ($E(G)$) for the vertex (resp. edge) set of G. The number of elements in $V(G)$, denoted by n ($= |V(G)|$), is called the *order* of G. Usually, we shall assume that $V(G) = \{1, 2, \ldots, n\}$.

Let e_{ij} be the edge connecting vertices i and j. The set $\{e_{i_1 j_1}, e_{i_2 j_2}, \ldots, e_{i_k j_k}\}$ of distinct edges, such that $i = i_1, j_1 = i_2, j_2 = i_3, \ldots, j_k = j$, is called *path* (of *length* k) connecting vertices i and j. The length of the shortest path connecting i and j is called the *distance* between these two vertices. The maximum distance between any two vertices in G is called the *diameter* of G, and it is denoted by D. If there exists a path between any two vertices in G, then G is *connected*; otherwise it is *disconnected*.

Two vertices are called *adjacent* (or *neighbors*) if they are connected by an edge; the corresponding relation between vertices is called the *adjacency relation*. The number of neighbors of a vertex i, denoted by d_i, is its *vertex degree*. The maximum vertex degree (of G) is denoted by Δ. A graph in which all vertex degrees are equal to r is *regular* of degree r (or r-*regular*, or just *regular* if r is unimportant).

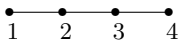
The *adjacency matrix* A is used to represent the adjacency relation, and so the graph G itself. The element a_{ij} of the adjacency matrix A is equal to 1 if vertices i and j are adjacent, and 0 otherwise.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A (of G) is called the *characteristic polynomial of* G, and is denoted by $P_G(x)$. The eigenvalues of A (i.e., the zeros of $\det(xI - A)$), and the spectrum of A (which consists of the n eigenvalues) are also called the *eigenvalues* and the *spectrum* of G, respectively. The eigenvalues of G are usually denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$; they are real because A is symmetric. Unless we indicate otherwise, we shall assume that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. We also use the notation $\lambda_i = \lambda_i(G)$ for $i = 1, 2, \ldots, n$. The largest eigenvalue, i.e., λ_1, is called the *index* of G.

If λ is an eigenvalue of G, then a non-zero vector $\mathbf{x} \in \mathbb{R}^n$, satisfying $A\mathbf{x} = \lambda\mathbf{x}$, is called an *eigenvector* of A (or of the labeled graph G) for λ; it is also called a λ-*eigenvector*. The relation $A\mathbf{x} = \lambda\mathbf{x}$ can be interpreted in the following way: if $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$, then for any vertex u we have $\lambda x_u = \sum_{v \sim u} x_v$, where the summation is over all neighbours v of u. If λ is an eigenvalue of G, then the set $\{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \lambda\mathbf{x}\}$ is a subspace of $\mathbb{R}^n$, called the *eigenspace* of G for λ; it is denoted by $\mathcal{E}(\lambda)$. Such eigenspaces are called *eigenspaces* of G.

For the index of G, since A is non-negative, there exists an eigenvector whose all entries are non-negative.

Example. Let G be the graph shown in Fig. 1 together with its adjacency matrix.



$$A = \begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{Vmatrix}$$

FIGURE 1. An example

For G we have

$$P_G(\lambda) = \begin{vmatrix} \lambda & -1 & 0 & 0 \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ 0 & 0 & -1 & \lambda \end{vmatrix} = \lambda^4 - 3\lambda^2 + 1\,.$$

Eigenvalues of G are

$$\frac{1+\sqrt{5}}{2} \approx 1.6180, \qquad \frac{-1+\sqrt{5}}{2} \approx 0.6180,$$
$$\frac{1-\sqrt{5}}{2} \approx -0.6180, \qquad \frac{-1-\sqrt{5}}{2} \approx -1.6180.$$

The following vector $\mathbf{x} = (1, \lambda, \lambda^2 - 1, \lambda^3 - 2\lambda)^T$ is a λ-eigenvector of G. □

Besides the spectrum of the adjacency matrix of a graph G we shall consider the spectrum of another matrix associated with G. The matrix $L = D - A$, where $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees, is known as the *Laplacian* of G. The matrix L is positive semi-definite, and therefore its eigenvalues are non-negative. The least eigenvalue is always equal to 0; the second least eigenvalue is also called the *algebraic connectivity* of of G [Fie].

The basic reference for the theory of graph spectra is the book [CvDSa]. Other books on graph spectra include [CvDGT], [CvRS1], [CvRS3], [CvRS4]. For any notion, not defined here, the reader is referred to [CvRS4] or [CvDSa].

As usual, K_n, C_n, S_n and P_n denote respectively the *complete graph*, the *cycle*, the *star* and the *path* on n vertices; K_{n_1,n_2} denotes the *complete bipartite* graph on $n_1 + n_2$ vertices.

A *tree* is a connected graph without cycles. A connected graph with n vertices and n edges is a *unicyclic graph*. It is called *even* (*odd*) if its unique cycle is even (resp. odd). A *dumbbell* is the graph obtained from two disjoint cycles by joining them by a path.

The *complement* of a graph G is denoted by $\overline{G}$, while mG denotes the union of m disjoint copies of G.

For $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting v, and all edges incident with it. More generally, for $U \subseteq V(G)$, $G - U$ is the subgraph of G obtained from G by deleting all vertices from U and edges incident to at least one vertex of U; we also say that G_U is induced by the vertex set $V(G) \setminus U$.

The *join* $G \nabla H$ of (disjoint) graphs G and H is the graph obtained from G and H by joining each vertex of G with each vertex of H. For any graph G, the *cone* over G is the graph $K_1 \nabla G$.

The *line graph* $L(H)$ of any graph H is defined as follows. The vertices of $L(H)$ are the edges of H and two vertices of $L(H)$ are adjacent whenever the corresponding edges of H have a vertex of H in common.

A set of disjoint edges in a graph G is called a *matching*. A set of disjoint edges which cover all vertices of the graph is called an 1-*factor* of G.

2. Some results

We present here some known results from the theory of graph spectra that will be used in other chapters.

In graph theory and in the theory of graph spectra, some special types of graphs are studied in detail and their characteristics are well known and summarized in the literature (see, for example, [CvDSa]). Here, we will survey some of them.

Recall, K_n is a complete graph, i.e., a graph with each two vertices connected by an edge (so, the number of edges is equal to $\binom{n}{2}$). The spectrum of K_n consists of $m = 2$ distinct eigenvalues: $\lambda_1 = n-1$ which is a simple eigenvalue, and $\lambda_i = -1$ for $i = 2, \ldots, n$.

A *path* P_n is a tree on n vertices (and $n - 1$ edges) without vertices of degree greater than two. Two "ending" vertices (for $n \geqslant 2$) have degree one, while the rest

of them (the internal vertices) have degree two. A spectral characteristic of paths is that they have all distinct eigenvalues. In fact, the spectrum of P_n consists of the following eigenvalues: $2\cos\frac{\pi}{n+1}i,\ \ i=1,2,\ldots,n$.

The C_n is a 2-regular connected graph. It contains the following eigenvalues: $2\cos\frac{2\pi}{n}i,\ \ i=0,1,\ldots,n-1$. It has $m=\lfloor\frac{n}{2}\rfloor+1$ distinct eigenvalues. Here $\lfloor x\rfloor$ denotes the largest integer smaller than or equal to x.

The star S_n is a tree having a vertex (central vertex) which is adjacent to all remaining vertices (all of them being of degree one). Each star on $n\geqslant 3$ vertices has $m=3$ distinct eigenvalues. It contains the following eigenvalues: $\pm\sqrt{n-1}$ which are both simple, and $\lambda_i=-1$ for $i=2,\ldots,n-1$.

A complete bipartite graph K_{n_1,n_2} consists of n_1+n_2 vertices divided into two sets of the cardinalities n_1 and n_2 with the edges connecting each vertex from one set to all the vertices in the other set. This means that the number of edges is n_1n_2. In particular, $S_n=K_{1,n-1}$. More generally, *bipartite* graphs consist of two sets of vertices with the edges connecting a vertex from one set to a vertex in the other set. The spectrum of K_{n_1,n_2} (for $n_1+n_2\geqslant 3$) also consists of $m=3$ distinct eigenvalues (simple eigenvalues $\pm\sqrt{n_1n_2}$, and 0 of multiplicity n_1+n_2-2).

In the theory of graph spectra an important role play the graphs with $\lambda_1=2$, known as Smith graphs. They are well studied, and all of them are given in [CvDSa], on Fig. 2.4, p. 79. There are 6 types of Smith graphs (namely, C_n ($n\geqslant 3$), W_n ($n\geqslant 6$), S_5 H_7, H_8 and H_9 – see also Fig. 2). Four of them are concrete graphs S_5, H_7, H_8 and H_9, while the remaining two types (cycles C_n and *double-head snakes* W_n, of order n, can have an arbitrary number of vertices); in Fig. 2 we reproduce those which are not cycles C_n, nor the star $S_5=K_{1,4}$.

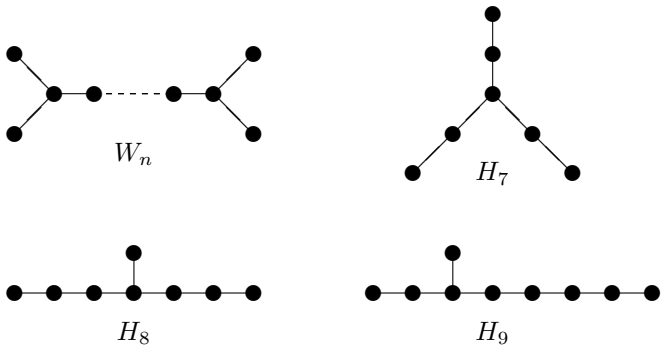


FIGURE 2. Some Smith graphs

In our study we need also graphs with $\lambda_1<2$. To obtain such graphs, it is enough to study (connected) subgraphs of Smith graphs. By removing vertices out of Smith graphs, we obtain paths P_n, $n=2,3,\ldots$; *single-head snakes* Z_n, $n=4,5,\ldots$, given in the upper row of Fig. 3 up to $n=7$; and the three other graphs given in the second row of Fig. 3 and denoted by E_6, E_7 and E_8. It is enough to consider only one vertex removal; removing further vertices leads to the graph already obtained in another way.

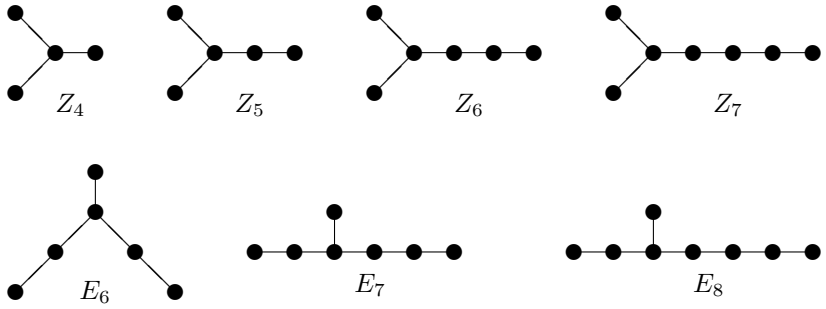


FIGURE 3. Subgraphs of some Smith graphs

By Theorem 3.13. from [CvDSa] for the diameter D of a graph G we have

$$D \leqslant m - 1, \tag{1}$$

where m is the number of distinct eigenvalues.

The largest eigenvalue λ_1 of G and the maximum vertex degree Δ are related in the following way (cf. [CvDSa, p. 112 and p. 85]):

$$\sqrt{\Delta} \leqslant \lambda_1 \leqslant \Delta. \tag{2}$$

A graph is called *strongly regular* with parameters (n, r, e, f) if it has n vertices and is r-regular, and if any two adjacent (non-adjacent) vertices have exactly e (resp. f) common neighbors [CvDSa]. One can show that the number n of vertices of a strongly regular graph is determined by the remaining three parameters. Note that a complement of a strongly regular graph is also a strongly regular graph. Usually, strongly regular graphs which are disconnected, or whose complements are disconnected are excluded from considerations (trivial cases). Under this assumption, the diameter of a strongly regular graph is always equal to 2, and also it has 3 distinct eigenvalues.

A graph is called *integral* if its spectrum consists entirely of integers. Each eigenvalue has integral eigenvectors and each eigenspace has a basis consisting of such eigenvectors.

Graphs with a small number of distinct eigenvalues have attracted much attention in the research community.

The number of distinct eigenvalues of a graph is correlated with its symmetry property [CvDSa]: the graphs with a small number of distinct eigenvalues are (very frequently) highly symmetric. They also have a small diameter, what follows from (1). Let m be the number of distinct eigenvalues of a graph G. Trivial cases are $m = 1$ and $m = 2$. If $m = 1$, all eigenvalues are equal to 0 and G consists of isolated vertices. In the case $m = 2$ G consists of, say $k \geqslant 1$ copies of complete graphs on $s \geqslant 2$ vertices (so the distinct eigenvalues are $s - 1$ (of multiplicity k) and -1 (of multiplicity $k(s - 1)$)).

Further, we shall consider only connected graphs. If $m = 3$ and G is regular, then G is strongly regular (cf. [CvDSa, p. 108]). For example, the well known

Petersen graph (see Fig. 4) is strongly regular with distinct eigenvalues $3, 1, -2$ of multiplicities $1, 5, 4$, respectively.

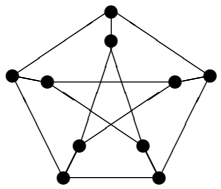


FIGURE 4. The Petersen graph

It is difficult to construct families of strongly regular graphs which contain graphs for any number of vertices. It could be rather expected that one can find sporadic examples with nice properties like it appears in the Petersen graph.

There are also some non-regular graphs with three distinct eigenvalues [Dam]. Such graphs usually have a vertex adjacent to all other vertices (like in stars), i.e., they are cones over some other graphs.

Several classes of regular graphs with four distinct eigenvalues are described in [Dam], but the whole set has not been described yet.

3. A survey of applications

In this section we shall give a short survey of applications of the theory of graph spectra.

The applications are numerous so that we cannot give a comprehensive survey in limited space that we have at the disposal. We shall rather limit ourselves to review representative examples of applications so that the reader can get an impression on the situation but also to become able to use the literature.

The books [CvDSa], [CvDGT] contain each a chapter on applications of graph eigenvalues.

The book [CvRS4] also contains a chapter on applications . There are sections on Physics, Chemistry, Computer Sciences and Mathematics itself.

We shall first mention applications to Chemistry, Physics, Computer Sciences and Mathematics itself (we devote a subsection of this section to each). Graph spectra are used in many other branches of science including Biology, Geography, Economics and Social Sciences and the fifth subsection contains some information about that. In all fields we are forced to give only examples of applications.

3.1. Chemistry. Motivation for founding the theory of graph spectra has come from applications in Chemistry and Physics.

The paper [Huc] is considered as the first paper where graph spectra appear though in an implicit form. The first mathematical paper on graph spectra [CoSi] was motivated by the membrane vibration problem i.e., by approximative solving of partial differential equations.

One of the main applications of graph spectra to Chemistry is the application in a theory of unsaturated conjugated hydrocarbons known as the *Hückel molecular*

orbital theory. Some basic facts of this theory are given at the beginning of the chapter "Studies on Graph Energy" in this book.

More detail on the Hückel molecular orbital theory the interested reader can find, for example, in books [CvDSa], [Bal], [CoLM], [Dia], [GrGT], [Gut], [GuTr], [Tri]. For more references to the Hückel theory as well as to other chemical applications see Section 4.

Three separate chapters of this book are devoted to applications in Chemistry.

3.2. Physics. Treating the membrane vibration problem by approximative solving of the corresponding partial differential equation leads to consideration of eigenvalues of a graph which is a discrete model of the membrane (see [CvDSa, Chapter 8]).

The spectra of graphs, or the spectra of certain matrices which are closely related to adjacency matrices appear in a number of problems in statistical physics (see, for example, [Kas], [Mon], [Per]). We shall mention the so-called *dimer problem*.

The dimer problem is related to the investigation of the thermodynamic properties of a system of diatomic molecules ("dimers") adsorbed on the surface of a crystal. The most favorable points for the adsorption of atoms on such a surface form a two-dimensional lattice, and a dimer can occupy two neighboring points. It is necessary to count all ways in which dimers can be arranged on the lattice without overlapping each other, so that every lattice point is occupied.

The dimer problem on a square lattice is equivalent to the problem of enumerating all ways in which a chess-board of dimension $n \times n$ (n being even) can be covered by $\frac{1}{2}n^2$ dominoes, so that each domino covers two adjacent squares of the chess-board and that all squares are so covered.

A graph can be associated with a given adsorption surface. The vertices of the graph represent the points which are the most favorable for adsorption. Two vertices are adjacent if and only if the corresponding points can be occupied by a dimer. In this manner an arrangement of dimers on the surface determines a 1-factor in the corresponding graph, and vice versa. Thus, the dimer problem is reduced to the task of determining the number of 1-factors in a graph. Enumeration of 1-factors involves consideration of walks in corresponding graphs and graph eigenvalues (see [CvDSa, Chapter 8]).

Not only the dimer problem but also some other problems can be reduced to the enumeration of 1-factors (i.e. dimer arrangements). The best known is the famous *Ising problem* arising in the theory of ferromagnetism (see, for example, [Kas], [Mon]).

The graph-walk problem is of interest in physics not only because of the 1-factor enumeration problem. The numbers of walks of various kinds in a lattice graph appear in several other problems: the random-walk and self-avoiding-walk problems (see [Kas], [Mon]) are just two examples.

3.3. Computer science. It was recognized in about last ten years that graph spectra have several important applications in computer science. Graph spectra appear in internet technologies, pattern recognition, computer vision and in many other areas. Here we mention applications in treating some of these and other

problems. (See Chapter *Multiprocessor Interconnection Networks* for applications in designing multiprocessor interconnection topologies).

One of the oldest applications (from 1970's) of graph eigenvalues in Computer Science is related to graphs called *expanders*. Avoiding a formal definition, we shall say that a graph has good *expanding properties* if each subset of the vertex set of small cardinality has a set of neighbors of large cardinality. Expanders and some related graphs (called *enlargers, magnifiers, concentrators* and *superconcentrators*, just to mention some specific terms) appear in treatment of several problems in Computer Science (for example, communication networks, error-correcting codes, optimizing memory space, computing functions, sorting algorithms, etc.). Expanders can be constructed from graphs with a small second largest eigenvalue in modulus. Such class of graphs includes the so called *Ramanujan graphs*. For an introduction to this type of applications see [CvSi] and references cited therein. Paper [LuPS] is one of the most important papers concerning Ramanujan graphs.

Referring to the book [CvDSa] as "the current standard work on algebraic graph theory", Van Mieghem gave in his book [Van] a twenty page appendix on graph spectra, thus pointing out the importance of this subject for communications networks and systems.

The paper [Spi] is a tutorial on the basic facts of the theory of graph spectra and its applications in computer science delivered at the 48th Annual IEEE Symposium on Foundations of Computer Science.

The largest eigenvalue λ_1 plays an important role in modelling virus propagation in computer networks. The smaller the largest eigenvalue, the larger the robustness of a network against the spread of viruses. In fact, it was shown in [WaCWF] that the epidemic threshold in spreading viruses is proportional to $1/\lambda_1$. Motivated by this fact, the authors of [DaKo] determine graphs with minimal λ_1 among graphs with given numbers of vertices and edges, and having a given diameter.

Some data on using graph eigenvalues in studying Internet topology can be found in [ChTr] and in the references cited therein.

Web search engines are based on eigenvectors of the adjacency and some related graph matrices [BrPa, Kle].

The indexing structure of object appearing in computer vision (and in a wide range of other domains such as linguistics and computational biology) may take the form of a tree. An indexing mechanism that maps the structure of a tree into a low-dimensional vector space using graph eigenvalues is developed in [ShDSZ].

Statistical databases are those that allow only statistical access to their records. Individual values are typically deemed confidential and are not to be disclosed, either directly or indirectly. Thus, users of a statistical database are restricted to statistical types of queries, such as SUM, MIN, MAX, etc. Moreover, no sequence of answered queries should enable a user to obtain any of the confidential individual values. However, if a user is able to reveal a confidential individual value, the database is said to be *compromised*. Statistical databases that cannot be compromised are called *secure*.

One can consider a restricted case where the query collection can be described as a graph. Surprisingly, the results from [Bra, BrMS] show an amazing connection

between compromise-free query collections and graphs with least eigenvalue -2. This connection was recognized in the paper [BraCv].

It is interesting to note that original Doob's description [Doo] in 1973 of the eigenspace of -2 in line graphs in terms of even cycles and odd dumbbells has been extended to generalized line graphs by Cvetković, Doob and Simić [CvDS] in 1981 in terms of the chain groups, not explicitly dealing with cycles and dumbbells. The independent discovery of Branković, Miller and Širáň [BrMS] in 1996 put implicitly some light on the description of the eigenspace in generalized line graphs a bit before Cvetković, Rowlinson and Simić in 2001 (the paper [CvRS2] was submitted in 1998), using the star complement technique and without being aware of [BrMS], gave the entire description of the eigenspace.

Another way to protect the privacy of personal data in databases is to randomize the network representing relations between individuals by deleting some actual edges and by adding some false edges in such a way that global characteristics of the network are unchanged. This is achieved using eigenvalues of the adjacency matrix (in particular, the largest one) and of the Laplacian (algebraic connectivity) [YiWu].

3.4. Mathematics. There are many interactions between the theory of graph spectra and other branches of mathematics. This applies, by definition, to linear algebra. Another field which has much to do with graph spectra is combinatorial optimization.

Combinatorial matrix theory studies matrices by the use of and together with several digraphs which can be associated to matrices. Many results and techniques from the theory of graph spectra can be applied for the foundations and development of matrix theory. A combinatorial approach to the matrix theory is given in the book [BrCv]. Particular topics, described in the book, include determinants, systems of linear algebraic equations, sparse matrices, the Perron–Frobenius theory of non-negative matrices, Markov chains and many others.

Relations between eigenvalues of graphs and *combinatorial optimization* have been known for last twenty years. The section titles of an excellent expository article [MoPo] show that many problems in combinatorial optimization can be treated using eigenvalues: 1. Introduction, 1.1. Matrices and eigenvalues of graphs; 2. Partition problems; 2.1 Graph bisection, 2.2. Connectivity and separation, 2.3. Isoperimetric numbers, 2.4. The maximum cut problem, 2.5. Clustering, 2.6. Graph partition; 3. Ordering, 3.1. Bandwidth and min-p-sum problems, 3.2. Cutwidth, 3.3 Ranking, 3.4. Scaling, 3.5. The quadratic assignment problem; 4. Stable sets and coloring, 4.1. Chromatic number, 4.2. Lower bounds on stable sets, 4.3. Upper bounds on stable sets, 4.4. k-colorable subgraphs; 5. Routing problems, 5.1. Diameter and the mean distance, 5.2. Routing, 5.3. Random walks; 6. Embedding problems; A. Appendix: Computational aspects; B. Appendix: Eigenvalues of random graphs. The paper [MoPo] contains a list of 135 references.

See [CvDSa], third edition, pp. 417–418, for further data and references.

The *travelling salesman problem* (TSP) is one of the best-known NP-hard combinatorial optimization problems, and there is an extensive literature on both its

theoretical and practical aspects. The most important theoretical results on TSP can be found in [LaLRS], [GuPu] (see also [CvDM]). Many algorithms and heuristics for TSP have been proposed. In the *symmetric* travelling salesman problem (STSP), it is assumed that the cost of travelling between two points is the same in both directions.

We shall mention here only one approach, which uses semi-definite programming (SDP) to establish a lower bound on the length of an optimal tour. This bound is obtained by relaxing the STSP and can be used in an algorithm of branch-and-bound type. The semi-definite relaxations of the STSP developed in [CvCK1] are based on a result of M. Fiedler [Fie] related to the Laplacian of graphs and algebraic connectivity (the second smallest eigenvalue of the Laplacian).

A semi-definite programming model for the travelling salesman problem was also obtained by Cvetković et al. [CvCK2, CvCK3].

The largest eigenvalue of a minimal spanning tree of the complete weighted graphs, with distances between cities serving as weights, can be used as a complexity index for the travelling salesman problem [CvDM].

3.5. Other sciences. Networks appearing in biology have been analyzed by spectra of normalized graph Laplacian in [Ban], [BaJo].

Research and development networks (R&D networks) are studied by the largest eigenvalue of the adjacency matrix in [KoBNS1], [KoBNS2].

Some older references on applications of graph spectra to Geography and social Sciences can be found in [CvDGT, Section 5.17].

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4. Selected bibliographies on applications of the theory of graph spectra

Subsections contain bibliographies related to Chemistry, Physics, Computer Science, Engineering, Biology and Economics.

4.1. Chemistry. In this bibliography are included books and expository articles that are either completely or to a significant extent concerned with some aspect(s) of chemical applications of graph spectral theory. Some books and expository articles in which graph–spectrum–related topics are mentioned only marginally (not necessarily in an explicit manner) are also included; these are marked by [XX].

Original research papers concerned with chemical applications of graph spectral theory are to numerous to be covered by this bibliography. Some of these papers, of exceptional (mainly historical) relevance, are nevertheless included; these are marked by [OR].

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A similar comment applies to the remaining sections (Computer Science, Engineering, Biology and Economics).

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MULTIPROCESSOR INTERCONNECTION NETWORKS

Abstract. Homogeneous multiprocessor systems are usually modelled by undirected graphs. Vertices of these graphs represent the processors, while edges denote the connection links between adjacent processors. Let G be a graph with diameter D, maximum vertex degree Δ, the largest eigenvalue λ_1 and m distinct eigenvalues. The products $m\Delta$ and $(D+1)\lambda_1$ are called the tightness of G of the first and second type, respectively. In the recent literature it was suggested that graphs with a small tightness of the first type are good models for the multiprocessor interconnection networks. We study these and some other types of tightness and some related graph invariants and demonstrate their usefulness in the analysis of multiprocessor interconnection networks. A survey of frequently used interconnection networks is given. Load balancing problem is presented. We prove that the number of connected graphs with a bounded tightness is finite and we determine explicitly graphs with tightness values not exceeding 9. There are 69 such graphs and they contain up to 10 vertices. In addition we identify graphs with minimal tightness values when the number of vertices is $n = 2, \ldots, 10$.

Mathematics Subject Classification (2000): 05C50, 68M07, 68M10, 68M14

Keywords: Multiprocessor Systems, Interconnection Topologies, Load Balancing, Spectra of Graphs, Graph Invariants.

Contents

1. Introduction

Usual models for multiprocessor interconnection networks [18] are (undirected, connected) graphs [29, 31]. Vertices of these graphs represent the processors, while edges denote the connection links between neighboring (adjacent) processors. The processors within a multiprocessor system communicate by sending or receiving messages through these communication links. The two main parameters of the graph that play an important role in the design of multiprocessor topologies are maximum vertex degree Δ and the diameter D. In other words, Δ directly corresponds to the number of neighboring processors (adjacent vertices in the graph model), while D represents the length of the longest path in processor graph, i.e. maximum distance between two processors. The main drawback of multiprocessor systems is the communication overhead [4, 33], the time required to exchange data between different processing units. Therefore, interconnection networks have to satisfy two contradictory properties: to minimize the "number of wires" and to maximize the data exchange rate. This means that the paths connecting each two processors have to be as short as possible while the average number of connections per processor has to be as small as possible.

Recently, the link between the design of multiprocessor topologies and the theory of graph spectra [13] has been recognized [17]. The general idea of using graph eigenvalues in multiprocessor interconnection networks can be also found in [28]. The main conclusion of [17] is that the product of the number m of distinct eigenvalues of a graph adjacency matrix and Δ has to be as small as possible. We call this product the *tightness of the first type* for a graph. In [6] we introduced the *tightness of the second type* as the product $(D+1)\lambda_1$, where λ_1 is the largest eigenvalue of the graph. Moreover, we defined some other types of graph tightness, and investigated the relation between the tightness values and the suitability of

the corresponding multiprocessor architecture. We showed that the graphs with a small tightness of the second type are suitable for the design of multiprocessor topologies.

In the paper [5] we determined explicitly graphs with tightness values not exceeding $a = 9$. To explain why the value 9 has been chosen, note first that by Theorem 1 the number of connected graphs with a bounded tightness is finite. If the selected upper bound a is high, the number of corresponding graphs could be very big and some of these graphs may have large number of vertices. It turned out that the value $a = 9$ is very suitable: i) it is big enough to include the Petersen graph (Fig. 12), known to be a very good interconnection network (see, for example, [35]), and ii) it is small enough so that only 69 graphs obey the bound with the number of vertices in these graphs not exceeding 10.

For basic definitions and some general results in the theory of graph spectra the reader is referred to the introductory chapter of this publication.

The paper is organized as follows. Section 2 is devoted to relations between the load balancing problem and the theory of graph spectra. Definitions and basic properties of various types of tightness are given in Section 3. Section 4 contains a survey of frequently used multiprocessor interconnection networks. Some results on a special class of trees in the role of interconnection networks are given in Section 5. Graphs with small values for different types of tightness are classified in Section 6. Graphs with smallest tightness values (among all graphs of the same order not exceeding 10) are identified within Section 7.

2. Load balancing

The job which has to be executed by a multiprocessor system is divided into parts that are given to particular processors to handle them. We can assume that the whole job consists of a number of elementary jobs (items) so that each processor gets a number of such elementary jobs to execute. Mathematically, elementary jobs distribution among processors can be represented by a vector x whose coordinates are non-negative integers. Coordinates are associated to graph vertices and indicate how many elementary jobs are given to corresponding processors.

Vector x is usually changed during the work of the system because some elementary jobs are executed while new elementary jobs are permanently generated during the execution process. Of course, it would be optimal that the number of elementary jobs given to a processor is the same for all processors, i.e., that the vector x is an integer multiple of the vector j whose all coordinates are equal to 1. Since this is not always possible, it is reasonable that processors with a great number of elementary jobs send some of them to adjacent processors so that the job distribution becomes uniform if possible. In this way the so called problem of *load balancing* is important in managing multiprocessor systems. The load balancing problem requires creation of algorithms for moving elementary jobs among processors in order to achieve the uniform distribution.

We shall present an algorithm for the load balancing problem which is based on the Laplacian matrix of a graph. A similar algorithm can be constructed using the adjacency matrix.

Let G be a connected graph on n vertices. Eigenvalues and corresponding ortonormal eigenvectors of the Laplacian $L = D - A$ of G are denoted by $\nu_1, \nu_2, \ldots, \nu_n = 0$ and $u_1, u_2, \ldots, u_n$, respectively. Any vector x from R^n can be represented as a linear combination of the form $x = \alpha_1 u_1 + \alpha_2 u_2 + \cdots + \alpha_n u_n$.

Suppose now that G has distinct Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_m = 0$ with multiplicities $k_1, k_2, \ldots, k_m = 1$, respectively. Vector x can now be represented in the form $x = y_1 + y_2 + \cdots + y_m$ where y_i belong to the eigenspace of μ_i for $i = 1, 2, \ldots, m$. We also have $y_m = \beta j$ for some β.

Since $Lx = L(y_1 + y_2 + \cdots + y_m) = \mu_1 y_1 + \mu_2 y_2 + \cdots + \mu_m y_m$, we have $x^{(1)} = x - \frac{1}{\mu_1} Lx = \big(I - \frac{1}{\mu_1} L\big)x = \big(1 - \frac{\mu_2}{\mu_1}\big)y_2 + \cdots + \beta j$. We see that the component of x in the eigenspace of μ_1 has been cancelled by the transformation by the matrix $I - \frac{1}{\mu_1} L$ while the component in the eigencpace of μ_m remains unchanged. The transformation $I - \frac{1}{\mu_2} L$ will cause that the component of $x^{(2)} = \big(I - \frac{1}{\mu_2} L\big)x^{(1)}$ in the eigenspace of μ_2 disappears. Continuing in this way

$$x^{(k)} = \Big(I - \frac{1}{\mu_k} L\Big) x^{(k-1)}, \quad k = 1, 2, \ldots, m-1 \tag{1}$$

we shall obtain $x^{(m-1)} = \beta j$.

We have seen how a vector x can be transformed to a multiple of j using the iteration process (1) which involves the Laplacian matrix of the multiprocessor graph G. It remains to see what relations (1) mean in terms of load moving.

Let vector $x^{(k)}$ have coordinates $x_1^{(k)}, x_2^{(k)}, \ldots, x_n^{(k)}$. Relations (1) can be rewritten in the form

$$x_i^{(k)} = x_i^{(k-1)} - \frac{1}{\mu_k} \sum_{i*j} \Big(d_i x_i^{(k-1)} - x_j^{(k-1)}\Big) \tag{2}$$

where d_i is the degree of vertex i. This means that the current load at vertex i is changed in such a way that vertex (processor) i sends $\frac{1}{\mu_k}$-th part of its load to each of its d_i neighbors and, because this holds for every vertex, also receives $\frac{1}{\mu_k}$-th part of the load from each of its d_i neighbors.

In this way we have defined a load flow on the edge set of G. First, particular amounts of load flow should be considered algebraically, i.e., having in mind their sign. So, if $x_i^{(k-1)}$ is negative, then vertex i, in fact, receives the corresponding amount. For each edge ij we have two parts of the flow: the part which is sent (or received) by i and the part which is sent (or received) by j. These two amounts should be added algebraically and in this way we get final value of the flow through edge ij. This flow at the end has a non-negative value which is sent either from i to j or vice versa.

Although the load flow plan defined in this way by relations (1) theoretically solves the problem of load balancing, one should be careful when it has to be really applied. This is not the only flow plan which solves the problem. For example, one can apply relations (1) with various orders of eigevalues. Further, the flow plan that we get could be such that the load is sent to final destinations via long paths. Also, it is not clear that a flow plan is always realizable because it could happen that a

vertex has not enough elementary jobs to send which it should send according to the flow plan. These facts indicate that one should further consider the load balancing and find, if possible, flow plans which would be optimal according to some criteria. We shall not further elaborate the problem of load balancing and the interested reader can consult the literature (see, for example, [17] and references given there).

Here we point out the obvious fact that the number of iterations in (1) is equal to the number of non-zero distinct Laplacian eigenvalues of the underlying graph. Hence we see that from the point of view of complexity of the load balancing algorithms graphs with a small number of distinct Laplacian eigenvalues are suitable for modelling multiprocessor interconnection networks. In addition, maximum vertex degree Δ of G also affects computation of the balancing flow. Therefore, the complexity of the balancing flow calculations essentially depends on the product $m\Delta$ and that is why this quantity was proposed in [17] as a parameter relevant for the choice and the design of multiprocessor interconnection networks.

Although graphs with few distinct eigenvalues allow a quick execution of load balancing algorithms, it is not expected that infinite families of such graphs with small tightness can be constructed.

A graph is called *integral* if its spectrum consists entirely of integers. Each eigenvalue has integral eigenvectors and each eigenspace has a basis consisting of such eigenvectors.

In integral graphs load balancing algorithms, which use eigenvalues and eigenvectors, can be executed in integer arithmetics. The further study of integral graphs in connection to multiprocessor topologies seems to be a promising subject for future research.

See references [15, 16, 21, 24, 25] for a further study of the load balancing problem.

3. Various types of tightness of a graph

As we have already pointed out, the graph invariant obtained as the product of the number of distinct eigenvalues m and the maximum vertex degree Δ of G has been investigated in [17] related to the design of multiprocessor topologies. The main conclusion of [17] with respect to the multiprocessor design and, in particular to the load balancing within given multiprocessor systems was the following: if $m\Delta$ is small for a given graph G, the corresponding multiprocessor topology was expected to have good communication properties and has been called *well-suited*. It has been pointed out that there exists an efficient algorithm which provides optimal load balancing within $m - 1$ computational steps. The graphs with large $m\Delta$ were called *ill-suited* and were not considered suitable for design of multiprocessor networks.

Several families of graphs with a small product $m\Delta$ have been constructed. One such family is based on hypercubes. It is interesting that the ubiquitous Petersen graph appears also as a good candidate for multiprocessor interconnection networks.

On the other hand there are many known and widely used multiprocessor topologies based on graphs which appear to be ill-suited according to [17]. Such an example is the star graph $S_n = K_{1,n-1}$.

In order to extend and improve the application of the theory of graph spectra to the design of multiprocessor topologies, some other types of graph invariants (under common name tightness) have been defined in [6] and their suitability for describing the corresponding interconnection networks investigated.

As we can see, $m\Delta$ is the product of one spectral invariant m and one structural invariant Δ. Therefore, we will refer to this type of tightness as the *mixed tightness*. In [6], we introduced two alternative (homogeneous) definitions of tightness, the *structural* and the *spectral* one. Moreover, we introduced another mixed tightness, and therefore we end up with *type one mixed tightness* and *type two mixed tightness*. Here we recall all these definitions. New types of tightness involve another structural invariant (diameter) and another spectral invariant (the largest eigenvalue). Both invariants are important for communication properties of a network in general.

Definition 1. The *tightness* $t_1(G)$ of a graph G is defined as the product of the number of distinct eigenvalues m and the maximum vertex degree Δ of G, i.e., $t_1(G) = m\Delta$.

Definition 2. *Structural tightness* $\mathrm{stt}(G)$ is the product $(D+1)\Delta$ where D is diameter and Δ is the maximum vertex degree of a graph G.

Definition 3. *Spectral tightness* $\mathrm{spt}(G)$ is the product of the number of distinct eigenvalues m and the largest eigenvalue λ_1 of a graph G.

Definition 4. *Second type mixed tightness* $t_2(G)$ is defined as a function of the diameter D of G and the largest eigenvalue λ_1, i.e., $t_2(G) = (D+1)\lambda_1$.

If the type of tightness is not relevant for the discussion, all four types of tightness will be called, for short, tightness. In general discussions we shall use $t_1, t_2, \mathrm{stt}, \mathrm{spt}$ independently of a graph to denote the corresponding tightness. An alternative term for tightness could be the word *reach*.

The use of the largest eigenvalue, i.e. the index, of a graph instead of the maximum vertex degree in description of multiprocessor topologies seems to be appropriate for several reasons. By Theorem 1.12 of [13] the index of a graph is equal to a kind of mean value of vertex degrees, i.e. to the so called dynamical mean value, which takes into account not only immediate neighbors of vertices, but also neighbors of neighbors, etc. The index is also known to be a measure of the extent of branching of a graph, and in particular of a tree (see [10] for the application in chemical context and [9] for a treatment of directing branch and bound algorithms for the travelling salesman problem). The index, known also as a spectral radius, is a mathematically very important graph parameter as presented, for example, in a survey paper [11].

According to the well-known inequality $d_{\min} \leqslant \bar{d} \leqslant \lambda_1 \leqslant d_{\max} = \Delta$, [13, p. 85] we have that $\mathrm{spt}(G) \leqslant t_1(G)$. Here $d_{\min}$ and $d_{\max}$ denote minimum and maximum vertex degrees, respectively and $\bar{d}$ is used to denote the average value of vertex degrees.

The relation between $\mathrm{stt}(G)$ and $t_1(G)$ is $t_1(G) \geqslant \mathrm{stt}(G)$, since $m \geqslant 1 + D$ (see Theorem 3.13. from [13]). For distance-regular graphs [3] $m = 1 + D$ holds.

We also have $t_2(G) \leqslant \mathrm{spt}(G)$ and $t_2(G) \leqslant \mathrm{stt}(G)$.

The two homogeneous tightness appear to be incomparable. To illustrate this, let us consider star graph with $n = 5$ vertices ($S_5 = K_{1,4}$) given on Fig. 1a, and the graph $\bar{S}_5$ obtained if new edges are added to the star graph as it is shown on Fig. 1b.

a) b)

FIGURE 1. a) Star graph with $n = 5$ vertices and b) extended star graph

From [13, pp. 272–275, Table 1], we can see that for S_5 it holds $D = 2$, $\Delta = 4$, $m = 3$ and $\lambda_1 = 2$ and hence $\mathrm{spt}(S_5) = m\lambda_1 = 6 < 12 = (D + 1)\Delta = \mathrm{stt}(S_5)$. On the other hand for the graph $\bar{S}_5$ we have $D = 2$, $\Delta = 4$, $m = 4$ and $\lambda_1 = 3.2361$ yielding to $\mathrm{spt}(\bar{S}_5) > \mathrm{stt}(\bar{S}_5)$.

The above mentioned table shows that this is not the only example. For $n = 5$, 21 different graphs exist. Only for 3 of them the two homogeneous tightness have the same value, while $\mathrm{stt}(G)$ is smaller for 9 graphs, and for the remaining 9 $\mathrm{spt}(G)$ has a smaller value.

For two graph invariants $\alpha(G)$ and $\beta(G)$ we shall say that the relation $\alpha(G) \prec \beta(G)$ holds if $\alpha(G) \leqslant \beta(G)$ holds for any graph G. With this definition we have the Hasse diagram for the $\prec$ relation between various types of tightness given on Fig. 2.

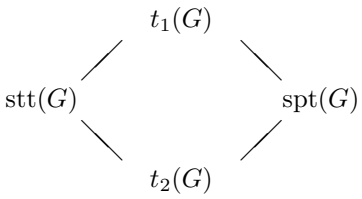

FIGURE 2. Partial order relation between different types of graph tightness

In order to study the behavior of a property or invariant of graphs when the number of vertices varies, it is important that the property (invariant) is scalable. *Scalability* means that for each n there exists a graph with n vertices having that property (invariant of certain value).

A family of graphs is called *scalable* if for any n there exists an n-vertex graph in this family. For example, in [17] the scalable families of sparse graphs (maximum vertex degree $O(\log n)$) with small number of distinct eigenvalues are considered. Obviously, sometimes it is difficult to construct scalable families of graphs for a given property.

We present a theorem which seems to be of fundamental importance in the study of the tightness of a graph.

Theorem 1. *For any kind of tightness, the number of connected graphs with a bounded tightness is finite.*

Proof. Let $t(G) \leqslant a$ for a given positive integer a, where $t(G)$ stands for any kind of tightness. In all four cases, we shall prove that there exists a number b such that both diameter D and maximum vertex degree Δ are bounded by b. We need two auxiliary results from the theory of graph spectra.

Having in view (1) and (2) from the introductory chapter of this publication, $t(G) \leqslant a$ implies

Case $t(G) = t_1(G)$. $m\Delta \leqslant a$, $m \leqslant a$ and $\Delta \leqslant a$, $D \leqslant a-1$, and we can adopt $b = a$;

Case $t(G) = \mathrm{stt}(G)$. $(D+1)\Delta \leqslant a$, $D \leqslant a-1$ and $\Delta \leqslant a$, here again $b = a$;

Case $t(G) = \mathrm{spt}(G)$. $m\lambda_1 \leqslant a$, $m \leqslant a$ and $\lambda_1 \leqslant a$, $D \leqslant a-1$, and $\Delta \leqslant \lambda_1^2 \leqslant a^2$, and now $b = a^2$;

Case $t(G) = t_2(G)$. $(D+1)\lambda_1 \leqslant a$, $D \leqslant a-1$, and $\Delta \leqslant a^2$, and again $b = a^2$.

It is well known that for the number of vertices n in G the following inequality holds

$$n \leqslant 1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{D-1}. \tag{3}$$

To derive this inequality vertices of G are enumerated starting from a particular vertex and adding maximum number of neighbors at particular distances from that vertex. Based on this relation and assuming that both D and Δ are bounded by a number b, we have

$$\begin{aligned} n &< 1 + \Delta + \Delta^2 + \Delta^3 + \cdots + \Delta^D \leqslant 1 + \Delta + \Delta^2 + \Delta^3 + \cdots + \Delta^b \\ &\leqslant 1 + b + b^2 + b^3 + \cdots + b^b. \end{aligned}$$

In such a way we proved that the number of vertices of a connected graph with a bounded tightness is bounded. Therefore, it is obvious that there can be only finitely many such graphs and the theorem is proved. □

Corollary 1. *The tightness of graphs in any scalable family of graphs is unbounded.*

Corollary 2. *Any scalable family of graphs contains a sequence of graphs, not necessarily scalable, with increasing tightness diverging to $+\infty$.*

The asymptotic behavior of the tightness, when n tends towards $+\infty$, is of particular interest in the analysis of multiprocessor interconnection networks. Typically, in suitable (scalable) families of graphs the tightness values have asymptotic behavior, for example, $O(\log n)$ or $O(\sqrt{n})$. Several cases are studied in [6] and reviewed also here in the next section.

4. A survey of frequently used interconnection networks

In this section we survey the graphs that are often used to model multiprocessor interconnection networks and examine the corresponding tightness values. Since the tightness is a product of two positive quantities, it is necessary for both of them to have small values to assure a small value of tightness.

1. An example of such a graph is the *d-dimensional hypercube* $Q(d)$. It consists of $n = 2^d$ vertices, each of them connected with d neighbors. The vertices are labelled starting from 0 to $n-1$ (considered as binary numbers). An edge connects two vertices with binary number differing in only one bit. For these graphs we have $m = d+1,\ D = d,\ \Delta = d,\ \lambda_1 = d$ and all four types of the tightness are equal to $(d+1)d = O((\log n)^2)$.

Since the connection is fully symmetric, for the diameter we have $D(Q(d)) = d$. The 1-, 2- and 3-dimensional hypercubes are illustrated on Fig. 3. □

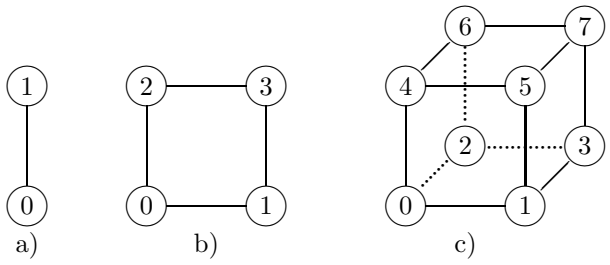

FIGURE 3. The examples of hypercube multiprocessor topologies

2. Another example is *butterfly* graph $B(k)$ containing $n = 2^k(k+1)$ vertices (Fig. 4). The vertices of this graph are organized in $k+1$ levels (columns) each containing 2^k vertices. In each column, vertices are labelled in the same way (from 0 to $2^k - 1$). An edge is connecting two vertices if and only if they are in the consecutive columns i and $i+1$ and their numbers are the same or they differ only in the bit at the i-th position. The maximum vertex degree is $\Delta = 4$ (the vertices from the two outer columns have degree 2 and the vertices in $k-1$ inner columns all have degree 4). Diameter D equals $2k$ while the spectrum is given in [17, Theorem 11]. Therefrom, the largest eigenvalue is $\lambda_1 = 4\cos(\pi/(k+1))$. However, it is not obvious how to determine parameter m. Therefore, we got only the values $\mathrm{stt} = 4(2k+1) = O(\log n)$ and $t_2 = 4(2k+1)\cos(\pi/(k+1)) = O(k) = O(\log n)$. □

Widely used interconnection topologies include some kind of trees, meshes and toruses [26]. We shall describe these structures in some details.

3. *Stars* $S_n = K_{1,n-1}$ are considered as ill-suited topologies in [17], since the tightness $t_1(S_n)$ is large. However stars are widely used in the multiprocessor system design, the so-called master–slave concept is based on the star graph structure. This fact may be an indication that the classification of multiprocessor interconnection networks based on the value for t_1 is not always adequate.

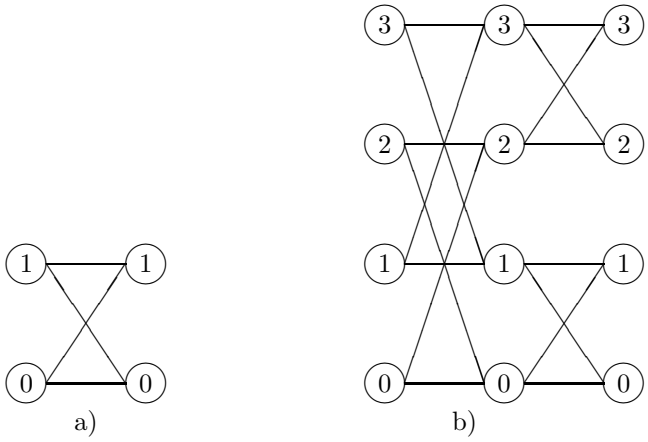

FIGURE 4. The examples of butterfly multiprocessor topologies

For S_n: $m = 3$, $\Delta = n - 1$, $D = 2$, $\lambda_1 = \sqrt{n-1}$ and we have

$$t_1(S_n) = 3(n-1),$$
$$\mathrm{stt}(S_n) = 3(n-1), \quad \mathrm{spt}(S_n) = 3\sqrt{n-1},$$
$$t_2(S_n) = 3\sqrt{n-1}.$$

Stars are only the special case in more general class of bipartite graphs. The main representative of this class are complete bipartite graphs K_{n_1,n_2} having vertices divided into two sets and edges connecting each vertex from one set to all vertices in the other set. For K_{n_1,n_2} we have $m = 3$, $\Delta = \max\{n_1, n_2\}$, $D = 2$, $\lambda_1 = \sqrt{n_1 n_2}$ and hence

$$t_1(K_{n_1,n_2}) = \mathrm{stt}(K_{n_1,n_2}) = 3\max\{n_1, n_2\},$$
$$\mathrm{spt}(K_{n_1,n_2}) = t_2(K_{n_1,n_2}) = 3\sqrt{n_1 n_2}.$$

In the case $n_1 = n_2 = n/2$ all tightness values are of order $O(n)$. However, for the star S_n we have $t_2(S_n) = O(\sqrt{n})$. This may be the indication that complete bipartite graphs are suitable for modelling multiprocessor interconnection networks only in some special cases. □

4. *Mesh* (or *grid*) (Fig. 5a) consists of $n = n_1 n_2$ vertices organized within layers. We can enumerate vertices with two indices, like the elements of an $n_1 \times n_2$ matrix. Each vertex is connected to its neighbors (the ones whose one of the indices is differing from its own by one). The inner vertices have 4 neighbors, the corner ones only 2, while the outer (but not corner ones) are of degree 3. Therefore, $\Delta = 4$, $D = n_1 + n_2 - 2$. Spectrum is given in [13, p. 74]. In particular, the largest eigenvalue is $\lambda_1 = 2\cos(\pi/(n_1+1)) + 2\cos(\pi/(n_2+1))$ and for the tightness of the second type we obtain $t_2 = (n_1 + n_2 - 1)(2\cos(\pi/(n_1+1)) + 2\cos(\pi/(n_2+1)))$. Hence, $t_2 = O(\sqrt{n})$ if $n_1 \approx n_2$. □

a) b)

FIGURE 5. a) Mesh of order 3×4 and b) corresponding torus architecture

5. *Torus* (Fig. 5b) is obtained if the mesh architecture is closed among both dimensions. We do not distinguish corner or outer vertices any more. The characteristics of a torus are $\Delta = 4$, $D = [n_1/2] + [n_2/2]$. Spectrum is given in [13, p. 75]. In particular, the largest eigenvalue is $\lambda_1 = 2\cos(2\pi/n_1) + 2\cos(2\pi/n_2)$ and thus $t_2 = ([n_1/2]+[n_2/2]+1)(2\cos(2\pi/n_1)+2\cos(2\pi/n_2))$. As in the previous case (for mesh) we have $t_2 = O(\sqrt{n})$ if $n_1 \approx n_2$. □

All these architectures satisfy both requirements of designing the multiprocessor topologies (small distance between processors and small number of wires). Those of them which have a small value for t_1 are called *well-suited interconnection topologies* in [17]. Other topologies are called *ill-suited*. Therefore, according to [17], well-suited and ill-suited topologies are distinguished by the value for the mixed tightness of the first type $t_1(G)$.

The star example suggests that $t_2(G)$ is a more appropriate parameter for selecting well-suited interconnection topologies than $t_1(G)$. Namely, the classification based on the tightness t_2 seems to be more adequate since it includes stars in the category of well-suited structures.

The obvious conclusion following from the Hasse diagram given on Fig. 3, is that the well-suited interconnection network according to the value for t_1 remain well-suited also when t_2 is taken into consideration. In this way, some new graphs become suitable for modelling multiprocessor interconnection networks. Some of these "new" types of graphs are already recognized by multiprocessor system designers (like stars and bipartite graphs). In the next section we propose a new family of t_2-based well-suited trees.

5. Complete quasi-regular trees

In this section we shall study properties of some trees and show that they are suitable for our purposes.

The complete quasi-regular tree $T(d,k)(d = 2,3,\dots,k = 1,2,\dots)$ is a tree consisting of a central vertex and k layers of other vertices, adjacencies of vertices being defined in the following way.

1. The central vertex (the one on the layer 0) is adjacent to d vertices in the first layer.

2. For any $i = 1, 2, \ldots, k-1$ each vertex in the i-th layer is adjacent to $d-1$ vertices in the $(i+1)$-th layer (and one in the $(i-1)$-th layer).

The graph $T(3,3)$ is given in Fig. 6.

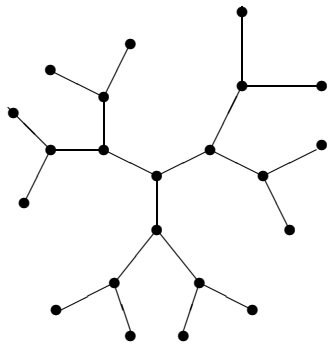

FIGURE 6. Quasi-regular tree $T(3,3)$

The graph $T(d,k)$ for $d > 2$, has $n = 1+d((d-1)^k-1)/(d-2)$ vertices, maximum vertex degree $\Delta = d$, diameter $D = 2k$ and the largest eigenvalue $\lambda_1 < d$. (The spectrum of $T(d,k)$ has been determined in [23]). We have $k = O(\log n)$ and, since $t_2(T(d,k)) = (D+1)\lambda_1 < (D+1)\Delta = \mathrm{stt}(T(d,k)) = (2k+1)d$, we obtain $t_2(T(d,k)) = O(\log n)$. This is asymptotically better than in the hypercube $Q(d)$ case, where $t_2(Q(d)) = O((\log n)^2)$ or in the case for star graph where $t_2(K_{1,n-1}) = O(\sqrt{n})$ (see Section 4). Note that the path P_n with $t_2(P_n) = 2n\cos(\pi/(n+1)) = O(n)$ also performs worse.

The coefficient of the main term in the expression for $t_2(T(d,k))$ is equal to $d/\log(d-1)$ with values of 4.328, 3.641, 3.607, 3.728, 3.907, 4.111, 4.328 and 4.551 for $d = 3, 4, 5, 6, 7, 8, 9, 10$, respectively. The coefficient is further an increasing function of d. Therefore the small values of d are desirable and we shall discuss in details only the case $d = 3$ since it is suitable for resolving the stability issues. The other cases with small values for d can be analyzed analogously.

To examine the suitability of graphs $T(3,k)$, we compared its tightness values with the corresponding ones for two interesting classes of trees: paths P_n and stars $S_n = K_{1,n-1}$ containing the same number of vertices $n = 3 \cdot 2^k - 2$. The results for small values of k are summarized in the Table 1. 5.

Since for paths and quasi-regular trees the mixed tightness of the second type has almost the same value as the mixed tightness of the first type, we put only the values for the first type mixed tightness for paths, while for $T(n,k)$ the structural tightness is given.

The last column (for stars) contains the values for two tightness, first for the mixed tightness of the first type and then the value for the mixed tightness of the second type in the parentheses.

As can be seen from the Table 1, the tightness values for paths P_n are significantly larger than the values $\mathrm{stt}(T(3,k))$. Star architecture seems to be better for small values of k, but starting from $k = 6$, we have $t_2(T(3,k)) < \mathrm{stt}(T(3,k)) < t_2(S_n)$.

TABLE 1. Tightness values for some trees

k	n	P_n	$T(3,k)$	S_n	
		$t_1(\geqslant t_2)$	$\mathrm{stt}(\geqslant t_2)$	t_1	(t_2)
1	4	$4 \cdot 2$	$3 \cdot 3$	$3 \cdot 3$	$(3 \cdot \sqrt{3})$
2	10	$10 \cdot 2$	$5 \cdot 3$	$3 \cdot 9$	$(3 \cdot \sqrt{9} = 3 \cdot 3)$
3	22	$22 \cdot 2$	$7 \cdot 3$	$3 \cdot 21$	$(3 \cdot \sqrt{21} < 3 \cdot 5)$
4	46	$46 \cdot 2$	$9 \cdot 3$	$3 \cdot 45$	$(3 \cdot \sqrt{45} < 3 \cdot 7)$
5	94	$94 \cdot 2$	$11 \cdot 3$	$3 \cdot 93$	$(3 \cdot \sqrt{93} < 3 \cdot 10)$
6	190	$190 \cdot 2$	$13 \cdot 3$	$3 \cdot 189$	$(3 \cdot \sqrt{189} > 3 \cdot 13)$
7	382	$382 \cdot 2$	$15 \cdot 3$	$3 \cdot 381$	$(3 \cdot \sqrt{381} > 3 \cdot 19)$

The intention when comparing complete quasi-regular trees $T(3,k)$ with paths P_n and stars S_n is to examine their place between two kinds of trees, extremal for many graph invariants. In particular, among all trees with a given number of vertices, the largest eigenvalue λ_1 and maximum vertex degree Δ have minimal values for the path and maximal for the star, while, just opposite, the number of distinct eigenvalues m and the diameter D have maximal values for the path and minimal for the star. Since the tightness (of any type) is a product of two graph invariants having, in the above sense, opposite behavior it is expected that its extreme value is attained "somewhere in the middle". Therefore, for a tree of special structure (like the quasi-regular trees are) we expect both tendencies to be in an equilibrium.

It is not difficult to extend the family of complete quasi-regular trees to a scalable family. A *quasi-regular tree* is a tree obtained from a complete quasi-regular tree by deleting some of its vertices of degree 1. If none or all vertices of degree 1 are deleted from a complete quasi-regular tree we obtain again a complete quasi-regular tree. Hence, a complete quasi-regular tree is also a quasi-regular tree. While a complete quasi-regular tree is unique for the given number of vertices, there are several non-isomorphic quasi-regular trees with the same number of vertices which are not complete. Therefore, there are several ways to construct a scalable family of quasi-regular trees. The following way is a very natural one.

Consider a complete quasi-regular tree $T(d,k)$ and perform the breadth first search through the vertex set starting from the central vertex. Adding to $T(d,k-1)$ pendant vertices of $T(d,k)$ in the order they are traversed in the mentioned breadth first search defines the desired family of quasi-regular trees.

The constructed family has the property that each its member has the largest eigenvalue λ_1 among all quasi-regular trees with the same number of vertices [32]. At first glance this property is something what we do not want since we are looking for graphs with the tightness t_2 as small as possible. Instead we would prefer, unlike the breadth first search, to keep adding pendant vertices to $T(d,k-1)$ in such a balanced way around that we always get a quasi-regular tree with largest eigenvalue as small as possible. Such a way of adding vertices is not known and its finding represents a difficult open problem in the spectral graph theory.

A scalable family of trees with $O((\log n)^2)$ distinct eigenvalues has been studied in [17]. An open question remains to compare the performances of these two families.

In our context interesting are also *fullerene graphs* corresponding to carbon compounds called *fullerenes*. Mathematically, fullerene graphs are planar regular graphs of degree 3 having as faces only pentagons and hexagons. It follows from the Euler theorem for planar graphs that the number of pentagons is exactly 12. Although being planar, fullerene graphs are represented (and this really corresponds to actual positions of carbon atoms in a fullerene) in 3-space with its vertices embedded in a quasi-spherical surface.

A typical fullerene C_{60} is given in Fig. 7. It can be described also as a truncated icosahedron and has the shape of a football.

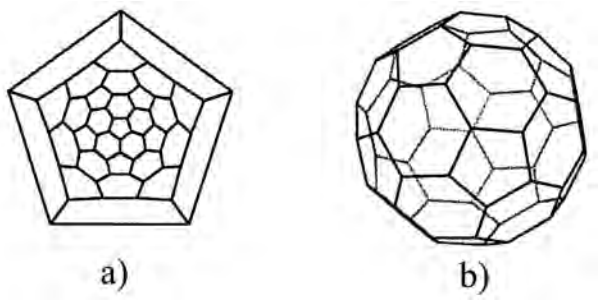

FIGURE 7. a) Planar and b) 3D visualization of the icosahedral fullerene C_{60}

Without elaborating details we indicate the relevance of fullerene graphs to our subject by comparing them with quasi-regular trees.

For a given number of vertices the largest eigenvalues of the two graphs are roughly equal (equal to 3 in fullerenes and close to 3 in quasi-regular trees) while the diameters are also comparable. This means that the tightness t_2 is approximately the same in both cases. In particular, the values of relevant invariants for the fullerene graph C_{60} are $n = 60$, $D = 9$ (see [19]), $m = 15$ (see [20]), $\Delta = \lambda_1 = 3$. Hence, $\mathrm{stt} = t_2 = 30$. A quasi-regular tree on 60 vertices has diameter $D = 9$ and we also get $\mathrm{stt} = 30$.

Note that the tightness t_1 is not very small since it is known that fullerene graphs have a large number of distinct eigenvalues [20].

It is also interesting that fullerene graphs have a nice 3D-representation in which the coordinates of the positions of vertices can be calculated from the eigenvectors of the adjacency matrix (the so called *topological coordinates* which were also used in producing the atlas [20]).

6. Graphs with small tightness values

In this section we classify graphs with small tightness values. In particular, we find graphs with tightness values not exceeding $a = 9$. To explain why the value

9 has been chosen, note first that by Theorem 1 from [6] (reproduced also here as Theorem 1) the number of connected graphs with a bounded tightness is finite. If the selected upper bound a is high, the number of corresponding graphs could be very big and some of these graphs may have large number of vertices. It turned out that the value $a = 9$ is very suitable: we established that exactly 69 graphs obey the bound with the number of vertices in these graphs not exceeding 10. The obtained graphs should be considered as reasonably good models for multiprocessor interconnection networks. A more modest task, finding graphs with tightness values not exceeding 8 is solved in [8].

Subsection 6.1 is devoted to preliminary considerations. The main results are contained in 6.2. The remaining four subsections contain the proofs related to the four types of tightness.

6.1. Preliminaries. Let $\mathcal{G}_c$ be the set of connected graphs with at least two vertices. Let us introduce the following notation:

$$T_1^a = \{G : G \in \mathcal{G}_c,\ t_1(G) \leqslant a\}, \quad T_{\rm stt}^a = \{G : G \in \mathcal{G}_c,\ {\rm stt}(G) \leqslant a\},$$
$$T_{\rm spt}^a = \{G : G \in \mathcal{G}_c,\ {\rm spt}(G) \leqslant a\}, \quad T_2^a = \{G : G \in \mathcal{G}_c,\ t_2(G) \leqslant a\}.$$

It is obvious that $T_1^a \subseteq T_{\rm stt}^a \subseteq T_2^a$ and $T_1^a \subseteq T_{\rm spt}^a \subseteq T_2^a$ because of the partial order between tightness values given on Fig. 3. Having in view inclusions between these sets we can represent them in the form

$$T_1^a = A,$$
$$T_{\rm stt}^a = A \cup B, \quad T_{\rm spt}^a = A \cup C,$$
$$T_2^a = A \cup B \cup C \cup D,$$

where A, B, C, D are sets of graphs illustrating the influence of each particular tightness definition. Moreover, according to Theorem 1, each of these sets is finite. From the definitions, the tightness of any kind is equal to 0 for the graph K_1 and equal to 2 for K_2. The trivial graph K_1 is not included in the above defined sets and therefore a should be at least 2 in order to have non-empty sets.

For $a = 2$ we have $T_1^2 = T_{\rm stt}^2 = T_{\rm spt}^2 = T_2^2 = \{K_2\}$ since for K_2 it holds $D = 1$, $\Delta = 1$, $m = 2$ and $\lambda_1 = 1$.

Further we have $T_1^4 = T_1^2 \cup \{K_3\} = T_{\rm stt}^4 = T_{\rm spt}^4 = T_2^4$. Namely, we have $t_1(K_3) = m\Delta = 2{\cdot}2 = 4$, $t_{\rm stt}(K_3) = (D{+}1)\Delta = 2{\cdot}2 = 4$, $t_{\rm spt}(K_3) = m\lambda_1 = 2{\cdot}2 = 4$, and $t_2(K_3) = (D+1)\lambda_1 = 2 \cdot 2 = 4$.

For $a = 5$, $T_1^5 = T_1^4$ and $T_{\rm stt}^5 = T_{\rm stt}^4$, but $T_{\rm spt}^5 = T_{\rm spt}^4 \cup \{P_3\}$ and $T_2^5 = T_2^4 \cup \{P_3\}$ which is easy to see from the characteristics of $P_3 = S_3 = K_{1,2}$.

For the further analysis, we need higher order graphs and we use the following sources. Diagrams and some relevant data for graphs with up to 5 vertices can be found in [13], the information about connected graphs with $n = 6$ vertices is presented in [14], while graphs containing $n = 7$ vertices are given in [12].

We used publicly available library of programs **nauty** [27] to generate all connected graphs with up to 10 vertices. **nauty** is a program for computing automorphism groups of graphs and digraphs. It can also produce a canonical graph labelling. **nauty** is an open source available function library written in a portable subset of **C**, and runs on a considerable number of different systems. We used its functions for generating all connected graphs on a given number of vertices. The implemented algorithm for generation of graphs is very efficient and provides a compact representation which is not readable by ordinary users. **nauty** library also provides several functions for converting this compact representation into "user friendly" form.

Since there are not too many graphs of order up to 5, we present them in Fig. 8. Starting from the results given in Table 1 in [13, pp. 272–275], we calculated values of different tightness for these graphs and summarized the obtained results in the Table 2. Column 1 gives the number n of vertices while column 2 contains the number e of edges. In the third column of the Table 6.1 graph labels consistent with Fig. 8 are given. Columns 4 to 7 contain values of the parameters used for tightness calculation, while in the remaining four columns corresponding tightness values are presented.

Looking at Table 2 we can easily identify graphs with the smallest value for the tightness of any type. For example, if $n = 5$, tightness t_1 has the smallest value for pentagon G_{27}, while the star G_{28} has a much greater value. However, according to the tightness t_2 star and pentagon are equally good as the interconnection topologies. For $n = 4$ the star is even better topology than the circuit, at least if we rely on tightness t_2.

Using the above mentioned sources, we can exhaustively enumerate sets T_1^a, T_{stt}^a, T_{spt}^a, T_2^a for few other values of a. For example, when we set $a = 6$, we get $T_1^6 = T_1^5 \cup \{G_3, G_4, G_7, G_{27}\} = \{K_2, K_3, G_3, G_4, G_7, G_{27}\} = T_{\text{stt}}^6$, while $T_{\text{spt}}^6 = T_{\text{spt}}^5 \cup \{G_4, G_7, G_8, G_{27}, G_{28}\} = \{K_2, K_3, P_3, G_4, G_7, G_8, G_{27}, G_{28}\} = T_2^6$. Note that graphs K_2, K_3, P_3 appear in Table 2 under the names G_1, G_2, G_3 respectively.

However, it is interesting to try a theoretical analysis which could be applied to more general cases. The following derivation can serve as a paradigm for more complex cases.

Let us now discuss the case T_1^6. More precisely, we are looking for graphs $G \in \mathcal{G}_c$ such that $t_1(G) = m\Delta \leqslant 6 = a$. Since both values ($m$ and Δ) are integers, we can distinguish the following cases:

- a°**:** $m = 1$. This is a trivial case satisfied only for K_1 which is excluded from considerations.
- b°**:** $m = 2$, $\Delta \leqslant 3$. Two distinct eigenvalues appear only in complete graphs, and consequently this case involves K_2, K_3 and K_4.
- c°**:** $m = 3$, $\Delta \leqslant 2$. The graphs satisfying this conditions are two circuits and 3-vertex path, namely, C_4, C_5 and P_3.

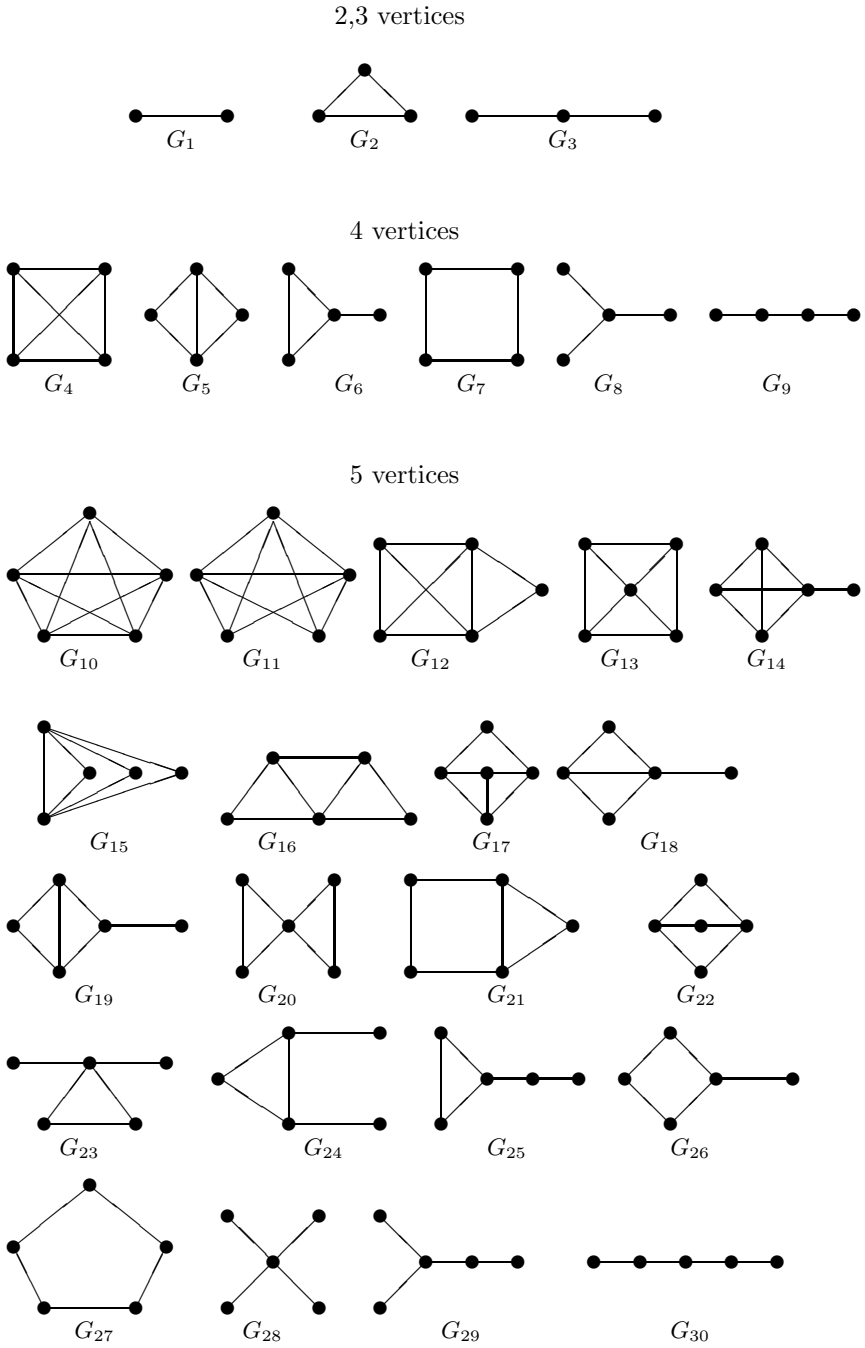

FIGURE 8. Graphs with up to 5 vertices

TABLE 2. Tightness values for small order graphs

n	e	graph	D	Δ	m	λ_1	t_1	stt	spt	t_2
2	1	G_1	1	1	2	1	2	2	2	2
3	3	G_2	1	2	2	2	4	4	4	4
	2	G_3	2	2	3	1.41	6	6	4.23	4.23
4	6	G_4	1	3	2	3	6	6	6	6
	5	G_5	2	3	4	2.56	12	9	10.24	7.68
	4	G_6	2	3	4	2.17	12	9	8.68	6.51
	4	G_7	2	2	3	2	6	6	6	6
	3	G_8	2	3	3	1.73	9	9	5.19	5.19
	3	G_9	3	2	4	1.618	8	8	6.472	6.472
5	10	G_{10}	1	4	2	4	8	8	8	8
	9	G_{11}	2	4	4	3.6458	16	12	14.5832	10.9374
	8	G_{12}	2	4	4	3.3234	16	12	13.2936	9.9702
	8	G_{13}	2	4	4	3.2361	16	12	12.9444	9.7083
	7	G_{14}	2	4	4	3.0861	16	12	12.3444	9.2583
	7	G_{15}	2	4	4	3	16	12	12	9
	7	G_{16}	2	4	5	2.9354	20	12	14.677	8.8062
	7	G_{17}	2	3	5	2.8558	15	9	14.279	8.5674
	6	G_{18}	2	4	5	2.6855	20	12	13.4275	8.0565
	6	G_{19}	3	3	5	2.6412	15	12	13.206	10.5648
	6	G_{20}	2	4	4	2.5616	16	12	10.2464	7.6848
	6	G_{21}	2	3	5	2.4812	15	9	12.406	7.4436
	6	G_{22}	2	3	3	2.4495	9	9	7.3485	7.3485
	5	G_{23}	2	4	5	2.3429	20	12	11.7145	7.0287
	5	G_{24}	3	3	5	2.3028	15	12	11.514	9.2112
	5	G_{25}	3	3	5	2.2143	15	12	11.07	8.8572
	5	G_{26}	3	3	5	2.1358	15	12	10.679	8.5432
	5	G_{27}	2	2	3	2	6	6	6	6
	5	G_{28}	2	4	3	2	12	12	6	6
	4	G_{29}	3	3	5	1.8478	15	12	9.239	7.3912
	4	G_{30}	4	2	5	1.7321	10	10	8.6605	8.6605

d°**:** $m = 4, 5, 6$, $\Delta \leqslant 1$. This case involves only disconnected graphs which are excluded from consideration.

Now, it is easy to see that

$$T_1^6 = \{K_2, K_3, P_3, K_4, C_4, C_5\} = \{G_1, G_2, G_3, G_4, G_7, G_{27}\},$$

and therefore we completed set T_1^6 in another way.

6.2. Main results. In paper [5] we determined all graphs for which the tightness value (all four types) does not exceed 9. These graphs happen to be of small order (not exceeding 10 vertices). In this way we made a catalog of models for small well-suited (according to each tightness) multiprocessor networks. In fact we proved

that $T_2^9 = Q \cup R' \cup S' \cup V'$, where $T_1^9 = Q$, $T_{\text{stt}}^9 = Q \cup R'$, $T_{\text{spt}}^9 = Q \cup S'$ and $|T_2^9| = 69$.

Here we have

$$\begin{aligned} Q &= \{K_2, K_3, K_4, K_5, P_3, P_4, C_4, C_5, C_6, C_7, K_{3,1}, K_{3,2}, K_{3,3}, PG\}, \\ R' &= \{G_5, G_6, G_{17}, G_{21}, CP(51), CP(69), CP(72), CP(93), N(7,337), \\ &\qquad N(7,514), N(7,624), N(8,6660), N(8,8469)\}, \\ S' &= \{P_5, K_{1,4}, K_{1,5}, K_{1,6}, K_{1,7}, K_{1,8}, K_{1,9}, \} \end{aligned}$$

and V' is given by Proposition 1. PG denotes the well known Petersen graph.

Proposition 1. *The set V' consists of the following* 35 *graphs.*

$$\begin{array}{lll} n=5: & G_{15}, G_{16}, G_{18}, G_{20}, G_{23}, & G_{25}, G_{26}, G_{29} = Z_5; \\ n=6: & CP(61), CP(66), CP(68), CP(71), & CP(102), CP(105), \\ & CP(73) = K_{2,4}, CP(75), CP(79), & CP(108), CP(109) = W_6; \\ & CP(94), & \\ n=7: & N(7,3), N(7,8), N(7,23), N(7,75), & N(7,5), N(7,92); \\ & N(7,156), N(7,219), N(7,324), & \\ & N(7,448); & \\ n=8: & N(8,3), N(8,30), N(8,342), & \\ & N(8,1039); & \\ n=9: & N(9,3). & \end{array}$$

While listing these graphs, we separated graphs belonging to the set A_1 from the ones contained in the set A_2, defined and determined in subsection 6.6.

Some of the listed graphs are given in Figs. 8 and 9 to 12.

Enumeration gives $|Q| = 14$, $|R'| = 13$, $|S'| = 7$ and $|V'| = 35$. Thus we identified 69 graphs of order not exceeding 10 among which one should look for suitable multiprocessor topologies.

The proofs of the presented main results will be given in the four subsections that follow.

Note that a consequence of the results presented in this work is that for all graphs with eleven or more vertices the value of the tightness of any kind is greater than 9.

Replacing t_1 with stt in the criterion for a good interconnection network (i.e., replacing the number of distinct eigenvalues m with the quantity $D+1$ where D is the diameter) gives rise to graphs from the set R'. Graphs from R' have diameter 2 and maximum vertex degree 3.

Introducing spt instead of t_1 (i.e., replacing maximum vertex degree Δ with the largest eigenvalue λ_1, a kind of average vertex degree [6]) causes the acceptance of graphs from the set S' as good models. The set S' consists mainly of stars.

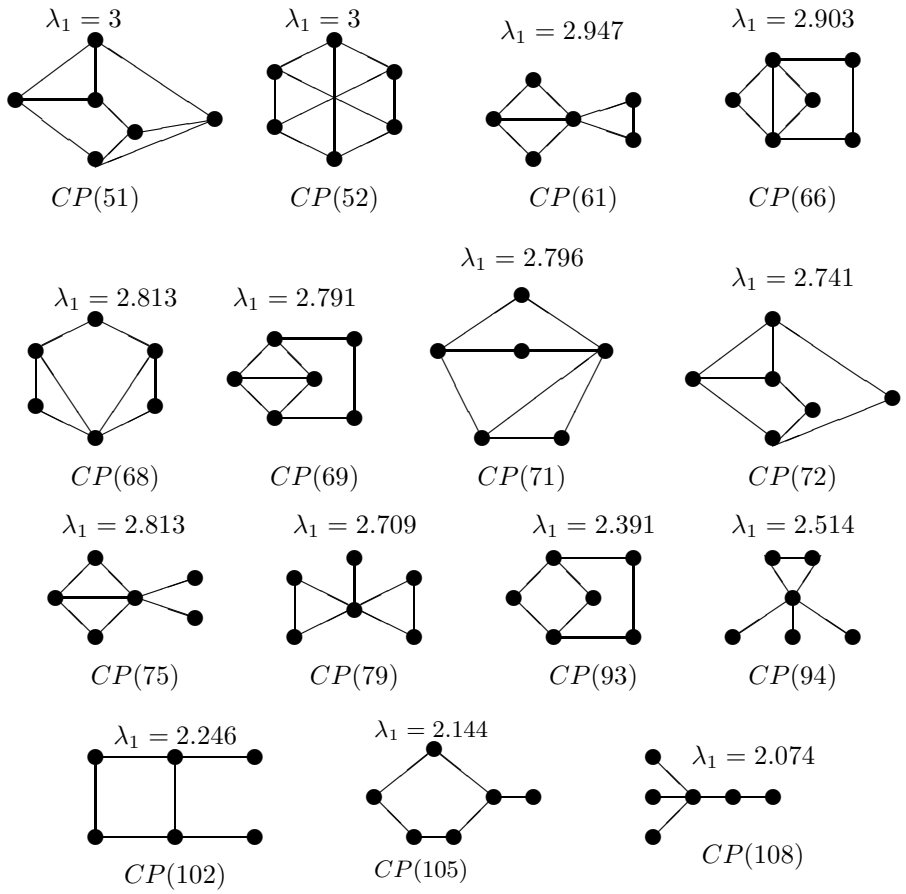

FIGURE 9. Some graphs with small tightness values on $n = 6$ vertices

If we finally pass to t_2, we get additional 35 graphs from the set V'. These graphs are characterized by a suitable combination of small values for diameter D and for the largest eigenvalue λ_1.

Among our 69 graphs there are exactly 14 integral graphs; for example, the Petersen graph, $K_{1,9}$ and $N(7, 219)$.

The fact that multiprocessor systems with small number of processors are very actual in both theoretical and practical research indicates the possible usefulness of the list with 69 graphs having small tightness values.

In addition to some theoretical importance we point out the following two arguments.

1° Interconnection networks with up to 10 nodes are widely used in the parallel research community. A lot of parallel algorithms that use small number of processors have been developed. Among recent results we emphasize [1] where the authors use 2-processors, circuit interconnection network of 4 processors as well as the 8

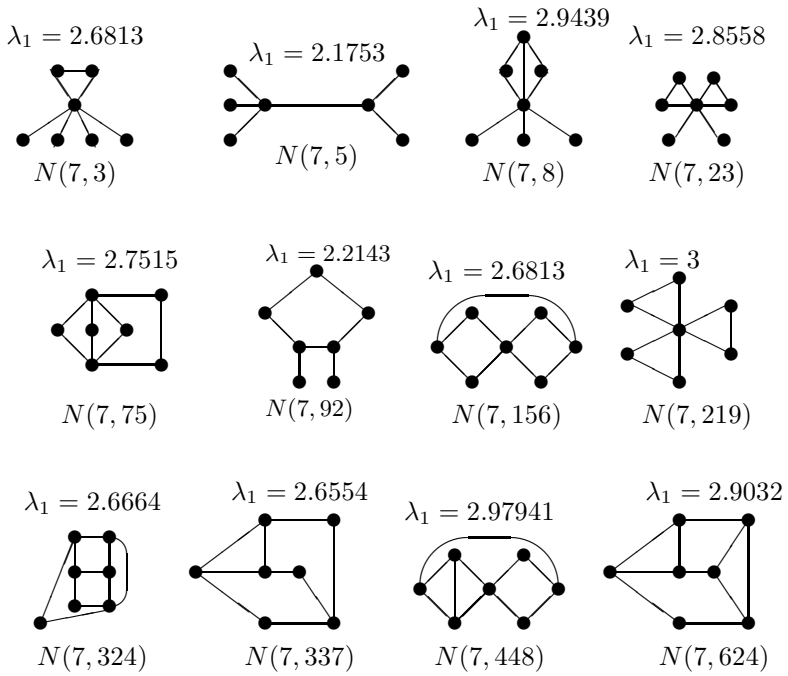

FIGURE 10. Some graphs with small tightness values on $n = 7$ vertices

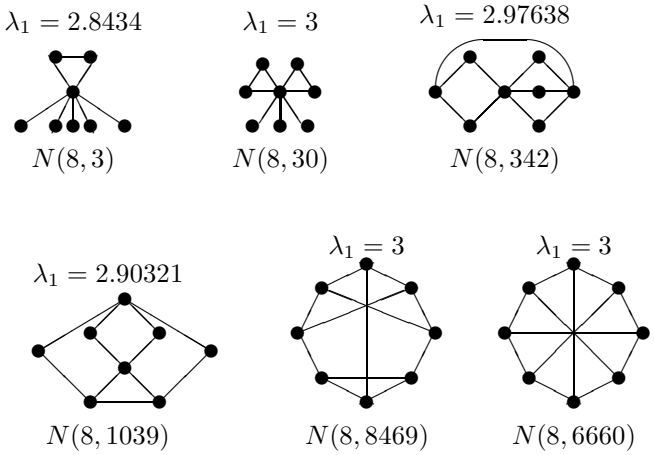

FIGURE 11. Some graphs with small tightness values on $n = 8$ vertices

processor mesh and 3D-hypercube for molecular dynamic simulations. The authors of [30] report best results of parallel Variable Neighborhood Search algorithm for job shop scheduling problems running on the ring (circuit) of ten processors. In

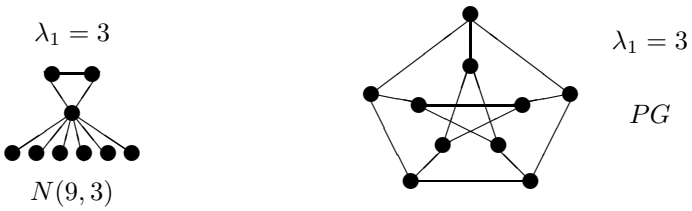

FIGURE 12. Some graphs with small tightness values on $n = 9, 10$ vertices

general, the designers of special parallel algorithms using a small number of processors can select some of the graphs from our list based on their own additional criteria (e.g. diameter, maximum vertex degree, load balancing properties, etc.). Another potential application of our graphs is in automatic mapping of a parallel program to the underlying network topology (like the one described in [22]).

2° The 69 graphs can be used to built real multiprocessor interconnection networks with a large number of processors using some graph operations and graph embedding. Two examples can be found in [35]: i) the Cartesian product of the Petersen graph with itself yields a good network with 100 vertices, ii) the Petersen graph can be embedded in a hypercube so that good properties of both graphs are combined.

These results provide further evidence that the tightness $t_2(G)$ is more suitable than the tightness $t_1(G)$ (previously used in the literature) for describing and classifying multiprocessor interconnection networks.

6.3. Type 1 mixed tightness. Since T_1^6 is already determined, here we look for T_1^9. Following cases are of interest:

- a°: $m = 2$, $\Delta \leqslant 4$. Here we have complete graphs K_2, K_3, K_4, K_5.
- b°: $m = 3$, $\Delta \leqslant 3$. In this case we can first calculate the upper bound for the number of vertices based on the relation (3). Since $\Delta = 3$ and $D \leqslant 2$ we have $n \leqslant 1 + 3 + 3 \cdot 2 = 10$. This case includes strongly regular and complete bipartite graphs, since there are no non-regular connected graphs with three distinct eigenvalues on less than 11 vertices other than complete bipartite graphs [34]. Hence, we get C_4, C_5, P_3, $K_{3,1}$, $K_{3,2}$, $K_{3,3}$, and the famous Petersen graph (PG), given on Fig. 12.
- c°: $m = 4$, $\Delta \leqslant 2$. In this case we have only C_6, C_7 and P_4.

We can summarize above considerations in the following theorem.

Theorem 2. *The only connected graphs with type* 1 *mixed tightness not exceeding* 9 *are the following* 14 *graphs:*

the Petersen graph,
complete graphs K_n for $n \leqslant 5$,
paths P_n for $n \leqslant 4$,
circuits C_n for $n \leqslant 7$, and
complete bipartite graphs $K_{3,n}$ for $n \leqslant 3$.

6.4. Structural tightness. This type of tightness also takes integer values, since $\mathrm{stt} = (D+1)\Delta$. Considering the set T^9_{stt}, the following cases should be analyzed:

$$a^\circ: \quad D=1,\ \Delta \leqslant 4, \qquad b^\circ: \quad D=2,\ \Delta \leqslant 3, \qquad c^\circ: \quad D=3, \Delta \leqslant 2.$$

We readily get all graphs as in Theorem 2. The only new possibility appears in case b° and corresponding graphs have $D=2$ and $\Delta=3$. Let R be the set of graphs satisfying these conditions ($D=2$, $\Delta=3$).

Based on the data presented in Table 2 in the subsection 6.1 set R contains graphs G_5, G_6 and G_8 with $n=4$ vertices and G_{17}, G_{21}, G_{22} for $n=5$. For $n=6$ the table of graphs from [14] yields the graphs (labelled there 51, 52, 69, 72, 93, here with prefix CP and parentheses) presented on Fig. 9. For $n=7,8,9$ we need a careful analysis. Among others, we have to look at cubic graphs (regular graphs of degree 3) on 8 vertices. Table 3 of [13, pp. 292–305], gives two such graphs (denoted there by 3.4 and 3.6) and they are presented here on Fig. 11 as $N(8,6660)$, $N(8,8469)$. ($N(x,y)$ denotes the y-th graph on x vertices generated by program **nauty**.) The stt tightness value for these two graphs is equal to 9.

The set R is completely determined by the following lemma.

Lemma 1. *The set R consists of the following* 17 *graphs: G_5, G_{17} given on Fig.* 8, *$CP(69)$ and $CP(93)$, from Fig.* 9, *all graphs presented on Fig.* 14, *graph $K'_{3,3}$ obtained from $K_{3,3}$ by subdividing one of its edges, the graphs $N(8,6660)$, $N(8,8469)$ on Fig.* 11, *$K_{3,1}$, $K_{3,2}$, $K_{3,3}$ and the Petersen graph.*

Proof. By formula (3) graphs from R have at most 10 vertices. Consider a graph $G \in R$. It has a vertex of degree 3 and suppose that it is labelled by 1. The three neighbors are 2, 3, 4 (see Fig. 13a).

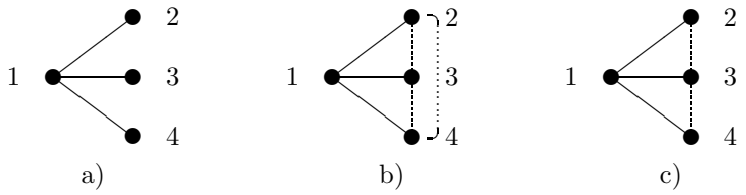

FIGURE 13. Some steps for construction of graphs from set R

Let f be the number of edges in the subgraph of G induced by 2, 3, 4. We have the following possibilities:

(1) $f=3$. The three newly added edges are represented on Fig. 13b) by dotted lines. This implies $G=K_4$ which is excluded since $D=1$.
(2) $f=2$. Now we start from the graph given on Fig. 13c) and add new vertices and edges in such a way that conditions $D=2$, $\Delta=3$ are not violated. We readily get $G=G_5$, or $G=G_{17}$ given on Fig. 8, or G is isomorphic to $CP(69)$ from Fig. 9.
(3) $f=1$. We can construct all these graphs by successively adding edges and vertices as long as all conditions are satisfied. The obtained graphs up to

7 vertices are presented on Fig. 6.4. Finally, we get the graph $N(8, 8469)$ from Fig. 11 on $n = 8$ vertices.

(4) $f = 0$. We first have $K_{3,1}$, $K_{3,2}$, $K_{3,3} = CP(52)$, $CP(93)$. For $n = 7$ we again come across graph $N(7, 337)$, and the graph $K'_{3,3} = N(7, 514)$. For $n = 8$ the graphs $N(8, 6660)$, $N(8, 8469)$ from Fig. 11 appear. The Petersen graph on 10 vertices belongs here. There are no graphs on 9 vertices. □

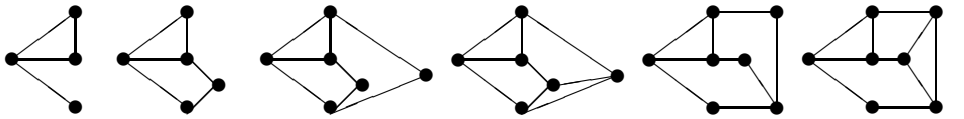

FIGURE 14. Some graphs from set R

Now we can formulate the main result of this subsection.

Theorem 3. *The set T^9_{stt} consists of graphs from the set T^9_1 and the graphs from the set R.*

Let $T^9_1 = Q$ and $R' = R \setminus Q$. The set R' consists of 13 graphs since $K_{3,1}$, $K_{3,2}$, $K_{3,3}$ and the Petersen graph belong to Q.

Corollary 3. $T^9_{\mathrm{stt}} = Q \cup R'$.

According to the structural tightness stt we have graphs from the set R (with $D = 2$ and $\Delta = 3$) as additional candidates for models of good interconnection networks. The set T^9_{stt} consists of 27 graphs.

6.5. Spectral tightness. As for the definition of spt, we have to analyze product of two positive numbers, one of them not always being integer. This may cause our analysis to be more difficult, but we can use the well known theoretical results from the theory of graph spectra.

Within this analysis the graphs with $\lambda_1 \leqslant 2$ (Smith graphs and their subgraphs, described in Section 2 of the introductory chapter) play an important role. We calculated all relevant parameters for Smith graphs and their subgraphs and summarized them in Table 3. As a useful tool for this study we explored newGRAPH programming package [2] to calculate values of m and λ_1 of obtained subgraphs. Values for C_n are not represented in Table 3, since we always have $D = \lfloor \frac{n}{2} \rfloor$, $\Delta = 2$, $m = \lfloor \frac{n}{2} \rfloor + 1$, $\lambda_1 = 2$.

Once we have all relevant parameters summarized in a table, it is easy to collect all Smith graphs and their subgraphs satisfying some given conditions.

If we want to determine T^9_{spt}, we have to analyze 6 cases:

a°: $m = 1$, $\lambda_1 \leqslant 9$. There are no graphs satisfying these conditions.

b°: $m = 2$, $\lambda_1 \leqslant 4.5$. Graphs K_2, K_3, K_4, K_5 satisfy these conditions.

c°: $m = 3$, $\lambda_1 \leqslant 3$. These conditions are satisfied for C_4, C_5, the Petersen graph, $K_{1,2} = P_3$, $K_{2,3}$, $K_{3,3}$, $K_{1,3}$, $K_{1,4}, \ldots, K_{1,9}$.

TABLE 3. Parameters of some Smith graphs and some subgraphs of Smith graphs

graph	D	Δ	m	λ_1	graph	D	Δ	m	λ_1
W_6	3	3	5	2.00000	Z_4	2	3	3	1.73205
W_7	4	3	5	2.00000	Z_5	3	3	5	1.84776
W_8	5	3	7	2.00000	Z_6	4	3	5	1.90211
W_9	6	3	7	2.00000	Z_7	5	3	7	1.93185
W_{10}	7	3	9	2.00000	Z_8	5	3	7	1.94986
H_7	4	3	5	2.00000	E_6	4	3	6	1.93185
H_8	6	3	7	2.00000	E_7	5	3	7	1.96962
H_9	7	3	9	2.00000	E_8	6	3	8	1.98904
P_2	1	1	2	1.00000	P_6	5	2	6	1.80194
P_3	2	2	3	1.41421	P_7	6	2	7	1.84776
P_4	3	2	4	1.61803	P_8	7	2	8	1.87939
P_5	4	2	5	1.73205	$K_{1,4}$	2	4	3	2

d°: $m = 4$, $\lambda_1 \leqslant 2.25$. Since $m = 4$, we have $D = 2$ or $D = 3$. Since $\lambda_1 \leqslant 2.25$, graphs with $D = 3$ are contained in the set A_2, defined in the subsection 6.6, and this set is determined in Lemma 3. Looking at the largest eigenvalue of the graphs from A_2 we easily established that only P_4, C_6, C_7 fulfill the above conditions. One can show that graphs with $D = 2$, $m = 4$ and $\lambda_1 \leqslant 2.25$ do not exist.

e°: $m = 5$, $\lambda_1 \leqslant 1.8$. According to the data presented in Table 3, we get only P_5.

f°: $m \geqslant 6$. This implies $\lambda_1 \leqslant 1.5$ and in Table 3 there are no such graphs.

Comparing results obtained here with the ones for $T^8_{\rm spt}$ and T^9_1 we can formulate the following theorem.

Theorem 4. *We have* $T^9_{\rm spt} = T^9_1 \cup \{P_5, K_{1,4}, K_{1,5}, K_{1,6}, K_{1,7}, K_{1,8}, K_{1,9}\}$.

Corollary 4. *We have*

$$T^9_{\rm spt} = Q \cup S', \quad \textit{where} \quad S' = \{P_5, K_{1,4}, K_{1,5}, K_{1,6}, K_{1,7}, K_{1,8}, K_{1,9}\}.$$

Note that $Q \cap S' = \emptyset$ and $|S'| = 7$. The set $T^9_{\rm spt}$ contains 21 graphs.

6.6. Type 2 mixed tightness.

Considering tightness t_2 we also perform case analysis in a similar way. In fact, the analysis of T^9_2 involves the following cases:

a°: $D = 1$, $\lambda_1 \leqslant 4.5$. We have K_2, K_3, K_4, K_5.

b°: $D = 2$, $\lambda_1 \leqslant 3$. Denote the set of graphs satisfying these conditions by A_1. According to (2) from the introductory chapter we have $\Delta \leqslant 9 = \lambda_1^2$ and by formula (3) we get $n \leqslant 1 + 9 + 9 \cdot 8 = 82$. For example, $K_{1,9} \in A_1$. The set A_1 is completely determined in Lemma 2.

c°: $D = 3$, $\lambda_1 \leqslant 2.25$. Denote the set of graphs satisfying these conditions by A_2. The restrictions for this case are $\Delta \leqslant 5$ since $\lambda_1^2 < 6$ and we have

$n \leqslant 1 + 5 + 5 \cdot 4 + 5 \cdot 4^2 = 106$. Graphs belonging to the set A_2 are listed in Lemma 3.

d°**:** $D = 4$, $\lambda_1 \leqslant 1.8$. Results from Table 3 lead us to P_5 only.

e°**:** $D \geqslant 5$, $\lambda_1 \leqslant 1.5$. There are no graphs satisfying these conditions.

Lemma 2. *The set A_1 consists of* 52 *graphs given below.*

$$
\begin{aligned}
n = 3: &\quad G_3 = P_3;\\
n = 4: &\quad G_5, G_6, G_7 = C_4, G_8 = S_4;\\
n = 5: &\quad G_{15}, G_{16}, G_{17}, G_{18}, G_{20}, G_{21}, G_{22}, G_{23}, G_{27} = C_5, G_{28} = S_5;\\
n = 6: &\quad CP(51), CP(52), CP(61), CP(66), CP(68), CP(69), CP(71),\\
&\quad CP(72), CP(73) = K_{2,4}, CP(75), CP(79), CP(93), CP(94),\\
&\quad CP(107) = S_6;\\
n = 7: &\quad N(7,1) = S_7, N(7,3), N(7,8), N(7,23), N(7,75), N(7,156),\\
&\quad N(7,219), N(7,324), N(7,337), N(7,448), N(7,514), N(7,624);\\
n = 8: &\quad N(8,1) = S_8, N(8,3), N(8,30), N(8,342), N(8,1039),\\
&\quad N(8,6660), N(8,8469);\\
n = 9: &\quad N(9,1) = S_9, N(9,3);\\
n = 10: &\quad N(10,1) = S_{10}, N(10,27956) = PG.
\end{aligned}
$$

Sketch of the proof. Difficulties in proving theorems on this type of tightness arise from the fact that the diameter and the largest eigenvalue have different behavior when adding edges to a connected graph: D does not increase while λ_1 increases.

After having generated graphs in the form of their adjacency matrices using **nauty**, we have used our own programs to compute for each graph the maximum vertex degree Δ, the diameter D and the spectrum (from which we obtained m and λ_1). Based on these invariants we have also calculated all four types of tightness for each graph. Experimental details are given in [7].

By an exhaustive search we know that the 52 graphs listed in the statement of the lemma are the only graphs from A_1 having at most 10 vertices. We should show that no other graphs belong to A_1. Recall that $A_1 = \{G \in \mathcal{G}_c : D = 2, \lambda_1 \leqslant 3\}$ and we know that $\Delta \leqslant 9$ and $n \leqslant 82$. However, an exhaustive search among graphs with n vertices is very difficult for $n = 11$ and $n = 12$ and practically impossible for $n > 12$ because of an enormous number of graphs. Therefore, the proof should use theoretical tools.

Since $D = 2$, we can assume that adding edges to a graph from A_1 leaves the diameter unchanged. Namely, if the diameter decreased to the value of 1, we would have a complete graph which does not belong to A_1 and such cases could be ignored. On the other hand, λ_1 (and, consequently, the spectral tightness) increases.

By the way of contradiction, suppose that there exists a graph $H \in A_1$ with at least 11 vertices.

The maximum degree of H cannot be 9 since in this case H would contain $K_{1,9}$ with an additional edge or vertex. Such a subgraph would have $\lambda_1 > 3$ which is impossible.

In a similar way, the maximum degree of H cannot be 8, 7 or 6. In these cases H would contain one of the stars $K_{1,8}, K_{1,7}, K_{1,6}$ and graphs $N(9,3)$, $N(8,3)$, $N(8,30)$, $N(7,3)$, $N(7,8)$, $N(7,23)$, $N(7,219)$, shown on Figs. 10, 11 and 12, could appear when building up the graph H. However, soon we would infer, in the main stream of the proof, that H contains graphs $N(9,3)$, $N(8,30)$, $N(7,219)$, respectively. Since in all three cases $\lambda_1 = 3$, we again can construct impossible situations.

Now formula (3) gives that H can have at most 26 vertices.

The proof can be completed by further theoretical reductions of possible values for the maximum vertex degree combined by an exhaustive search among graphs with more than 10 vertices but with a small maximum vertex degree. □

Lemma 3. *The set A_2 consists of* 12 *graphs listed below.*

$$\begin{aligned}
n = 4: &\quad G_9 = P_4;\\
n = 5: &\quad G_{25}, G_{26}, G_{29} = Z_5;\\
n = 6: &\quad CP(102), CP(105), CP(106) = C_6, CP(108), CP(109) = W_6;\\
n = 7: &\quad N(7,5), N(7,92), N(7,292) = C_7.
\end{aligned}$$

Proof. By an exhaustive search we know that the 12 graphs listed in the statement of the lemma are the only graphs from $A_2 = \{G \in \mathcal{G}_c : D = 3, \lambda_1 \leqslant 2.25\}$ having at most 10 vertices. We shall show that no other graphs belong to A_2.

By the way of contradiction, suppose that there exists a graph $H \in A_2$ with at least 11 vertices.

Maximum degree of H cannot be 5 since in this case H would contain $K_{1,5}$ with an additional vertex since $D = 3$. Such a subgraph would have $\lambda_1 > 2.25$ which is impossible.

If $\Delta = 4$, H contains a subgraph isomorphic to $K_{1,4}$. Adding an edge to $K_{1,4}$ rises λ_1 to 2.3429 since we obtain G_{23}. However, $K_{1,4}$ can be extended with new vertices to graphs $CP(108)$ and $N(7,5)$. No other extensions of vertices and edges are feasible.

Next we have to consider the case $\Delta \leqslant 3$. Now formula (3) gives that H can have at most 10 vertices which completes the proof. □

Hence we can formulate the following theorem.

Theorem 5. *We have $T_2^9 = T_1^9 \cup A_1 \cup A_2 \cup \{P_5\}$.*

Corollary 5. *It holds $T_2^9 = Q \cup R' \cup S' \cup V$, where $V = A_1 \cup A_2$.*

Proof. Starting from $T_2^9 = T_1^9 \cup A_1 \cup A_2 \cup \{P_5\}$, and the definition of V we have $T_2^9 = Q \cup V \cup \{P_5\}$. By definition R' (and R) is a subset of A_1 and it can be added to the union. According to Corollary 4, graph P_5 belongs to S'. Other graphs from S' belong to A_1 according to Lemma 2. □

Remark 1. If we introduce $V' = ((V \setminus Q) \setminus R) \setminus S$ we can represent the set T_2^9 as a union of four disjoint sets: $T_2^9 = Q \cup R' \cup S' \cup V'$.

Hence, $|V'| = 35$. Therefore, T_2^9 contains $14 + 13 + 7 + 35 = 69$ graphs.

7. Graphs with smallest tightness values

One of the goals in this work is to identify graphs with smallest tightness values for all four types of tightness.

Based on the Theorem 2 we are in a position to find the best configurations w.r.t. t_1 up to 10 vertices.

Theorem 6. *Among connected graphs G on n ($n \leqslant 10$) vertices the value $t_1(G)$ is minimal for the following graphs:*

K_2 *for* $n = 2$, C_5 *for* $n = 5$, C_8 *for* $n = 8$,
K_3 *for* $n = 3$, C_6 *for* $n = 6$, C_9 *for* $n = 9$,
K_4 *for* $n = 4$, C_7 *for* $n = 7$, *the Petersen graph for* $n = 10$.

Proof. By Theorem 2, all connected graphs G with $t_1(G)$ at most 9 are known. Among them it is easy to identify graphs with minimal tightness for $n \leqslant 7$ and $n = 10$. The cases $n = 8, 9$ remain. Since m and Δ are both integers, the next unexamined value for t_1 is ten. We easily find that for C_8 and C_9, having $m = 5$ and $\Delta = 2$, tightness value $t_1 = 10$. □

In a similar way we can identify extremal graphs for other types of tightness based on the results presented in the previous section. The obtained graphs are summarized in Table 4. Together with extremal graphs, the corresponding tightness values are given in parentheses.

TABLE 4. Minimal graphs with their tightness values

n	t_1	stt	spt	t_2
2	K_2 (2)	K_2 (2)	K_2 (2)	K_2 (2)
3	K_3 (4)	K_3 (4)	K_3 (4)	K_3 (4)
4	K_4, C_4 (6)	K_4, C_4 (6)	S_4 (5.196)	S_4 (5.196)
5	C_5 (6)	C_5 (6)	C_5, S_5 (6)	C_5, S_5 (6)
6	C_6 (8)	C_6 (8)	S_6 (6.708))	S_6 (6.708))
7	C_7 (8)	C_7 (8)	S_7 (7.348)	S_7 (7.348)
8	C_8 (10)	$N(8, 6660), N(8, 8469)$ (9)	S_8 (7.937)	S_8 (7.937)
9	C_9 (10)	C_9 (10)	S_9 (8.485)	S_9 (8.485)
10	PG (9)	PG (9)	PG, S_{10} (9)	PG, S_{10} (9)

Several interesting observations can be made.

For $n = 2$ and $n = 3$ complete graphs (in a trivial way) are minimal graphs for all four types of tightness. Starting from $n = 4$, tightness spt and t_2 start to suggest stars as best interconnection networks while tightness t_1 and stt start to suggest circuits as the best ones. Surprises come for $n = 8$ and $n = 10$.

For $n = 8$ according to the tightness stt we get two cubic graphs $N(8, 6660)$ and $N(8, 8469)$ (graphs in which all vertex degrees are equal to 3) of diameter 2. These graphs break the circuit sequence of minimal graphs for stt. They also represent the only case (among small graphs) when t_1 and stt have different minimal values.

For $n = 10$ the Petersen graph (PG) appears in all four cases. It is also a cubic graph of diameter 2. In addition, it is strongly regular, which means that any two adjacent vertices have a fixed number (0 in this case) of common neighbors and any two non-adjacent vertices have a fixed number (1 in this case) of common neighbors. Such an extraordinary structure is the reason why the Petersen graph appears frequently in graph theory as example or counterexample in numerous studies. Here it appears that the Petersen graph should be considered as a very good multiprocessor interconnection network. It is also remarkable that tightness t_1 and stt cannot be smaller than 10 for $n = 9$ and that only with one vertex more, when $n = 10$ their value can become 9 for the Petersen graph.

However, by tightness spt and t_2, the star on 10 vertices is as equally good topology as the Petersen graph.

The results for spt and t_2 perhaps suggest that stars are candidates for optimal topologies in general. However, such a conclusion is correct only for small graphs. In [6] it was shown that stars have tightness spt and t_2 asymptotically equal to $O(\sqrt{n})$ while hypercubes have equal values for all four types of tightness with asymptotical behavior $O((\log n)^2)$. On the other hand, 3-dimensional hypercube seems to be less suitable not only than the star S_8; $N(8, 6660)$, $N(8, 8469)$, C_8 and some other graphs also have smaller tightness values. Moreover, graphs $N(8, 6660)$ and $N(8, 8469)$ provide a smaller diameter with the same maximum vertex degree.

The problem of finding graphs with the smallest tightness values for a given number of vertices remains open in general.

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SELECTED TOPICS FROM THE THEORY OF GRAPH ENERGY: HYPOENERGETIC GRAPHS

Abstract. The energy $E = E(G)$ of a graph G is the sum of the absolute values of the eigenvalues of G. The motivation for the introduction of this invariant comes from chemistry, where results on E were obtained already in the 1940's. A graph G with n vertices is said to be "hypoenergetic" if $E(G) < n$. In this chapter we outline some selected topics from the theory of graph energy. The main part of this chapter is concerned with the characterization of graphs satisfying the inequalities $E(G) < n$ and $E(G) \geqslant n$, that, respectively, are "hypoenergetic" and "non-hypoenergetic".

Mathematics Subject Classification (2000): 05C50; 05C90; 92E10

Keywords: energy (of graph); hypoenergetic graph; spectrum (of graph); chemistry

Contents

1. Introduction: the chemical connection

Researches on what we call the *energy of a graph* can be traced back to the 1940s or even to the 1930s. In the 1930s the German scholar Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called "unsaturated conjugated hydrocarbons". Details of this approach, often referred to as the "Hückel molecular orbital (HMO) theory" can be found in appropriate textbooks [1, 2, 3].

The Schrödinger equation (or, more precisely: the time-independent Schrödinger equation) is a second-order partial differential equation of of the form

$$\hat{H}\,\Psi = \mathcal{E}\,\Psi \tag{1}$$

where Ψ is the so-called wave function of the system considered, $\hat{H}$ the so-called Hamiltonian operator of the system considered, and $\mathcal{E}$ the energy of the system considered. When applied to a particular molecule, the Schrödinger equation enables one to describe the behavior of the electrons in this molecule and to establish their energies. For this one needs to solve Eq. (1), which evidently is an eigenvalue–eigenvector problem of the Hamiltonian operator. In order that the solution of (1) be feasible (yet not completely exact), one needs to express Ψ as a linear combination of a finite number of pertinently chosen basis functions. If so, then Eq. (1) is converted into:

$$\mathbf{H}\,\Psi = E\,\Psi$$

where now $\mathbf{H}$ is a matrix - the so-called Hamiltonian matrix.

The HMO model enables to approximately describe the behavior of the so-called π-electrons in an unsaturated conjugated molecule, especially of conjugated hydrocarbons. In Fig. 1 is depicted the chemical formula of biphenylene – a typical conjugated hydrocarbon H. It contains $n = 12$ carbon atoms over which the $n = 12$ π-electrons form waves.

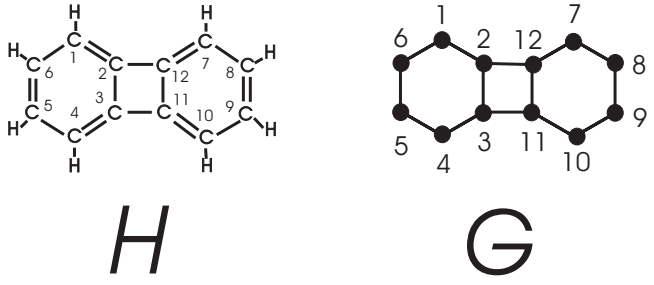

FIGURE 1. Biphenylene H is a typical unsaturated conjugated hydrocarbon. Its carbon–atom skeleton is represented by the molecular graph G. The carbon atoms in the chemical formula H and the vertices of the graph G are labelled by $1, 2, \ldots, 12$ so as to be in harmony with Eqs. (2) and (3).

In the HMO model the wave functions of a conjugated hydrocarbon with n carbon atoms are expanded in an n-dimensional space of orthogonal basis functions, whereas the Hamiltonian matrix is a square matrix of order n, defined so that:

$$[\mathbf{H}]_{ij} = \begin{cases} \alpha, & \text{if } i = j \\ \beta, & \text{if the atoms } i \text{ and } j \text{ are chemically bonded} \\ 0, & \text{if there is no chemical bond between the atoms } i \text{ and } j. \end{cases}$$

The parameters α and β are assumed to be constants, equal for all conjugated molecules. Their physical nature and numerical value are irrelevant for the present considerations; for details see in [1, 2, 3].

For instance, the HMO Hamiltonian matrix of biphenylene is:

$$\mathbf{H} = \begin{bmatrix} \alpha & \beta & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta \\ 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & 0 & 0 & 0 & \beta & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha & \beta & 0 & 0 & 0 & \beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 \\ 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta \\ 0 & \beta & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & \beta & \alpha \end{bmatrix} \tag{2}$$

which can be written also as

(3)

$$\mathbf{H} = \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1 \end{bmatrix} + \beta \begin{bmatrix} 0&1&0&0&0&1&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0&0&1 \\ 0&1&0&1&0&0&0&0&0&0&1&0 \\ 0&0&1&0&1&0&0&0&0&0&1&0 \\ 0&0&0&1&0&1&0&0&0&0&0&0 \\ 1&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0&0&1 \\ 0&0&0&0&0&0&1&0&1&0&0&0 \\ 0&0&0&0&0&0&0&1&0&1&0&0 \\ 0&0&0&0&0&0&0&0&1&0&1&0 \\ 0&0&1&0&0&0&0&0&0&1&0&1 \\ 0&1&0&0&0&0&1&0&0&0&1&0 \end{bmatrix}.$$

The first matrix on the right-hand side of Eq. (3) is just the unit matrix of order $n = 12$, whereas the second matrix can be understood as the adjacency matrix of a graph on $n = 12$ vertices. This graph is also depicted in Fig. 1, and in an evident manner corresponds to the underlying molecule (in our example: to biphenylene).

From the above example it is evident that also in the general case within the HMO model one needs to solve the eigenvalue–eigenvector problem of an approximate Hamiltonian matrix of the form

$$\mathbf{H} = \alpha\, \mathbf{I}_n + \beta\, \mathbf{A}(G) \tag{4}$$

where α and β are certain constants, $\mathbf{I}_n$ is the unit-matrix of order n, and $\mathbf{A}(G)$ is the adjacency matrix of a particular graph G on n vertices, that corresponds to the carbon-atom skeleton of the underlying conjugated molecule.

As a curiosity we mention that neither Hückel himself nor the scientists who did early research in HMO theory were aware of the identity (4), which was first noticed only in 1956 [4].

As a consequence of (4), the energy levels E_j of the π-electrons are related to the eigenvalues λ_j of the graph G by the simple relation $E_j = \alpha + \beta\, \lambda_j$; $j = 1, 2, \ldots, n$.

In addition, the molecular orbitals, describing how the π-electrons move within the molecule, coincide with the eigenvectors ψ_j of the graph G.

In the HMO approximation, the total energy of all π-electrons is given by

$$E_\pi = \sum_{j=1}^{n} g_j\, E_j$$

where g_j is the so-called "occupation number", the number of π-electrons that move in accordance with the molecular orbital ψ_j. By a general physical law, g_j may assume only the values 0, 1, or 2.

Details on E_π and the way in which the molecular graph G is constructed can be found in the books [5, 6, 7] and reviews [8, 9, 10]. There also more information on the chemical applications of E_π can be found. For what follows, it is only important that because the number of π-electrons in the conjugated hydrocarbon considered

is equal to n, it must be $g_1 + g_2 + \cdots + g_n = n$ which immediately implies

$$E_\pi = \alpha\, n + \beta \sum_{j=1}^{n} g_j\, \lambda_j \ .$$

In view of the fact that α and β are constants, and that in chemical applications n is also a constant, the only non-trivial part in the above expression is

$$E = \sum_{j=1}^{n} g_j\, \lambda_j \ . \tag{5}$$

The right-hand side of Eq. (5) is just what in the chemical literature is referred to as "total π-electron energy"; if necessary, then one says "total π-electron energy in β-units".

If the π-electron energy levels are labelled in a non-decreasing order: $E_1 \leqslant E_2 \leqslant \cdots \leqslant E_n$ then the requirement that the total π-electron energy be as low as possible is achieved if for even n,

$$g_j = \begin{cases} 2, & \text{for } j = 1, 2, \ldots, n/2 \\ 0, & \text{for } j = n/2 + 1,\ n/2 + 2, \ldots, n \end{cases}$$

whereas for odd n,

$$g_j = \begin{cases} 2, & \text{for } j = 1, 2, \ldots, (n-1)/2 \\ 1, & \text{for } j = (n+1)/2 \\ 0, & \text{for } j = (n+1)/2 + 1, (n+1)/2 + 2, \ldots, n. \end{cases}$$

For the majority (but not all!) chemically relevant cases,

$$g_j = \begin{cases} 2, & \text{whenever } \lambda_j > 0 \\ 0, & \text{whenever } \lambda_j < 0. \end{cases}$$

If so, then Eq. (5) becomes: $E = E(G) = 2 \sum_{+} \lambda_j$ where $\sum_{+}$ indicates summation over positive eigenvalues. Because for all graphs, the sum of eigenvalues is equal to zero, we can rewrite the above equality as

$$E = E(G) = \sum_{j=1}^{n} |\lambda_j| \ . \tag{6}$$

2. The energy of a graph

In the 1970s one of the present authors noticed that practically all results that until then were obtained for the total π-electron energy, in particular those in the papers [11, 12, 13, 14], tacitly assume the validity of Eq. (6) and, in turn, are not restricted to the molecular graphs encountered in the HMO theory, but hold for all graphs. This observation motivated one of the present authors to put forward [15] the following

Definition 1. If G is a graph on n vertices, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the *energy* of G is

$$E = E(G) = \sum_{j=1}^{n} |\lambda_j| \ . \tag{7}$$

The difference between Eq. (6) and Definition 1 is that Eq. (6) has a chemical interpretation and therefore the graph G in it must satisfy several chemistry-based conditions (e.g., the maximum vertex degree of G must not exceed 3). On the other hand, the graph energy is defined for all graphs and mathematicians may study it without being restricted by any chemistry-caused limitation.

Initially, the graph-energy concept did not attract any attention of mathematicians, but somewhere around the turn of the century they did realize its value, and a vigorous and world-wide mathematical research of E started. The current activities on the mathematical studies of E are remarkable: According to our records, in the year 2006 the number of published papers was 11. In 2007 this number increased to 28. In 2008 (until mid October!) already 42 papers on graph energy were published.

Details on graph energy can be found in the reviews [16, 17] and in the references cited therein. A regularly updated bibliography on graph energy (covering only the 21st century) is available at the web site `http://www.sgt.pep.ufrj.br/`.

In this chapter we are going to outline only a single aspect of the theory of graph energy, namely the results pertaining the condition $E(G) < n$.

3. Hypoenergetic graphs

Definition 2. A graph G on n vertices is said to be *hypoenergetic* if

$$E(G) < n \ . \tag{8}$$

Graphs for which

$$E(G) \geqslant n \tag{9}$$

are said to be *non-hypoenergetic*.

In the chemical literature it has been noticed long time ago that for the vast majority of (molecular) graphs the energy exceeds the number of vertices. In 1973 the theoretical chemists England and Ruedenberg published a paper [18] in which they asked "*why is the delocalization energy negative?*". Translated into the language of graph spectral theory, their question reads: "*why does the graph energy exceed the number of vertices?*", understanding that the graph in question is "molecular".

Recall that in connection with the chemical applications of E, a "molecular graph" means a connected graph in which there are no vertices of degree greater than three [6]. The authors of [18] were, indeed, quite close to the truth. Today we know that only five such graphs violate the relation (9), see below.

On the other hand, there are large classes of graphs for which the condition (9) is satisfied. We first mention three elementary results of this kind.

Theorem 3.1. *If the graph G is non-singular (i.e., no eigenvalue of G is equal to zero), then G is non-hypoenergetic.*

Proof. By the inequality between the arithmetic and geometric means,

$$\frac{1}{n}\,E(G) \geqslant \left(\prod_{i=1}^{n} |\lambda_i|\right)^{1/n} = |\det \mathbf{A}(G)|^{1/n}.$$

The determinant of the adjacency matrix is necessarily an integer. Because G is non-singular, $|\det \mathbf{A}(G)| \geqslant 1$. Therefore, also $|\det \mathbf{A}(G)|^{1/n} \geqslant 1$, implying (9). □

Theorem 3.2. *If G is a graph with n vertices and m edges, and if $m \geqslant n^2/4$, then G is non-hypoenergetic.*

Proof. It is known [19] that for all graphs, $E \geqslant 2\sqrt{m}$. Theorem 3.2 follows from $2\sqrt{m} \geqslant n$. □

Theorem 3.3. [20] *If the graph G is regular of any non-zero degree, then G is non-hypoenergetic.*

Proof. Let λ_1 be the greatest graph eigenvalue. Then $\lambda_1 |\lambda_i| \geqslant \lambda_i^2$ holds for $i = 1, 2, \ldots, n$, which summed over all i, yields $E \geqslant 2m/\lambda_1$. For a regular graph of degree r, $\lambda_1 = r$ and $2m = nr$. □

In the case of regular graphs, the equality $E(G) = n$ is attained if and only if G consists of a copies of the complete bipartite graph $K_{b,b}$, where $a \geqslant 1$ and $n = 2ab$.

Without proof we state here a few other, recently obtained, results related to the inequalities (8 and (9).

Theorem 3.4. [21] *For almost all graphs $E(G) = [4/(3\pi) + O(1)]\; n^{3/2}$ and therefore almost all graphs are non-hypoenergetic.*

Theorem 3.5. [22] *All hexagonal systems are non-hypoenergetic.*

Theorem 3.6. [23, 24, 25] *Denote by $\Delta = \Delta(G)$ the maximum vertex degree of the graph G.*

(a) *Among trees with $\Delta \leqslant 3$, there are exactly four hypoenergetic species, depicted in Fig. 2.*

(b) *Among trees with $\Delta = 4$, there are infinitely many hypoenergetic species. The same holds also if $\Delta > 4$.*

(c) *Among connected quadrangle-free graphs with $\Delta \leqslant 3$, exactly those four depicted in Fig. 2, are hypoenergetic.*

Conjecture 3.7. *$K_{2,3}$ is the only hypoenergetic connected quadrangle-containing graph with $\Delta \leqslant 3$. There are exactly four connected graphs with $\Delta \leqslant 3$ for which the equality $E(G) = n$ holds; these are depicted in Fig. 2.*

In connection with Theorem 3.6 it must be mentioned that if the maximum vertex degree (Δ) is sufficiently large, then it is not difficult to find hypoenergetic graphs. For instance, the n-vertex star (with $\Delta = n-1$) is hypoenergetic for all $n \geqslant 3$. In view of this, the recently reported result [26] that there exist hypoenergetic

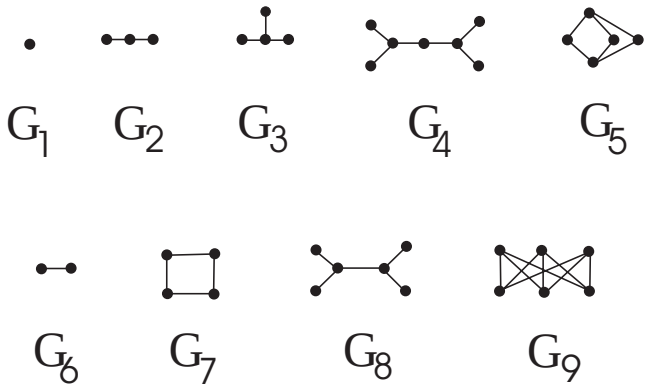

FIGURE 2. G_1, G_2, G_3, G_4 are the only hypoenergetic trees with maximum vertex degree Δ not exceeding 3 [23, 24, 25]. It is conjectured that $G_5 \cong K_{2,3}$ is the only hypoenergetic connected cyclic graph with $\Delta \leqslant 3$. It is also conjectured that G_6, G_7, G_8, G_9 are the only connected graphs with $\Delta \leqslant 3$, having the property $E(G) = n$.

connected unicyclic graphs for all $n \geqslant 7$ and hypoenergetic connected bicyclic graphs for all $n \geqslant 8$ is no surprise whatsoever.

By Theorem 3.3, the problem considered in this chapter has been completely solved for regular graphs [20]. Hexagonal systems (mentioned in Theorem 3.5) have vertex degrees equal to 2 and 3, and therefore belong to a special class of biregular graphs. From the proof of Theorem 3.5 [22] it can be seen that also other types of biregular graphs have the same property, i.e., satisfy inequality (9). Work along these lines has recently been extended [27, 28, 29]. In what follows we report our researches on biregular and triregular graphs in due detail. These considerations may be of particular value for beginners in the field. Namely, these show how by means of relatively elementary graph-theoretic and algebraic reasoning one can obtain not quite trivial results on graph energy.

4. A lower bound for energy and its applications

In this section we obtain a lower bound for graph energy, which will be needed in the subsequent considerations. Our starting point is the Cauchy–Schwarz inequality

$$\sum_{i=1}^{n} x_i\, y_i \leqslant \sqrt{\sum_{i=1}^{n}(x_i)^2 \sum_{i=1}^{n}(y_i)^2}$$

which holds for any real numbers $x_i, y_i,\ \ i = 1, 2, \ldots, n$. Setting $x_i = |\lambda_i|^{1/2}$ and $y_i = |\lambda_i|^{3/2}$, we get

$$\left(\sum_{i=1}^{n}(\lambda_i)^2\right)^4 \leqslant \left(\sum_{i=1}^{n}|\lambda_i| \sum_{i=1}^{n}|\lambda_i|^3\right)^2$$

By another application of the Cauchy–Schwarz inequality,

$$\sum_{i=1}^{n} |\lambda_i|^3 = \sum_{i=1}^{n} |\lambda_i| \cdot (\lambda_i)^2 \leqslant \sqrt{\sum_{i=1}^{n} (\lambda_i)^2 \sum_{i=1}^{n} (\lambda_i)^4}$$

which substituted back into the previous inequality yields

$$\left(\sum_{i=1}^{n} (\lambda_i)^2 \right)^4 \leqslant \left(\sum_{i=1}^{n} |\lambda_i| \right)^2 \sum_{i=1}^{n} (\lambda_i)^2 \sum_{i=1}^{n} (\lambda_i)^4 \ . \tag{10}$$

The k-th spectral moment of a graph G with eigenvalues $\lambda_1, \lambda_2 \ldots, \lambda_n$ is

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k \ .$$

In view of this and the definition of graph energy, Eq. (7), the inequality (10) can be rewritten as

$$E \geqslant M_2 \sqrt{M_2/M_4} \ . \tag{11}$$

The lover bound (11) was independently discovered several times: two times for general graphs [30, 31] and two times for bipartite graphs [32, 33]. Recently a generalized version thereof was obtained [34].

The importance of the bound (11) lies in the fact that the structure-dependency of the spectral moments M_2 and M_4 is well known. If G is a graph with n vertices and m edges, if its vertex degrees are $d_1, d_2, \ldots, d_n$, and if it possesses q quadrangles, then

$$M_2(G) = 2m \tag{12}$$

$$M_4(G) = 2 \sum_{i=1}^{n} (d_i)^2 - 2m + 8q. \tag{13}$$

Combining (11), (13), and (12), we arrive at:

Theorem 4.1. *Let G be a graph with n vertices and m edges, possessing q quadrangles, and let $d_1, d_2, \ldots, d_n$ be its vertex degrees. If the condition*

$$M_2(G) \sqrt{\frac{M_2(G)}{M_4(G)}} \equiv 2m \sqrt{\frac{2m}{\sum_{i=1}^{n} (d_i)^2 - 2m + 8q}} \geqslant n \tag{14}$$

is obeyed, then G is non-hypoenergetic.

The application of Theorem 4.1 will be the basis for all the considerations that follow. Therefore it should be always kept in mind that condition (14) is a *sufficient*, but not a *necessary* condition for the validity of the inequality (9).

5. On the energy of biregular graphs

Let a and b be integers, $1 \leqslant a < b$. A graph is said to be (a, b)-biregular if the degrees of its vertices assume exactly two different values: a and b. A few examples of biregular graphs are shown in Fig. 3.

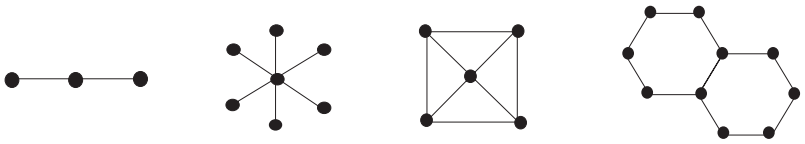

FIGURE 3. Examples of biregular graphs: a (1,2)-biregular tree (the 3-vertex path), a (1,6)-biregular tree (the 7-vertex star), a (3,4)-biregular graph, and a (2,3)-biregular graph (a hexagonal system).

5.1. Biregular trees. Let T be an (a, b)-biregular tree. Since trees necessarily possess vertices of degree 1 (pendent vertices), it must be $a = 1$ and $1 < b \leqslant n-1$, where n is the number of vertices. This tree has at least 3 vertices and $m = n - 1$ edges. With k we denote the number of pendent vertices. (Condition $n \geqslant 3$ is clear since the smallest biregular tree has exactly 3 vertices. See Fig. 3.)

From now on we will search for necessary and sufficient conditions under which the inequality (14) holds.

For trees, of course, $q = 0$. We begin with the equalities

$$k + n_b = n \tag{15}$$

and

$$1 \cdot k + b \cdot n_b = 2m = 2(n-1), \tag{16}$$

where n_b is the number of vertices of T of degree b. From (15) and (16) we have

$$k = \frac{2 + n(b-2)}{b-1}; \qquad n_b = \frac{n-2}{b-1} \, .$$

Further,

$$\sum_{i=1}^{n} d_i^2 = 1^2 \cdot k + b^2 \cdot n_b = \frac{2 + n(b-2)}{b-1} + b^2 \, \frac{n-2}{b-1} = n(b+2) - 2(b+1) \, .$$

By Eqs. (13) and (12), for a biregular tree T we have

$$M_2 = 2(n-1) \tag{17}$$

and

$$M_4 = 2[n(b+2) - 2(b+1)] - 2(n-1) = 2b(n-2) + 2(n-1) \, . \tag{18}$$

Substituting the expressions (17) and (18) back into (14) we get

$$\sqrt{\frac{4(n-1)^3}{b(n-2) + (n-1)}} \geqslant n \, . \tag{19}$$

From (19) we obtain

$$b \leqslant \frac{3n^3 - 11n^2 + 12n - 4}{n^2(n-2)}$$

or simplified

$$b \leqslant \frac{3n^2 - 5n + 2}{n^2} \ . \tag{20}$$

Bearing in mind that $b \geqslant 2$, the right-hand side of the latter inequality must be at least 2, so $n \geqslant 5$. If we examine the function

$$f(x) = \frac{3x^2 - 5x + 2}{x^2}, \quad f : [5, +\infty > \to \mathbb{R}$$

and its first derivative

$$f'(x) = \frac{5x - 4}{x^3}$$

we will see that $f'(x) > 0 \quad \forall x \in [5, +\infty)$, so f is a monotonically increasing function. Further, upper bound for f is 3 because $\lim_{x\to+\infty} f(x) = 3$, and lower bound for f is $f(5) = 52/25 = 2.08$.

Inequality (20) holds if and only if $b = 2$ and $n \geqslant 5$. We have the following:

Theorem 5.1. *Let T be a $(1, b)$-biregular tree with n vertices. Then* (14) *holds if and only if $b = 2$ and $n \geqslant 5$.*

Note that according to Theorem 5.1 the only biregular trees that satisfy condition (14) are the paths with at least 5 vertices.

5.2. Unicyclic biregular graphs. For connected unicyclic (a, b)-biregular graphs we have $m = n$, $a = 1$, and $b \geqslant 3$. Further, $M_2 = 2n$ whereas M_4 we obtain in the following way. We have $k + n_b = n$ and $1 \cdot k + b \cdot n_b = 2n$, from which

$$k = \frac{n(b-2)}{b-1} \qquad ; \qquad n_b = \frac{n}{b-1}$$

and

$$\sum_{i=1}^{n} d_i^2 = 1^2 \cdot k + b^2 \cdot n_b = \frac{n(b-2)}{b-1} + b^2 \frac{n}{b-1} = n(b+2) \ .$$

It follows that $M_4 = 2\sum_{i=1}^{n} d_i^2 - 2n + 8q = 2n(b+2) - 2n + 8q = 2n(b+1) + 8q$.

Now, the inequality (14) becomes

$$\sqrt{\frac{8n^3}{2n(1+b) + 8q}} \geqslant n$$

and we obtain $b \leqslant 3 - 4q/n$. Because the graph G is unicyclic, the number of quadrangles q can be either 0 or 1. For $q = 0$ we obtain $b \leqslant 3$, and with condition $b \geqslant 3$ we conclude $b = 3$. For $q = 1$ we obtain $b \leqslant 3 - 4/n$. Considering that $n \geqslant 8$ (the smallest unicyclic biregular graph with $q = 1$ has exactly 8 vertices) we obtain $b < 3$. We conclude that there is no unicyclic biregular graph with $q = 1$, for which the inequality (14) holds.

Theorem 5.2. *Let G be a connected unicyclic (a, b)-biregular graph with n vertices. Then* (14) *holds if and only if $a = 1$, $b = 3$, and $q = 0$.*

A few examples of biregular graphs that satisfy Theorem 5.2 are shown in Fig. 4.

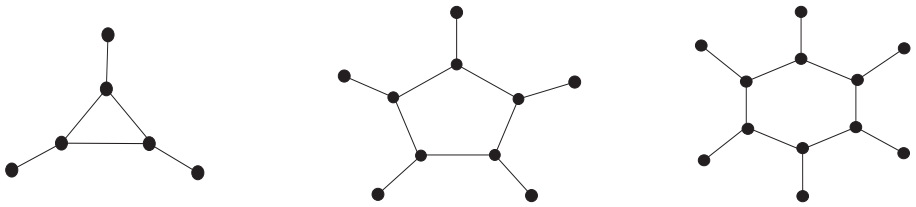

FIGURE 4. Examples of connected quadrangle-free (1,3)-biregular unicyclic graphs.

5.3. Bicyclic biregular graphs. For bicyclic (a, b)-biregular graphs we have $m = n + 1$ and the inequality (14) becomes

$$\sqrt{\frac{4(n+1)^3}{(2a+2b-1)(n+1)-abn+4q}} \geqslant n \ . \tag{21}$$

There are three possible cases (cf. Fig. 5):
(a) the cycles are disjoint (they have no common vertices),
(b) the cycles have a single common vertex
(c) the cycles have two or more common vertices.

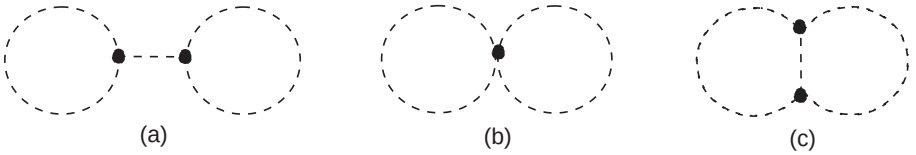

FIGURE 5. Types of bicyclic graphs.

5.3.1. Biregular bicyclic graphs with disjoint cycles. If we have a bicyclic (a, b)-biregular graph with disjoint cycles, then there are two types of such graphs: with $a = 1$, $b \geqslant 3$, and with $a = 2$, $b = 3$, see Fig. 6.

If $a = 1$ and $b \geqslant 3$, then inequality (21) becomes

$$\sqrt{\frac{4(n+1)^3}{b(n+2)+n+1+4q}} \geqslant n$$

from which

$$b \leqslant \frac{3n^3 + (11-4q)n^2 + 12n + 4}{n^3 + 2n^2} \ . \tag{22}$$

For $q = 0$ we obtain

$$b \leqslant \frac{3n^3 + 11n^2 + 12n + 4}{n^3 + 2n^2}$$

or simplified

$$b \leqslant \frac{3n^2 + 5n + 2}{n^2} \ . \tag{23}$$

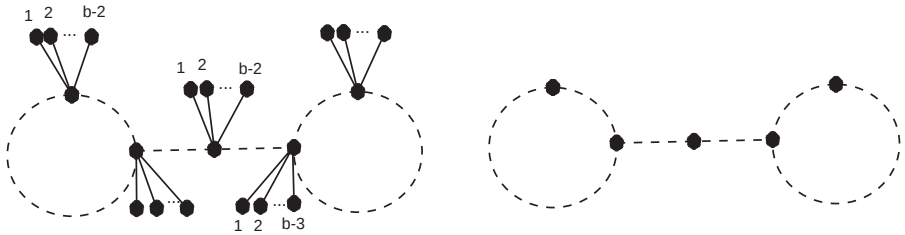

FIGURE 6. Sketches of $(1,b)$-, and $(2,3)$-biregular bicyclic graphs with disjoint cycles. The vertices that connect cycles in a $(1,b)$-biregular graph ($b \geqslant 3$) are connected also with $b-3$ pendent vertices, whereas all other vertices in such a graph are connected with $b-2$ pendent vertices. In a $(2,3)$-biregular graph there are only two vertices of degree 3, those that connect cycles, while every other vertex is of degree 2.

For $b \geqslant 3$, the right-hand side of the latter inequality must be at least 3. Another condition is $n \geqslant 10$, since the smallest bicyclic $(1,b)$-biregular graph with disjoint cycles has exactly 10 vertices.

If we examine the function

$$f(x) = \frac{3x^2+5x+2}{x^2}\,, \quad f : [10,+\infty) \to \mathbb{R}$$

and its first derivative $f'(x) = -(5x+4)/x^3$ we conclude that $f'(x) < 0$, $\forall x \in [10,+\infty)$. Thus f is a monotonically decreasing function. The lower bound for f is 3 because $\lim_{x\to+\infty} f(x) = 3$, and the upper bound for f is $f(10) = 88/25 = 3.52$. We conclude that it must be $b = 3$.

For $q = 1$ we have

$$b \leqslant \frac{3n^3+7n^2+12n+4}{n^3+2n^2}\,. \tag{24}$$

Analogously, and by taking into account that $n \geqslant 12$ we conclude that $b = 3$.

For $q = 2$ we have

$$b \leqslant \frac{3n^3+3n^2+12n+4}{n^3+2n^2}\,. \tag{25}$$

For $n \geqslant 14$ the right-hand side of the inequality (25) is less than 3 and thus there is no bicyclic $(1,b)$-biregular graph with $q = 2$, such that the inequality (14) holds.

For bicyclic $(2,3)$-biregular graphs we have

$$\sqrt{\frac{4(n+1)^3}{3n+9+4q}} \geqslant n$$

which implies $n^3 + (3-4q)n^2 + 12n + 4 \geqslant 0$.

For $q = 0, 1, 2$ we have

$$n^3 + 3n^2 + 12n + 4 \geqslant 0,$$

$$n^3 - n^2 + 12n + 4 \geqslant 0,$$
$$n^3 - 5n^2 + 12n + 4 \geqslant 0$$

respectively. Each of these three inequalities holds for arbitrary $n \in \mathbb{N}$.

Theorem 5.3. *Let G be a connected bicyclic (a, b)-biregular graph with disjoint cycles and let n be the number of its vertices. Then the inequality* (14) *holds if and only if either $a = 1$, $b = 3$, $q = 0$ or $a = 1$, $b = 3$, $q = 1$ or $a = 2$, $b = 3$.*

Some of the graphs satisfying the Theorem 5.3 are depicted in Fig. 7.

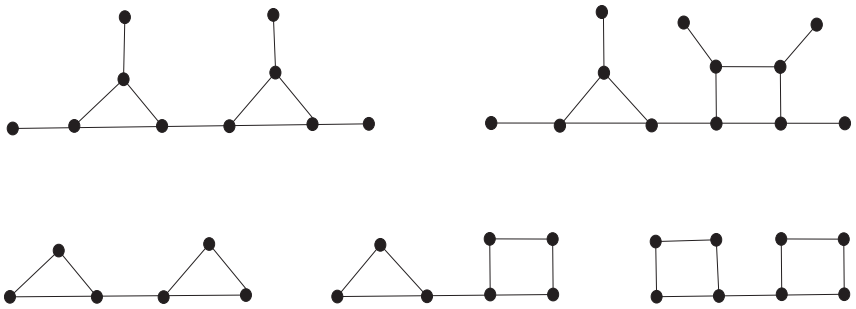

FIGURE 7. Connected bicyclic $(1, 3)$-biregular graphs with disjoint cycles, with $q = 0$ and $q = 1$, and bicyclic $(2, 3)$-biregular graphs with disjoint cycles, with $q = 0$, $q = 1$, $q = 2$. In all these examples the number of vertices is as small as possible.

5.3.2. Biregular bicyclic graphs whose cycles have a common vertex. If in a bicyclic (a, b)-biregular graph, the cycles share one common vertex, then we have two types of such graphs: with $a = 1$, $b \geqslant 4$, and with $a = 2$, $b = 4$, see Fig. 8.

For the first type of such graphs, the inequalities (23), (24), and (25) together with the condition $b \geqslant 4$ are not fulfilled.

For bicyclic $(2, 4)$-biregular graphs we have

$$\sqrt{\frac{4(n+1)^3}{3n + 11 + 4q}} \geqslant n$$

which is equivalent to $n^3 + (1 - 4q)n^2 + 12n + 4 \geqslant 0$. Taking $q = 0, 1, 2$, we obtain inequalities that are satisfied for arbitrary $n \in \mathbb{N}$. This implies:

Theorem 5.4. *Let G be a connected bicyclic (a, b)-biregular graph with n vertices in which the cycles share a single common vertex. Then condition* (14) *is obeyed if and only if $a = 2$ and $b = 4$.*

A few examples graphs specified in Theorem 5.4 are shown in Fig. 9.

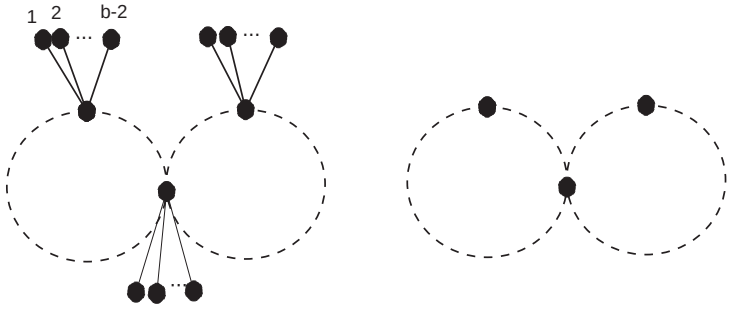

FIGURE 8. Connected bicyclic $(1, b \geqslant 4)$- and $(2, 4)$-biregular graph in which cycles have one common vertex. For the $(1, b)$-biregular graph, $b \geqslant 4$, every vertex except the one belonging to both cycles is connected with $b - 2$ pendent vertices. The vertex belonging to both cycles is connected with $b - 4$ pendent vertices. So, every vertex belonging to the cycles has degree b. In the $(2, 4)$-biregular graphs there are no pendent vertices, so there is only one (common) vertex of degree 4 and every other vertex is of degree 2.

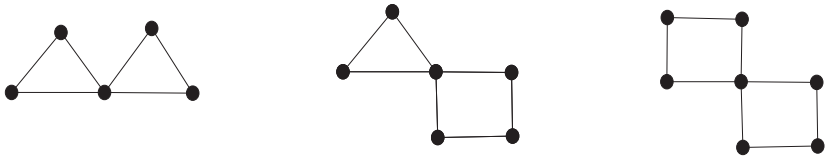

FIGURE 9. Bicyclic $(2, 4)$-biregular graphs in which the cycles have one common vertex, with $q = 0, 1, 2$ quadrangles. In these examples the number of vertices is as small as possible.

5.3.3. Biregular bicyclic graphs whose cycles have several common vertices. If the cycles of a bicyclic (a, b)-biregular graph posses two or more common vertices, then we have two types of such graphs: with $a = 1$, $b \geqslant 3$, and with $a = 2$, $b = 3$, see Fig. 10.

For the graphs depicted in Fig. 10 we obtain the same results as for bicyclic graphs with disjoint cycles, but we must add the case when $q = 3$ because there exists a unique bicyclic biregular graph in which the number of quadrangles is exactly 3. This is the complete bipartite graph on $2 + 3$ vertices, $K_{2,3}$, shown in Fig. 11. From (22) for $b = 3$, we get the inequality $-7n^3 + 12n + 4 \geqslant 0$ that is not fulfilled for $n = 5$.

Theorem 5.5. *Let G be a connected bicyclic (a, b)-biregular graph with n vertices, whose cycles have two or more common vertices. Then inequality* (14) *holds if and only if $a = 1$, $b = 3$, $q = 0, 1$ or $a = 2$, $b = 3$, $q = 0, 1, 2$.*

Examples of graphs for which Theorem 5.5 holds are shown in Fig. 12.

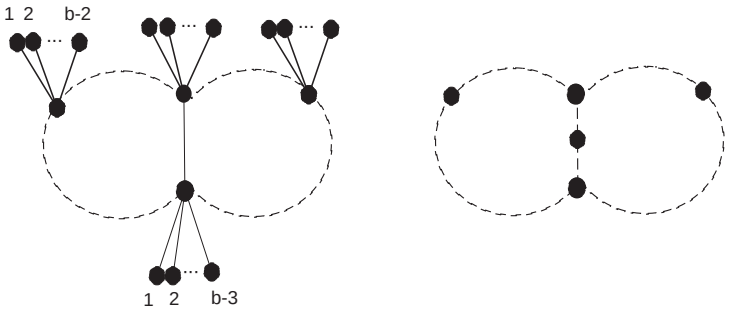

FIGURE 10. Connected bicyclic $(1, b \geqslant 3)$- and $(2, 3)$-biregular graphs in which the cycles have two or more common vertices. Notice that the graphs of first type have only two common vertices, whereas the graphs of the second type can have arbitrarily many common vertices (but more than one, of course).

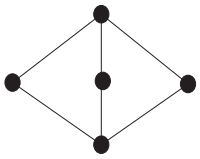

FIGURE 11. The only bicyclic biregular graph in which the number of quadrangles q is 3. For this graph inequality (14) is violated.

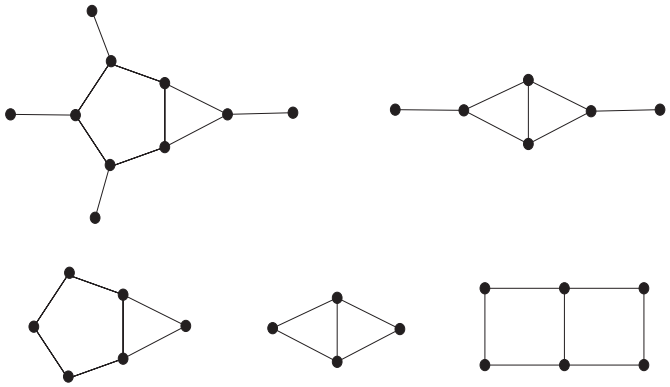

FIGURE 12. Bicyclic $(1, 3)$-biregular graphs in which cycles have two common vertices and $q = 0, 1$, and bicyclic $(2, 3)$-biregular graphs with $q = 0, 1, 2$.

6. On the energy of triregular graphs

6.1. Triregular graphs. Let x, a, and b be integers, $1 \leqslant x < a < b$. A graph is said to be (x, a, b)-triregular if its vertices assume exactly three different values: x, a, and b. A few examples of triregular graphs are shown in Fig. 13.

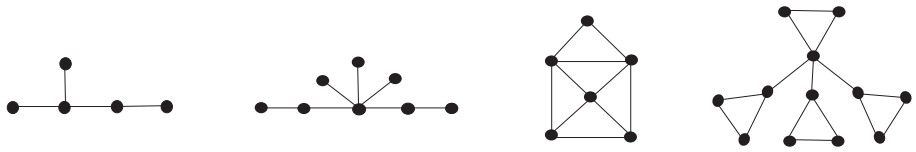

FIGURE 13. (1,2,3)-, (1,2,5)-, (2,3,4)-, and (2,3,5)-triregular graph, respectively.

As we did for biregular graphs, we will investigate the validity of the inequality (14) for triregular trees and connected triregular unicyclic and bicyclic graphs.

For a connected (x, a, b)-triregular graph with n vertices and m edges we have

$$n_x + n_a + n_b = n \tag{26}$$

and

$$xn_x + an_a + bn_b = 2m \tag{27}$$

where n_x is the number of vertices of degree x, n_a is the number of vertices of degree a and n_b is the number of vertices of degree b. From (26) and (27) follows

$$n_a = \frac{n_x(x-b) + (bn - 2m)}{b-a} \quad ; \quad n_b = \frac{n_x(a-x) - (an - 2m)}{b-a} \ . \tag{28}$$

Again, by d_i we denote the degree of i-th vertex. Then

$$\sum_{i=1}^{n} d_i^2 = x^2 \cdot n_x + a^2 \cdot n_a + b^2 \cdot n_b$$

which combined with Eqs. (28) yields

$$\sum_{i=1}^{n} d_i^2 = n_x(a-x)(b-x) + 2m(a+b) - abn \ .$$

From this,

$$\begin{aligned} M_4 &= 2[n_x(a-x)(b-x) + 2m(a+b) - abn] - 2m + 8q \\ &= 2[n_x(a-x)(b-x) + m(2a+2b-1) - abn + 4q] \ . \end{aligned}$$

Together with $M_2 = 2m$, inequality (14) becomes

$$\sqrt{\frac{4m^3}{n_x(a-x)(b-x) + m(2a+2b-1) - abn + 4q}} \geqslant n$$

from which

$$n_x \leqslant \frac{4m^3 + n^2[abn - 4q - m(2a+2b-1)]}{n^2(a-x)(b-x)}. \tag{29}$$

Theorem 6.1. *Let G be connected (x, a, b)-triregular graph with n vertices and m edges. Let n_x be the number of vertices of degree x. Then inequality* (14) *holds if and only if*

$$n_x \leqslant \frac{4m^3 + n^2[abn - 4q - m(2a + 2b - 1)]}{n^2(a - x)(b - x)} \ .$$

6.2. Triregular trees. Let T be a triregular n-vertex tree with vertex degrees 1, a, and b, $1 < a < b \leqslant n - 2$. Then $n \geqslant 5$ and the number of edges is $m = n - 1$. Condition $n \geqslant 5$ is necessary because the smallest triregular tree has 5 vertices, $a = 2$ and $b = 3$, see Fig. 13.

Now, by applying Theorem 1.1 we get

$$n_1 \leqslant \frac{(5 + ab - 2a - 2b)n^3 + (2a + 2b - 13)n^2 + 12n - 4}{n^2(a - 1)(b - 1)}$$

and since for every triregular tree $n_1 \geqslant a+b-2$, the right-hand side of the inequality must be greater than $a + b - 2$. Thus, we require

$$\frac{(5 + ab - 2a - 2b)n^3 + (2a + 2b - 13)n^2 + 12n - 4}{n^2(a - 1)(b - 1)} \geqslant a + b - 2 \ . \tag{30}$$

For $(1, 2, 3)$-triregular tree the relation (30) yields

$$\frac{n^3 - 3n^2 + 12n - 4}{2n^2} \geqslant 3$$

which implies $n^3 - 9n^2 + 12n - 4 \geqslant 0$ and this inequality holds for every $n \geqslant 8$.

Theorem 6.2. *Let T be a $(1, a, b)$-triregular tree, $1 < a < b$, and let n be the number of its vertices. Then relations* (14) *holds if and only if*

$$\frac{(5 + ab - 2a - 2b)n^3 + (2a + 2b - 13)n^2 + 12n - 4}{n^2(a - 1)(b - 1)} \geqslant a + b - 2 \ .$$

Corollary 6.3. *Let T be a $(1, 2, 3)$-triregular tree and let n be the number of its vertices. Then* (14) *holds if and only if $n \geqslant 8$.*

The next figure shows all $(1, 2, 3)$-triregular trees with $n < 8$. According to Corollary 6.3, these trees do not satisfy inequality (14).

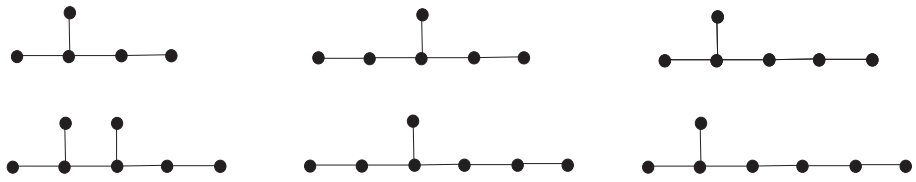

FIGURE 14. $(1, 2, 3)$-triregular trees not satisfying inequality (14).

As another example, if we consider $(1, 3, 4)$-triregular trees, then from (30) we obtain $3n^3 - 29n^2 + 12n - 4 \geqslant 0$, and this holds for $n \geqslant 10$. Since the smallest such

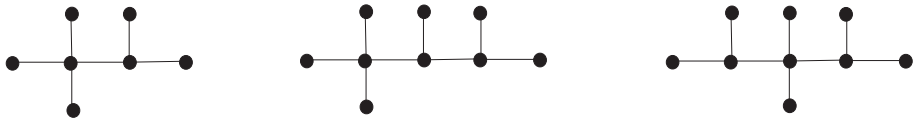

FIGURE 15. $(1, 2, 4)$-triregular trees not satisfying inequality (14).

tree has exactly 7 vertices, we conclude that inequality (14) is not true for such trees with $n = 7, 9$, which are depicted in Fig. 15.

In the same way for $(1, 3, 5)$-triregular trees we will have $4n^3-45n^2+12n-4 \geqslant 0$, which holds for $n \geqslant 11$. We conclude that (14) is violated for such tree with $n = 8, 10$, see Fig. 16.

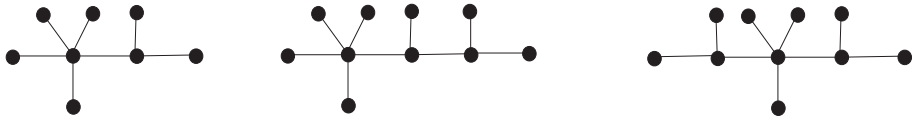

FIGURE 16. $(1, 3, 5)$-triregular trees not satisfying inequality (14).

In the case of $(1, 4, 5)$-, $(1, 4, 6)$-, $(1, 4, 7)$-, and $(1, 5, 6)$-triregular trees, the analogous conditions under which (14) holds are $n \geqslant 12$, $n \geqslant 13$, $n \geqslant 14$, and $n \geqslant 14$, respectively.

6.3. Triregular unicyclic graphs. For unicyclic (x, a, b)-triregular graph it must be $x = 1$, $m = n$ and the number of quadrangles q is either 0 or 1.

Inequality (29) together with conditions $m = n$ and $x = 1$ yields

$$n_1 \leqslant \frac{n(5 + ab - 2a - 2b) - 4q}{(a - 1)(b - 1)} \ .$$

Now, in order to proceed, we will need a lower bound for n_1 in any unicyclic triregular graph:

Lemma 6.4. *Let G be a unicyclic $(1, a, b)$-triregular graph with n vertices and n_1 pendent vertices. Then $n_1 \geqslant b - a + N(a - 2)$, where N is the size (= number of vertices) of the (unique) cycle of G.*

Notice that for $a = 2$ the lower bound for n_1 does not depend on N. We then have $n_1 \geqslant b - 2$.

Proof. Consider first the case $a = 2$, $b \geqslant 3$. We construct a graph specified in Lemma 6.4 with minimal number of pendent vertices. Start with the N-vertex cycle, in which each vertex is of degree 2 as shown in Fig. 17a. Choose only one vertex in the cycle and connect it with $b - 2$ vertices, each of degree 1 as shown in Fig. 17b. By this we obtain a unicyclic $(1, 2, b)$-triregular graph with minimal number of pendent vertices, equal to $b - 2$.

For $a > 2$, to each vertex in a cycle we must add another $a - 2$ pendent vertices, so at the moment we have $N(a-2)$ pendent vertices and each vertex of the cycle is

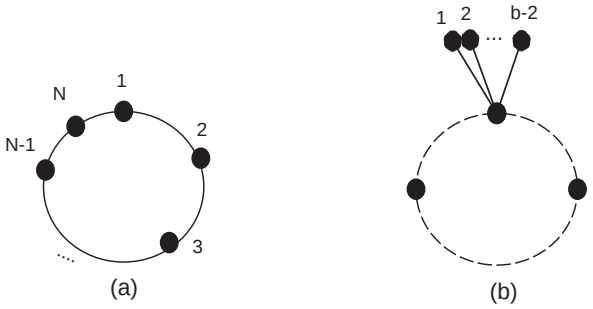

FIGURE 17. Details related to the proof of Lemma 6.4 for $a = 2$.

of degree a, see Fig. 18a. Then we choose only one vertex of the cycle and connect it with additional $b - a$ pendent vertices. This vertex is of degree b and any other vertex of the cycle is of degree a as shown in Fig. 18b. By this we constructed a graph with minimal number of pendent vertices, equal to $b - a + N(a - 2)$. □

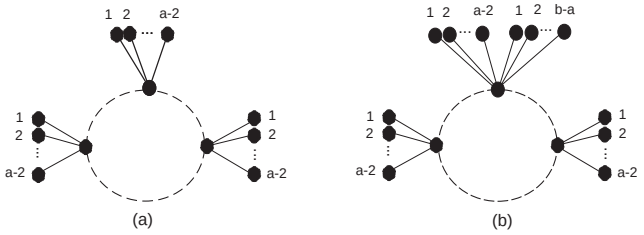

FIGURE 18. Details related to the proof of Lemma 6.4 for $a > 2$.

For $q = 0$ we have

$$n_1 \leqslant \frac{n(5 + ab - 2a - 2b)}{(a - 1)(b - 1)}$$

and from Lemma 6.4 it follows

$$\frac{n(5 + ab - 2a - 2b)}{(a - 1)(b - 1)} \geqslant b - a + N(a - 2), \quad N \neq 4$$

that is

$$n \geqslant [b - a + N(a - 2)] \frac{(a - 1)(b - 1)}{(5 + ab - 2a - 2b)} \ .$$

Theorem 6.5. *Let G be an n-vertex unicyclic $(1, a, b)$-triregular graph, $2 \leqslant a < b$. Let G be quadrangle-free and its cycle be of size N, $N \neq 4$. Then inequality (14) holds if and only if*

$$n \geqslant [b - a + N(a - 2)] \frac{(a - 1)(b - 1)}{(5 + ab - 2a - 2b)} \ .$$

Corollary 6.6. *Let G be an n-vertex unicyclic $(1,2,b)$-triregular graph, $b \geqslant 3$. Let G be quadrangle-free and its cycle be of size N, $N \neq 4$. Then inequality* (14) *holds if and only if $n \geqslant (b-1)(b-2)$.*

For example, for a (1,2,4)-triregular unicyclic graph with $n = 5$ this inequality does not hold, but it is true for every unicyclic quadrangle-free (1,2,3)-triregular graph, see Fig. 19.

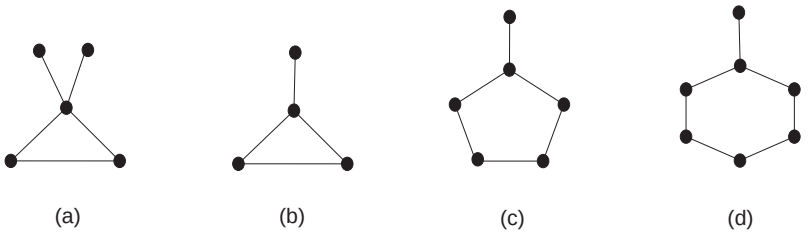

FIGURE 19. Diagram (a) represents the unique unicyclic quadrangle-free $(1,2,4)$-triregular graph for which inequality (14) does not hold. Diagrams (b), (c), and (d) pertain to the smallest unicyclic $(1,2,3)$-triregular graphs with $N = 3, 5, 6$, respectively.

For $q = 1$ we have

$$n_1 \leqslant \frac{n(5+ab-2a-2b)-4}{(a-1)(b-1)} \ .$$

This time $N = 4$ and, by lemma 6.4, we have the condition $n_1 \geqslant 3a+b-8$ so the right-hand side of the above inequality must be at least $3a+b-8$. In view of this

$$\frac{n(5+ab-2a-2b)-4}{(a-1)(b-1)} \geqslant 3a+b-8 \ .$$

Expressing n in the above inequality we arrive at:

Theorem 6.7. *Let G be an n-vertex unicyclic $(1,a,b)$-triregular graph, $2 \leqslant a < b$, whose cycle is of size* 4. *Then inequality* (14) *holds if and only if*

$$n \geqslant \frac{(a-1)(b-1)(3a+b-8)+4}{(a-1)(b-1)+4-(a+b)} \ .$$

Corollary 6.8. *Let G be an n-vertex unicyclic $(1,2,b)$-triregular graph, $2 < b$, whose cycle is of size* 4. *Then inequality* (14) *holds if and only if $n \geqslant (b-1)(b-2)+4$.*

Corollary 6.9. *Let G be an n-vertex unicyclic $(1,2,3)$-triregular graph, whose cycle is of size* 4. *Then inequality* (14) *holds if and only if $n \geqslant 6$.*

A few examples illustrating Theorem 6.7 and its corollaries are given in Fig. 20.

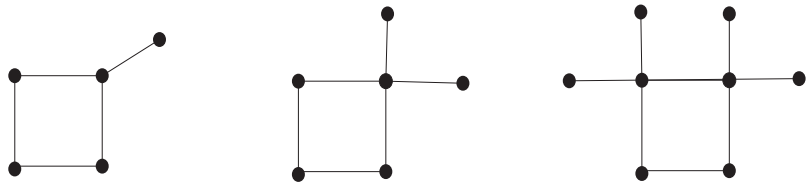

FIGURE 20. Diagram (a) represents the unique unicyclic $(1, 2, 3)$-triregular graph with $q = 1$ for which inequality (14) does not hold. Diagrams (b) and (c) are the unique unicyclic $(1, 2, 4)$-triregular graphs with $q = 1$ and with number of vertices $n = 6, 8$, respectively for which inequality (14) does not hold.

6.4. Triregular bicyclic graphs. The examination of the validity of condition (14) in the case of triregular bicyclic graphs turns our to be quite complicated, and we have to proceed case-by-case. The lengthy analysis that follows may be a good example for a beginner of how by slightly modifying a graph-theoretic problem (in our case, by moving from "bicyclic" to "tricyclic") it may gain much on difficulty. The same analysis shows how graph-theoretic problems are (usually) solved by separately considering particular cases and subcases.

For a bicyclic (x, a, b)-triregular graph, $m = n + 1$, $x = 1$, and the number of quadrangles q can be 0, 1, 2, or 3. Inequality (29) together with conditions $m = n + 1$ and $x = 1$ yields

$$n_1 \leqslant \frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b - 4q)n^2 + 12n + 4}{n^2(a-1)(b-1)} \,. \tag{31}$$

As outlined earlier in connection with bicyclic biregular graphs, there are three types of bicyclic graphs; for details see Fig. 5. Each of these types will be considered separately. In cases (a) and (b), $q \in \{0, 1, 2\}$ whereas in case (c) $q \in \{0, 1, 2, 3\}$.

6.4.1. Triregular bicyclic graphs with disjoint cycles. Again, we will need a lower bound for the number of pendent vertices:

Lemma 6.10. *Let G be a bicyclic $(1, a, b)$-triregular graph, $2 \leqslant a < b$, with disjoint cycles and with n_1 pendent vertices. Then*

$$n_1 \geqslant \begin{cases} 1, & \text{if } a = 2,\ b = 3 \\ 2(b-3), & \text{if } a = 2,\ b > 3 \\ (a-2)(N+M-2) + (b-3) + (a-3), & \text{otherwise} \end{cases}$$

where N and M are the sizes of the two cycles of G.

Proof. In order to construct a graph G with disjoint cycles and minimal number of pendent vertices, we first connect the cycles with just one edge, so that all vertices belong to cycles, see Fig. 21a.

For $a = 2$ and $b = 3$ we choose one vertex of degree 2 and attach to it one pendent vertex, see Fig. 21b.

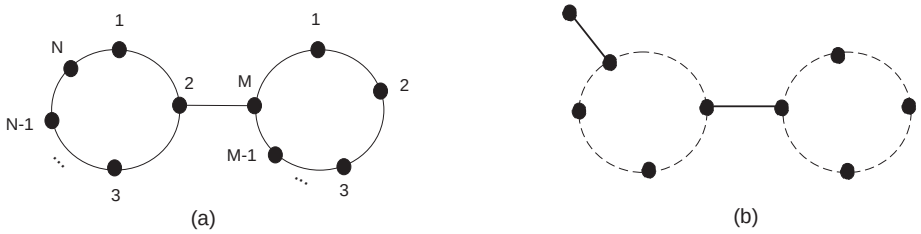

FIGURE 21. Details related to the proof of Lemma 6.10 for $a = 2$, $b = 3$.

For $a = 2$ and $b > 3$ we attach $b - 3$ pendent vertices to the vertices of degree 3. Since there are exactly two such vertices, we will have $2(b-3)$ pendent vertices, see Fig. 22.

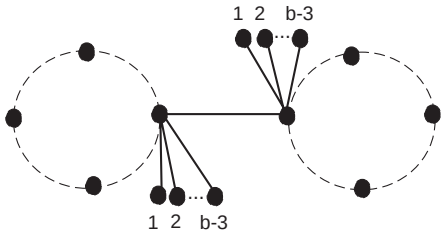

FIGURE 22. Details related to the proof of Lemma 6.10 for $a = 2$, $b > 3$.

For $2 < a < b$ we have to connect each vertex of degree 2 with $a - 2$ pendent vertices. There are $N + M - 2$ vertices of degree 2 so we arrive at $(a-2)(N + M - 2)$ pendent vertices. Then, we have to look at the vertices of degree 3. At the beginning, there are two such vertices. So, if $a = 3$ we leave one vertex alone and connect the other one with $b - 3$ pendent vertices in order to obtain one vertex of degree $b > 3$ (Fig. 23a). If $a > 3$, we connect each vertex of degree 2 with $a - 2$ pendent vertices, and to the remaining two vertices of degree 3 we attach $a-3$ and $b-3$ pendent vertices (Fig. 23b). In this way we obtain a $(1, a, b)$-triregular graph with minimal number of pendent vertices, equal to $(a-2)(N+M-2)+(b-3)+(a-3)$. □

Consider first $(1, 2, 3)$-triregular graphs. From (31) it follows that

$$n_1 \leqslant \frac{n^3 + (3 - 4q)n^2 + 12n + 4}{2n^2} .$$

By Lemma 6.10, the right hand side of this inequality must be at least 1. Therefore,

$$\frac{n^3 + (3 - 4q)n^2 + 12n + 4}{2n^2} \geqslant 1$$

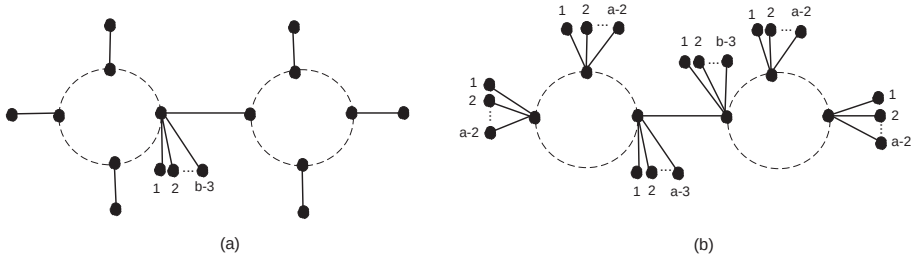

FIGURE 23. Details related to the proof of Lemma 6.10 for $a > 2$, $b > 3$.

and we obtain $n^3 + (1-4q)n^2 + 12n + 4 \geqslant 0$. For $q = 0, 1, 2$ this yields

$$n^3 + n^2 + 12n + 4 \geqslant 0,$$
$$n^3 - 3n^2 + 12n + 4 \geqslant 0,$$
$$n^3 - 7n^2 + 12n + 4 \geqslant 0,$$

respectively, and all these inequalities hold for arbitrary $n \in \mathbb{N}$. Thus we obtain:

Theorem 6.11. *Inequality* (14) *is obeyed by all bicyclic* $(1, 2, 3)$*-triregular graphs with disjoint cycles.*

In Fig. 24 are some examples of graphs specified in Theorem 6.11.

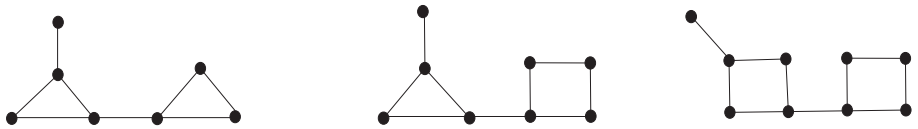

FIGURE 24. Bicyclic $(1, 2, 3)$-triregular graphs with disjoint cycles, with $q = 0, 1, 2$, and with minimal number of vertices.

Next, we consider the case $a = 2$, $b \geqslant 4$. From (31) it follows that

$$n_1 \leqslant \frac{n^3 + (9 - 2b - 4q)n^2 + 12n + 4}{n^2(b-1)} \, .$$

By Lemma 6.10, the right-hand side of the above inequality must be at least $2(b-3)$, which implies

$$\frac{n^3 + (9 - 2b - 4q)n^2 + 12n + 4}{n^2(b-1)} \geqslant 2(b-3)$$

and we obtain $n^3 + (3 + 6b - 2b^2 - 4q)n^2 + 12n + 4 \geqslant 0$. For $q = 0, 1, 2$ this becomes

$$2b^2 - 6b - 3 \leqslant \frac{n^3 + 12n + 4}{n^2} \, ,$$
$$2b^2 - 6b + 1 \leqslant \frac{n^3 + 12n + 4}{n^2} \, ,$$

$$2b^2 - 6b + 5 \leqslant \frac{n^3 + 12n + 4}{n^2} \ ,$$

respectively, resulting in:

Theorem 6.12. *Let G be a bicyclic $(1, 2, b)$-triregular graph with disjoint cycles, $b \geqslant 4$. Let n be the number of its vertices and q the number of its quadrangles. Then inequality* (14) *if and only if*

$$2b^2 - 6b - 3 \leqslant \frac{n^3 + 12n + 4}{n^2} \quad \textit{if} \ \ q = 0,$$
$$2b^2 - 6b + 1 \leqslant \frac{n^3 + 12n + 4}{n^2} \quad \textit{if} \ \ q = 1,$$
$$2b^2 - 6b + 5 \leqslant \frac{n^3 + 12n + 4}{n^2} \quad \textit{if} \ \ q = 2.$$

For example, for arbitrary bicyclic $(1, 2, 4)$-triregular graphs the first two inequalities hold for all values of n (for which such graphs exist), whereas the third one is not true only for $n = 10$, see Fig. 25.

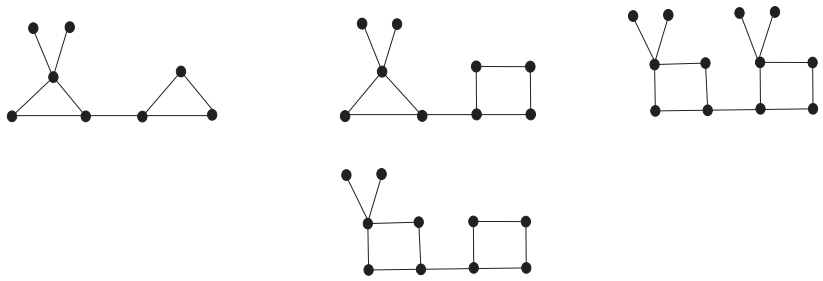

FIGURE 25. Examples of bicyclic $(1, 2, 4)$-triregular graphs with disjoint cycles. Only the graph with $q = 2$ and $n = 10$ violates inequality (14).

In the case $2 < a < b$, from (31) and Lema 6.10 it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b - 4q)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M)+b-a-2 \, .$$

For $q = 0$ we have $N, M \neq 4$, and we obtain

(32)
$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M) + b - a - 2 \ .$$

For $q = 1$ we have $N = 4$ and $M \neq 4$, and we obtain

(33) $$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M)+b-a-2 \, .$$

For $q = 2$ we obtain

(34) $$\frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 7a + b - 18 \ .$$

Theorem 6.13. *Let G be a bicyclic $(1, 2, b)$-triregular graph with disjoint cycles, $b \geqslant 4$. Let n be the number of its vertices and q the number of its quadrangles. Then* (14) *holds if and only if for $q = 0$, $q = 1$, and $q = 2$, the inequalities* (32), (33), *and* (34), *respectively, are satisfied.*

Consider now some special cases of Theorem 6.13.

If $a = 3$, $b = 4$, and $N = M = 3$, then

$$\frac{3n^3 - n^2 + 12n + 4}{6n^2} \geqslant 5 \qquad \text{i.e.,} \qquad 3n^3 - 31n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 10$. On the other hand, the smallest such graph has 11 vertices so the condition is obeyed by all considered graphs.

If $a = 3$, $b = 5$, and $N = M = 3$, then

$$\frac{4n^3 - 3n^2 + 12n + 4}{8n^2} \geqslant 6 \qquad \text{i.e.,} \qquad 4n^3 - 51n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 13$, so it is not true only for such graphs with 12 vertices, see Fig. 26.

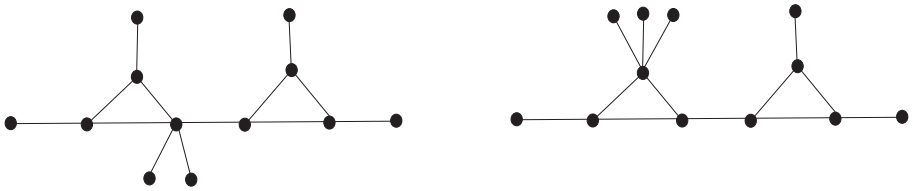

FIGURE 26. The only bicyclic $(1, 3, 5)$-triregular graphs with two disjoint cycles of size 3, which do not satisfy condition (14).

If $a = 3$, $b = 4$, and $N = 4$, $M = 3$, then

$$\frac{3n^3 - 5n^2 + 12n + 4}{6n^2} \geqslant 6 \qquad \text{i.e.,} \qquad 3n^3 - 41n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 14$. Consequently, it is not obeyed only by such graphs with 13 vertices, see Fig. 27a.

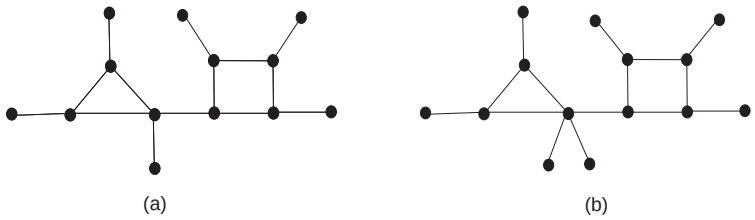

FIGURE 27. Some bicyclic triregular graphs violating condition (14).

If $a = 3$, $b = 5$, and $N = 4$, $M = 3$, then

$$\frac{4n^3 - 7n^2 + 12n + 4}{8n^2} \geqslant 7 \qquad \text{i.e.,} \qquad 4n^3 - 63n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 16$. Consequently, it is not obeyed only by such graphs with 14 vertices, see Fig. 27b.

If $a = 3$, $b = 4$, and $N = M = 4$, then

$$\frac{3n^3 - 9n^2 + 12n + 4}{6n^2} \geqslant 7 \qquad \text{i.e.,} \qquad 3n^3 - 51n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 17$. Consequently, it is not obeyed only by such graphs with 15 and 16 vertices, see Fig. 28a and 28b.

If $a = 3$, $b = 5$, and $N = M = 4$, then

$$\frac{4n^3 - 7n^2 + 12n + 4}{8n^2} \geqslant 8 \qquad \text{i.e.,} \qquad 4n^3 - 71n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 18$. Consequently, it is not obeyed only by such graphs with $n = 16$, see Fig. 28c.

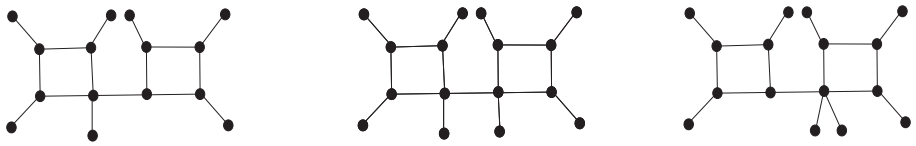

FIGURE 28. Some further bicyclic triregular graphs violating condition (14).

6.4.2. Triregular bicyclic graphs whose cycles have a common vertex. For any triregular graph considered in this section it must be $b \geqslant 4$. In analogy to Lemma 6.10 we can prove:

Lemma 6.14. *Let G be a bicyclic $(1, a, b)$-triregular graph, $2 \leqslant a < b$, in which cycles share a single vertex. Let n_1 be the number of pendent vertices. Then*

$$n_1 \geqslant \begin{cases} 2, & \text{if } a = 2,\ b = 4 \\ (a-2)(N+M-2) + b - 4, & \text{otherwise,} \end{cases}$$

where N and M are the sizes of the cycles.

Proof. Again, we begin with two cycles with one common vertex. Each cycle has, counting independently, N i.e., M vertices.

For $a = 2$ and $b = 4$, since we need to arrive at a graph with vertices of degree 1, 2, and 4, we have to add pendent vertices. We can do this by choosing only one vertex of degree 2 in a cycle and connect it with 2 pendent vertices. No matter how big the graph G is, 2 will be the minimal number of pendent vertices, see Fig. 29.

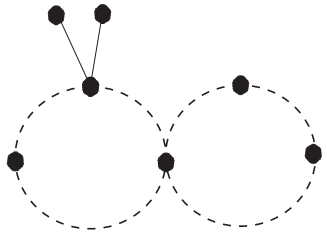

FIGURE 29. Details related to the proof of Lemma 6.14 for $a = 2$, $b = 4$.

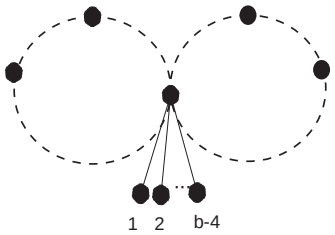

FIGURE 30. Details related to the proof of Lemma 6.14 for $a = 2$, $b > 4$.

For $a = 2$ and $b > 4$ we choose the vertex common to the two cycles and connect it with $b - 4$ pendent vertices, see Fig. 30.

For $2 < a < b$ we take every vertex of degree 2 in a cycle and connect it with $a-2$ pendent vertices to get vertices of degree a. There are exactly $N + M - 2$ vertices of degree 2 so we must add altogether $(a - 2)(N + M - 2)$ pendent vertices. Then we take the vertex common to the two cycles and connect it with $b - 4$ pendent vertices to get a vertex of degree b, see Fig. 31. Now, we have $(a - 2)(N + M - 2) + b - 4$ pendent vertices and from the construction it is clear that this number is minimal. □

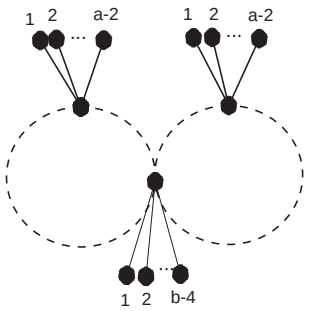

FIGURE 31. Details related to the proof of Lemma 6.14 for $a > 2$, $b > 3$.

The simplest case is a bicyclic $(1,2,4)$-triregular graph. From (31) it follows that

$$n_1 \leqslant \frac{n^3+(1-4q)n^2+12n+4}{3n^2} \ .$$

The right-hand side of this inequality must be at least 2, so we have

$$\frac{n^3+(1-4q)n^2+12n+4}{3n^2} \geqslant 2 \qquad \text{i.e.,} \qquad n^3+(-5-4q)n^2+12n+4 \geqslant 0 \ .$$

For $q=0$ we have

$$n^3-5n^2+12n+4 \geqslant 0 \tag{35}$$

and if we look at the left-hand side of the inequality as a real function with real arguments from $[7,+\infty>$ and its first derivative, we will conclude that (35) holds for any $n \geqslant 7$. (Why 7 as a lower bound? Because the smallest bicyclic (1,2,4)-triregular graph G in which cycles have one common vertex and with q=0 has exactly 7 vertices.) So, this inequality holds for any such graph.

For $q=1$ we have

$$n^3-9n^2+12n+4 \geqslant 0 \ . \tag{36}$$

In a same way as for $q=0$ we conclude that (36) holds for every $n \geqslant 8$, that is, for any bicyclic (1,2,4)-triregular graph G in which cycles have one common vertex and with $q=1$.

For $q=2$ we have

$$n^3-13n^2+12n+4 \geqslant 0 \tag{37}$$

Inequality (37) is true only for $n \geqslant 12$, but there are such graphs having fewer vertices. Consequently (37), and therefore also (14), is not true for such graphs with 9 and 11 vertices. These graphs are shown in Fig. 32.

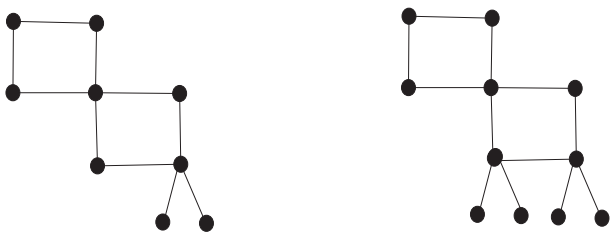

FIGURE 32. Bicyclic (1,2,4)-triregular graphs on 9 and 11 vertices. These violate inequality (14).

Theorem 6.15. *Let G be a bicyclic $(1,2,4)$-triregular graph with cycles sharing a single vertex. Let n be the number of its vertices and N, M the size of its cycles, of which q cycles are quadrangles. Then* (14) *holds if and only if the inequalities*

$$n^3-5n^2+12n+4 \geqslant 0,$$
$$n^3-9n^2+12n+4 \geqslant 0,$$

$$n^3 - 13n^2 + 12n + 4 \geqslant 0$$

are satisfied for $q = 0$, $q = 1$, and $q = 2$, respectively.

Consider the case of $(1, a, b)$-triregular graph, $2 < a < b$, $b \geqslant 4$. For $q = 0$, inequality (31) becomes

$$n_1 \leqslant \frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)}$$

and from Lemma 6.14 it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M) - 2a + b$$

where $N, M \neq 4$.

For example, if $a = 3$, $b = 4$, and $N = M = 3$, we have

$$\frac{3n^3 - n^2 + 12n + 4}{6n^2} \geqslant 4 \qquad \text{i.e.,} \qquad 3n^3 - 25n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 8$. The smallest such graph has 9 vertices so this is true for every graph of the considered type.

If $a = 3$, $b = 5$, and $N = M = 3$, then $4n^3 - 43n^2 + 12n + 4 \geqslant 0$ and this holds for $n \geqslant 11$, so it is not true only for such graph with 10 vertices, see Fig. 33.

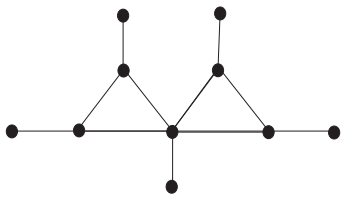

FIGURE 33. A 10-vertex graph for which condition (14) does not hold.

For $q = 1$, inequality (31) becomes

$$n_1 \leqslant \frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)}$$

and from Lemma 6.14 it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M) - 2a + b$$

where we took into account that $N = 4$ and $M \neq 4$.

For example, if $a = 3$, $b = 4$, and $M = 3$, then we have

$$\frac{3n^3 - 5n^2 + 12n + 4}{6n^2} \geqslant 5 \qquad \text{i.e.,} \qquad 3n^3 - 35n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 12$. Thus it does not hold only for such a graph with 11 vertices, see Fig. 34a.

If $a = 3$, $b = 5$, and $M = 3$, then $4n^3 - 55n^2 + 12n + 4 \geqslant 0$ which holds for $n \geqslant 14$. So this condition is violated only for a graph with 12 vertices, see Fig. 34b.

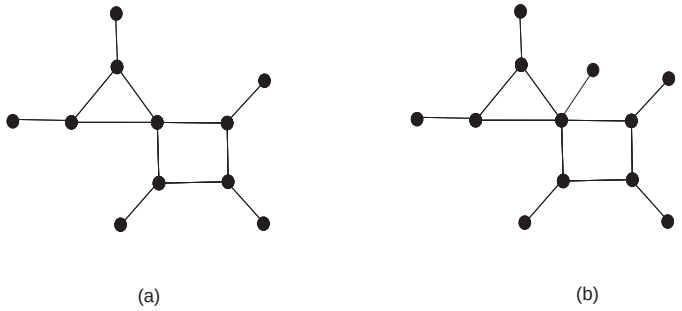

FIGURE 34. A bicyclic (1,3,4)-triregular graph on 11 vertices and a bicyclic (1,3,5)-triregular graph on 12 vertices for which condition (14) does not hold.

For $q = 2$ inequality (31) becomes

$$n_1 \leqslant \frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)}$$

and from Lemma 6.14, since $N = M = 4$, it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 6a + b - 16 \ .$$

For example, if $a = 3$, $b = 4$, then

$$\frac{3n^3 - 9n^2 + 12n + 4}{6n^2} \geqslant 6 \qquad \text{i.e.,} \qquad 3n^3 - 45n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 15$. Therefore graphs with $n = 13$ and $n = 14$ do not obey the above condition, see Fig. 35.

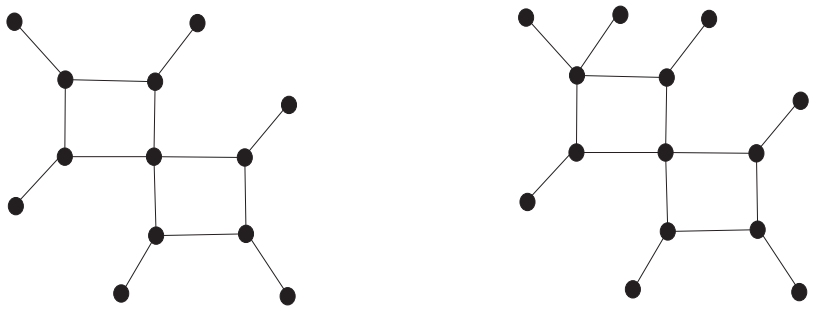

FIGURE 35. A 13- and a 14-vertex bicyclic (1,3,4)-triregular graph for which condition (14) does not hold.

If $a = 3$, $b = 5$, we have $4n^3 - 67n^2 + 12n + 4 \geqslant 0$, which holds for $n \geqslant 17$. Therefore graphs with $n = 14$ and $n = 16$ do not obey the above condition, see Fig. 36.

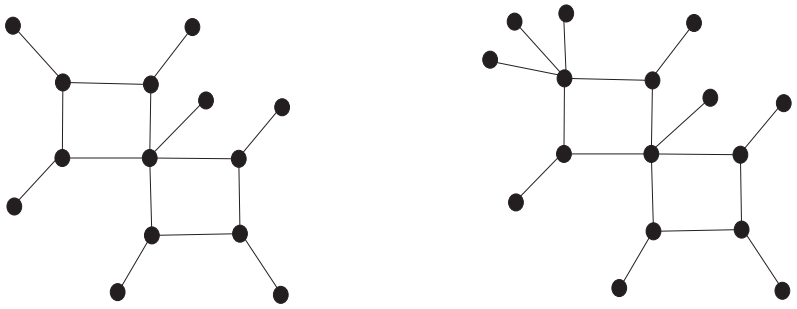

FIGURE 36. A 14- and a 16-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

Theorem 6.16. *Let G be a bicyclic $(1, a, b)$-triregular graph with cycles sharing a single vertex, $2 < a < b$. Let n be the number of its vertices, and N, M the size of its cycles, of which q cycles are quadrangles. Then* (14) *holds if and only if the inequalities*

$$\frac{(5+ab-2a-2b)n^3+(13-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M)-2a+b$$

$$\frac{(5+ab-2a-2b)n^3+(9-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M)-2a+b$$

$$\frac{(5+ab-2a-2b)n^3+(5-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant 6a+b-16$$

are satisfied for $q = 0$, $q = 1$, and $q = 2$, respectively.

6.4.3. Triregular bicyclic graphs whose cycles have several common vertices. Graphs of this type contain three cycles and only two of them are independent. As a consequence, the number q of quadrangles may assume also the value 3. Any two of the three cycles may be chosen as independent. We will always choose those having the smallest size. These cycle sizes will be denoted by N and M. In analogy to Lemma 6.14 we now have:

Lemma 6.17. *Let G be a bicyclic $(1, a, b)$-triregular graph, $2 \leqslant a < b$, in which the cycles have two or more common vertices. Let n_1 be the number of its pendent vertices. Then*

$$n_1 \geqslant \begin{cases} 1, & \text{if } \ a=2,\ b=3 \\ 2(b-3), & \text{if } \ a=2,]; b>3 \\ (a-2)(N+M-4)+(b-3)+(a-3), & \text{otherwise} \end{cases}$$

where N, M are the sizes of its independent cycles.

Proof. We begin with two cycles with arbitrary number of vertices in each, and connect them in a way so that they have two or more common vertices. Now, only two common vertices are of degree 3 and every other common vertex is of degree 2.

For $a = 2$ and $b = 3$ it is easy. We just add one pendent vertex to a vertex of degree 2 in a cycle, see Fig. 37.

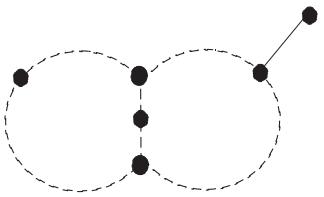

FIGURE 37. Details related to the proof of Lemma 6.17 for $a = 2$, $b = 3$.

For $a = 2$ and $b > 3$ we add $b - 3$ pendent vertices to vertices of degree 3. There are two such vertices, so we have to add altogether $2(b - 3)$ pendent vertices, see Fig. 38.

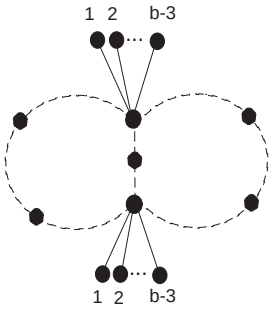

FIGURE 38. Details related to the proof of Lemma 6.17 for $a = 2$, $b > 3$.

For $2 < a < b$, the cycles must be connected so that they have only two common vertices (i.e., one common edge). We connect each of $N+M-4$ vertices of degree 2 with $a-2$ pendent vertices, in order to obtain vertices of degree a. Then, if $a = 3$, we add $b - 3$ pendent vertices to only one vertex of degree 3, to obtain a vertex of degree b (see Fig. 39a), but if $a > 3$ we add $a - 3$ pendent vertices to one vertex of degree 3 and $b - 3$ pendent vertices to another vertex of degree 3, see Fig. 39b.

We conclude that the minimal number of pendent vertices is $(a-2)(N+M-4)$ $+ (b-3) + (a-3)$. □

For $(1, 2, 3)$-, $(1, 2, b)$- and $(1, a, b)$-triregular graphs, $2 < a < b$, $b \geqslant 4$, we get results analogous to those for graphs with disjoint cycles, except that we must consider also the possibility $q = 3$.

The cycles of $(1, 2, 3)$-triregular graphs with $q = 3$ must have three common vertices and $N = M = 4$. From inequality (31) and Lemma 6.17 we obtain $n^3 + (1 - 4q)n^2 + 12n + 4 \geqslant 0$, which for $q = 3$ becomes $n^3 - 11n^2 + 12n + 4 \geqslant 0$. This

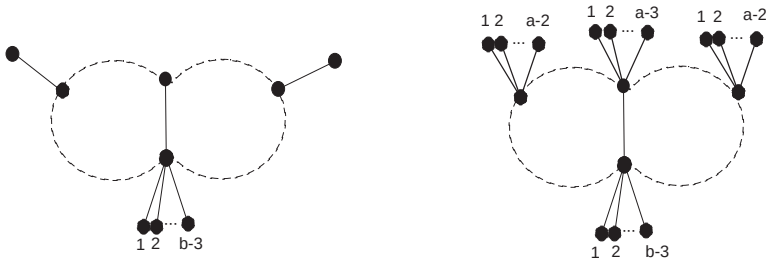

FIGURE 39. Details related to the proof of Lemma 6.17 for $a > 2$, $b > 3$.

inequality holds for $n \geqslant 10$. Therefore graphs with 6, 7, 8, and 9 vertices violate it, see Fig. 40.

Theorem 6.18. *Let G be a bicyclic $(1,2,3)$-triregular graph in which cycles have two or more common vertices and let n be the number of its vertices. Then inequality (14) holds for every G, except if $q = 3$ and if the number of vertices is $6, 7, 8$, or 9.*

Theorem 6.19. *Let G be an n-vertex bicyclic $(1,2,b)$-triregular graph with cycles sharing two or more common vertices, $b \geqslant 4$. Let q be the number of its quadrangles. Then inequality (14) holds if and only if*

$$2b^2 - 6b - 3 \leqslant \frac{n^3 + 12n + 4}{n^2} \qquad \text{if } \ q = 0,$$
$$2b^2 - 6b + 1 \leqslant \frac{n^3 + 12n + 4}{n^2} \qquad \text{if } \ q = 1,$$
$$2b^2 - 6b + 5 \leqslant \frac{n^3 + 12n + 4}{n^2} \qquad \text{if } \ q = 2,$$
$$2b^2 - 6b + 9 \leqslant \frac{n^3 + 12n + 4}{n^2} \qquad \text{if } \ q = 3.$$

For $(1,a,b)$-triregular graphs, $2 < a < b$, from (31) and Lemma 4 it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b - 4q)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M) + b - 3a + 2\,.$$

For $q = 0$ and $N, M \neq 4$, we obtain

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M) + b - 3a + 2\,.$$

For example, if $q = 0$, $a = 3$, $b = 4$, and $N = 3$, $M = 5$, we have

$$\frac{3n^3 - n^2 + 12n + 4}{6n^2} \geqslant 5 \qquad \text{i.e.,} \qquad 3n^3 - 31n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 10$. Since the smallest such graph has 11 vertices, this condition is satisfied by all graphs of this kind.

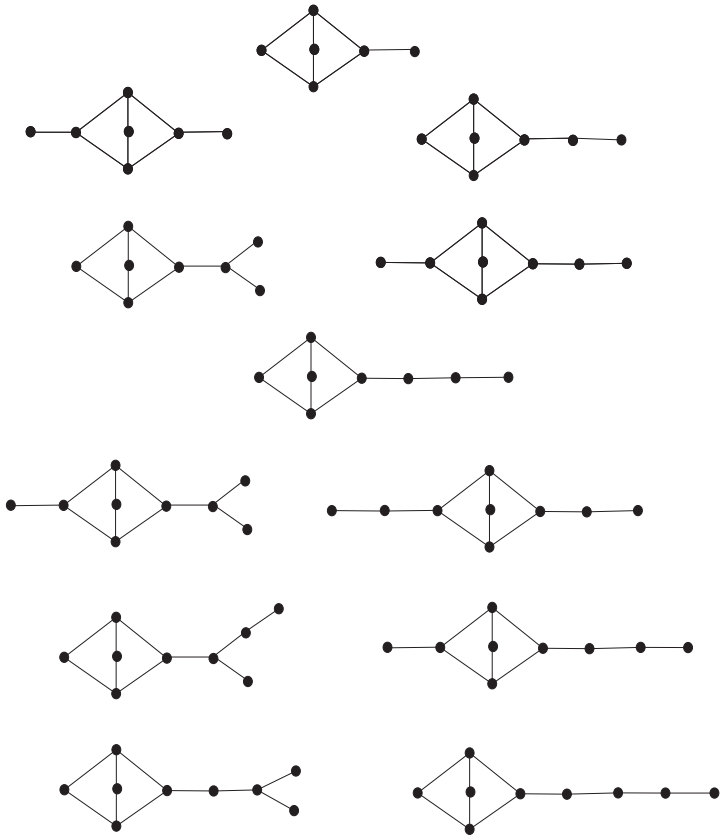

FIGURE 40. All bicyclic (1,2,3)-triregular graphs with $q = 3$, for which condition (14) does not hold. These have 6, 7, 8, and 9 vertices.

If $q = 0$, $a = 3$, $b = 5$, and $N = 3$, $M = 5$, we will have

$$\frac{4n^3 - 3n^2 + 12n + 4}{8n^2} \geqslant 6 \qquad \text{i.e.,} \qquad 4n^3 - 51n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 13$. Thus, it is not true only for such graph with 12 vertices, see Fig. 41. The next larger graph has 14 vertices and for it (as well as all other graphs of this kind) the inequality is satisfied.

If $q = 1$, then $N = 4$, $M \neq 4$ or $N = M = 3$. For $N = 4$ and $M \neq 4$ we have

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M) + b - 3a + 2$$

whereas for $q = 1$ and $N = M = 3$,

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 3a + b - 10\ .$$

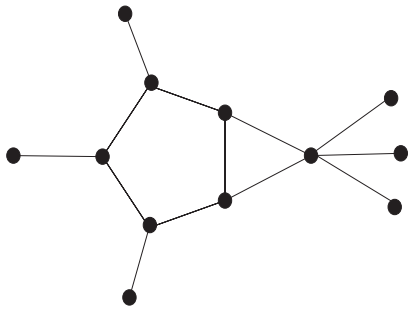

FIGURE 41. A 12-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

For example, if $q = 1$, $a = 3$, $b = 4$, and $N = 4$, $M = 3$, we have

$$\frac{3n^3 - 5n^2 + 12n + 4}{6n^2} \geqslant 4 \qquad \text{i.e.,} \qquad 3n^3 - 29n^2 + 12n + 4 \geqslant 0$$

and this holds for $n \geqslant 10$. Therefore only for such graphs with 9 vertices it is not true, see Fig. 42.

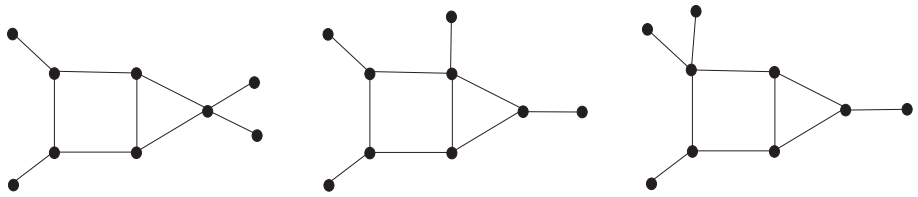

FIGURE 42. Bicyclic (1,3,4)-triregular graphs on 9 vertices for which condition (14) does not hold.

If $q = 1$, $a = 3$, $b = 5$, $N = 4$, and $M = 3$, then we have

$$\frac{4n^3 - 7n^2 + 12n + 4}{8n^2} \geqslant 5 \qquad \text{i.e.,} \qquad 4n^3 - 47n^2 + 12n + 4 \geqslant 0\ .$$

This inequality holds for $n \geqslant 12$, and therefore the graphs with 10 vertices violate it, see Fig. 43.

If $q = 1$, $a = 3$, $b = 4$, and $N = M = 3$, then we have

$$\frac{3n^3 - 5n^2 + 12n + 4}{6n^2} \geqslant 3 \qquad \text{i.e.,} \qquad 3n^3 - 23n^2 + 12n + 4 \geqslant 0\ .$$

This inequality holds for $n \geqslant 8$, and therefore the graph with 7 vertices violates it, see Fig. 44.

If $a = 3$, $b = 5$, and $N = M = 3$, we will have

$$\frac{4n^3 - 7n^2 + 12n + 4}{8n^2} \geqslant 4 \qquad \text{i.e.,} \qquad 4n^3 - 39n^2 + 12n + 4 \geqslant 0$$

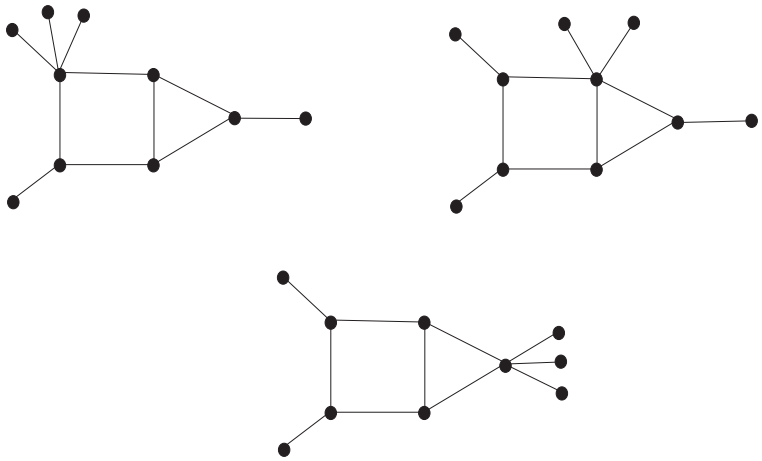

FIGURE 43. Bicyclic (1,3,5)-triregular graphs on 10 vertices for which condition (14) does not hold.

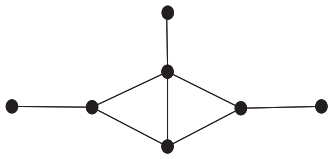

FIGURE 44. A 7-vertex bicyclic (1,3,4)-triregular graph for which condition (14) does not hold.

which holds for $n \geqslant 10$. Therefore, it is not true only for the graph of this kind on 8 vertices, see Fig. 45.

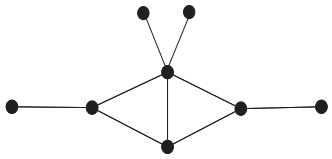

FIGURE 45. An 8-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

For $q = 2$ we obtain

$$\frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 5a + b - 14 \ .$$

For example, if $a = 3$, $b = 4$, we have

$$\frac{3n^3 - 9n^2 + 12n + 4}{6n^2} \geqslant 5 \qquad \text{i.e.,} \qquad 3n^3 - 39n^2 + 12n + 4 \geqslant 0$$

which holds for $n \geqslant 13$ and is thus violated by graphs with $n = 11$ and $n = 12$, see Fig. 46.

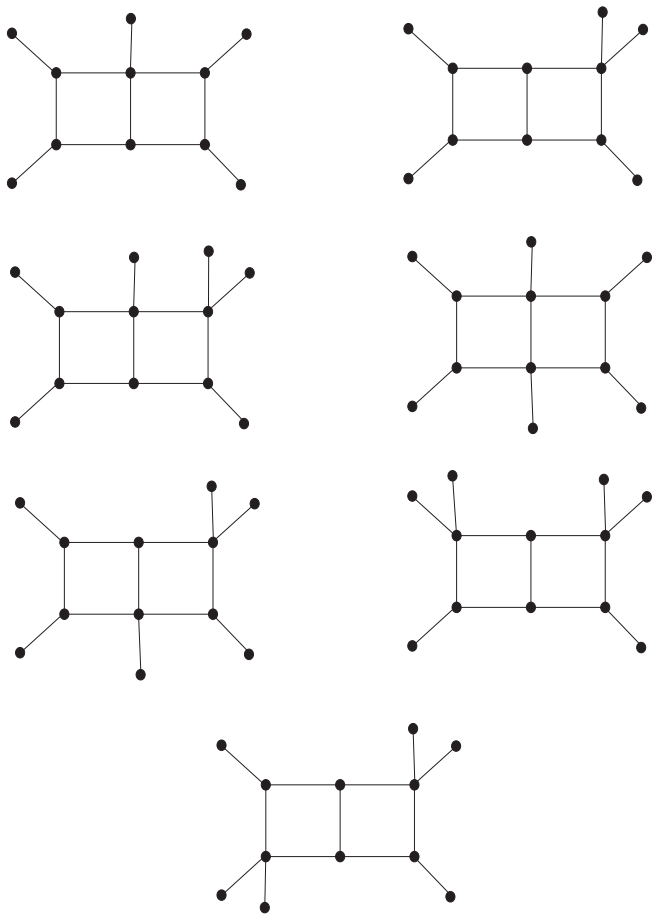

FIGURE 46. Bicyclic (1,3,4)-triregular graphs on 11 and 12 vertices, with $q = 2$, for which condition (14) does not hold.

If $a = 3$, $b = 5$, then

$$\frac{4n^3 - 7n^2 + 12n + 4}{8n^2} \geqslant 6 \qquad \text{i.e.,} \qquad 4n^3 - 55n^2 + 12n + 4 \geqslant 0$$

which holds for $n \geqslant 14$, and is thus violated by only two graphs with $n = 12$, see Fig. 47.

Theorem 6.20. *Let G be an n-vertex bicyclic $(1, a, b)$-triregular graph with cycles sharing at least two vertices, $2 < a < b$, $b \geqslant 4$. Let N, M be the sizes of its two independent cycles and q the number of its quadrangles. Then* (14) *holds if and only if the following conditions* (a), (b), (c), *or* (d) *are satisfied:*

FIGURE 47. Two 12-vertex bicyclic (1,3,5)-triregular graphs with $q = 2$ for which condition (14) does not hold.

(a) $q = 0$ *and*

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M) + b - 3a + 2$$

(b) $q = 1$, $N = 4$, $M \neq 4$, *and*

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M) + b - 3a + 2$$

(c) $q = 1$, $N = M = 3$, *and*

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 3a + b - 10$$

(d) $q = 2$ *and*

$$\frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geqslant 5a + b - 14\,.$$

7. Epilogue

In Sections 5 and 6 we established necessary and sufficient conditions for the validity of the inequality (14), for a great variety of types of acyclic, unicyclic, and bicyclic graphs. In these two sections the graph energy was not mentioned at all. Therefore, at this point it seems to be purposeful to re-state Theorem 4.1:

Theorem 4.1.bis. If the graph G satisfies the inequality (14), then the energy of G is greater than (or, exceptionally, equal to) the number of vertices of G, i.e., inequality (9) holds. Therefore G is necessarily not hypoenergetic. If, however, the graph G does not satisfy the inequality (14), then it may be hypoenergetic, but need not. Anyway, the search for hypoenergetic graphs must be done among those which violate inequality (14).

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NULLITY OF GRAPHS

Abstract. The nullity $\eta = \eta(G)$ of a graph G is the multiplicity of the number zero in the spectrum of G. The chemical importance of this graph-spectrum based invariant lies in the fact, that within the Hückel molecular orbital model, if $\eta(G) > 0$ for the molecular graph G, then the corresponding chemical compound is highly reactive and unstable, or nonexistent. This chapter outlines both the chemically relevant aspects of η (most of which were obtained in the 1970s and 1980s) and the general mathematical results on η obtained recently.

Mathematics Subject Classification (2000): 05C50; 05C90; 92E10

Keywords: nullity (of graph); zero eigenvalue (of graph); spectrum (of graph); chemistry

Contents

1. Graph nullity and its chemical applications

Let G be a graph of order n, having vertex set $V(G)$ and edge set $E(G)$. Let $A(G)$ be the adjacency matrix of G. The graph G is said to be singular (resp. non-singular) if its adjacency matrix $A(G)$ is singular (resp. non-singular). The *nullity* of G, denoted by $\eta = \eta(G)$, is the algebraic multiplicity of the number zero in the spectrum of G.

In order to explain the role of the nullity of graphs in chemistry, we need to recall a few basic facts from the quantum theory of molecules [11]. The behavior of the electrons in molecules is considered to be responsible for the majority of properties of chemical compounds. This behavior is governed by laws of quantum theory and is described by the so-called Schrödinger equation. Finding the solutions of the Schrödinger equation is one of the main tasks of quantum chemistry.

In an early stage of quantum chemistry, during the time when computers were not available, the German theoretical chemist Erich Hückel proposed an approximate method for solving the Schrödinger equation for a special (for chemistry very important) class of organic molecules, the so-called *unsaturated conjugated hydrocarbons* [23]. Nowadays, this method is known under the name *Hückel molecular orbital* (*HMO*) *theory* [4, 11, 35].

A quarter of century was needed to recognize that the mathematics on which the HMO theory is based is graph spectral theory [16, 30]. In a nutshell: The (approximate) energies $E_1, E_2, \ldots$ that the electrons may possess are related to the eigenvalues $\lambda_1, \lambda_2, \ldots$ of a so-called "*molecular graph*" as

$$E_j = \alpha + \beta\,\lambda_j \ , \ j = 1, 2, \ldots, n$$

where α and β are certain constants; for more detail see [15, 18]. Because $\beta < 0$, if the graph eigenvalues are labelled in the usual non-increasing manner as

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$$

then E_1 is the lowest energy level, E_2 is the second–lowest energy level, etc.

Each energy level in a molecule can be occupied by at most two electrons. Usually, the total number of electrons to which HMO theory is applied is equal to n, and n is most frequently an even number. Usually, $E_{n/2+1} < E_{n/2}$ or, what is the same, $\lambda_{n/2} > \lambda_{n/2+1}$.

If so, then in order to achieve the lowest-energy state of the underlying molecule, it has to possess two (= the maximum possible number) of electrons with energy E_1, two (= the maximum possible number) of electrons with energy $E_2, \ldots$ and two

(= the maximum possible number) of electrons with energy $E_{n/2}$. This will result in a stable arrangement of electrons; in the language of theoretical chemistry, the molecule will have a "*closed–shell electron configuration*".

If, however, $E_{n/2+1} = E_{n/2}$, then a total of four electrons could fill the two "degenerate" energy levels. Because the number of available electrons is only two, an irregular and unstable arrangement of electrons will result; in the language of theoretical chemistry, the molecule will have an "*open–shell electron configuration*".

The above described filling of the energy levels with electrons is in quantum chemistry referred to as the *Aufbau principle* (a word originating from German language). Details on this matter can be found elsewhere [28].

Molecules with an open-shell electron configuration are known to be highly reactive and in many cases are simply not capable of existence.

We now show how the nullity of the molecular graph is related to the closed/open-shell character of the underlying molecule.

Long before the above-sketched graph-spectral connections were envisaged, some important results in HMO theory were discovered. One of these is the so-called "*Pairing theorem*" [5]. According to it, for the majority of unsaturated conjugated hydrocarbons, the eigenvalues of the molecular graph are "paired", so that

$$\lambda_j = -\lambda_{n-j+1} \tag{1}$$

holds for all $j = 1, 2, \ldots, n$. In the language of HMO theory, the hydrocarbons to which the Pairing theorem applies are referred to as "*alternant*". With today's knowledge it is straightforward to recognize that an unsaturated conjugated hydrocarbon is "alternant" if and only if its molecular graph is bipartite. Indeed, the relation (1) is a well known spectral property of bipartite graphs [6].

An immediate consequence of the Pairing theorem is that a molecular graph with even number of vertices has either nullity zero (in which case $\lambda_{n/2} > 0 > \lambda_{n/2+1}$), or its nullity is an even positive integer (in which case $\lambda_{n/2} = \lambda_{n/2+1} = 0$). In HMO theory this means the following [27]:

- If the nullity of the molecular graph of an alternant unsaturated conjugated hydrocarbon is zero, then the respective molecule is predicted to have a stable, closed-shell, electron configuration and the respective compound predicted to have a low chemical reactivity and to be chemically stable.
- If the nullity of the molecular graph of an alternant unsaturated conjugated hydrocarbon is greater than zero, then the respective molecule is predicted to have an unstable, open-shell, electron configuration and the respective compound is expected to be highly reactive, chemically unstable and often not capable of existence.

Thus, the nullity of a molecular graph has a far-reaching inference on the expected stability of unsaturated conjugated hydrocarbons. This prediction of HMO theory has been experimentally verified in numerous cases. The most drastic such case is the fact that whereas there exist more than a thousand benzenoid hydrocarbons whose molecular graphs have nullity zero, not a single such hydrocarbon is nowadays known, whose molecular graph would have a non-zero nullity.

2. Elementary properties of nullity

Let $r(A(G))$ be the rank of $A(G)$. Clearly, $\eta(G) = n - r(A(G))$. The rank of a graph G is the rank of its adjacency matrix $A(G)$, denoted by $r(G)$. Then, $\eta(G) = n - r(G)$. Each of $\eta(G)$ and $r(G)$ determines the other (once n is specified).

Lemma 1. *Let G be a graph on n vertices. Then $\eta(G) = n$ if and only if G is a graph without edges (empty graph).*

For some classes of graphs the spectrum is known and thereby so is the nullity η. We list some examples.

Lemma 2. [6, 7, 31] (i) *The spectrum of the complete graph K_n consists of two distinct eigenvalues $n-1$ and -1, with multiplicities 1 and $n-1$, respectively. Thus, $\eta(K_n) = 1$ for $n = 1$ and $\eta(K_n) = 0$ for $n > 1$.*

(ii) *The eigenvalues of the path P_n are of the form $2\cos\frac{\pi r}{n+1}$, $r = 1, 2, \ldots, n$. According to this,*

$$\eta(P_n) = \begin{cases} 1, & \text{if } n \text{ is odd} \\ 0, & \text{if } n \text{ is even.} \end{cases}$$

(iii) *The eigenvalues of the cycle C_n are $2\cos\frac{2\pi r}{n}$, $r = 0, 1, \ldots, n-1$. Therefore,*

$$\eta(C_n) = \begin{cases} 2, & \text{if } n \equiv 0 \pmod 4, \\ 0, & \text{otherwise.} \end{cases}$$

Lemma 3. (i) *Let H be an induced subgraph of G. Then $r(H) \leqslant r(G)$.*

(ii) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_t$, where $G_1, G_2, \ldots, G_t$ are connected components of G. Then $r(G) = \sum_{i=1}^{t} r(G_i)$, i.e., $\eta(G) = \sum_{i=1}^{t} \eta(G_i)$.*

In the sequel we give some simple inequalities concerning $\eta(G)$ that are direct consequences of Lemmas 2 and 3.

Recall that the path P is a graph with $V(P) = \{v_1, v_2, \ldots, v_k\}$ and $E(P) = \{v_1v_2, v_2v_3, \ldots, v_{k-1}v_k\}$, where the vertices $v_1, v_2, \ldots, v_k$ are all distinct. We say that P is a path from v_1 to v_k, or a (v_1, v_k)-path. It can be denoted by P_k, where k is its *length*. The *distance* $d(x, y)$ in G of two vertices x, y is the length of a shortest (x, y)-path in G; if no such path exists, we define $d(x, y)$ to be infinite. The greatest distance between any two vertices in G is the *diameter* of G, denoted by $\mathrm{diam}(G)$.

Lemma 4. [10] *Let G be a simple graph on n vertices, and let the complete graph K_p be a subgraph of G, where $2 \leqslant p \leqslant n$. Then $\eta(G) \leqslant n - p$.*

A *clique* of a simple graph G is a complete subgraph of G. A clique S is maximum if G has no clique S' with $|V(S')| > |V(S)|$. The number of vertices in a maximum clique of G is called the clique number of G and is denoted by $\omega(G)$.

The following inequality is clear from the previous result.

Corollary 1. [10] *Let G be a simple non-empty graph on n vertices. Then $\eta(G) + \omega(G) \leqslant n$.*

From Lemma 3 and Lemma 2(iii) we arrive at:

Lemma 5. [10] *Let G be a simple graph on n vertices and let the cycle C_p be an induced subgraph of G, where $3 \leqslant p \leqslant n$. Then*

$$\eta(G) \leqslant \begin{cases} n-p+2, & \text{if } p \equiv 0 \pmod 4, \\ n-p, & \text{otherwise.} \end{cases}$$

The length of the shortest cycle in a graph G is the *girth* of G, denoted by $\mathrm{gir}(G)$. A relation between $\eta(G)$ and $gir(G)$ is given by:

Corollary 2. [10] *If G is a simple graph on n vertices, and G has at least one cycle, then*

$$\eta(G) \leqslant \begin{cases} n-\mathrm{gir}(G)+2, & \text{if } \mathrm{gir}(G) \equiv 0 \pmod 4, \\ n-\mathrm{gir}(G), & \text{otherwise.} \end{cases}$$

If we bear in mind Lemma 2(ii) and Lemma 3, the following result is obvious.

Lemma 6. [10] *Let G be a simple graph on n vertices and let the path P_k be an induced subgraph of G, where $2 \leqslant k \leqslant n$. Then*

$$\eta(G) \leqslant \begin{cases} n-k+1, & \text{if } k \text{ is odd,} \\ n-k, & \text{otherwise.} \end{cases}$$

Corollary 3. [10] *Suppose that x and y are two vertices in G and that there exists an (x,y)-path in G. Then*

$$\eta(G) \leqslant \begin{cases} n-d(x,y), & \text{if } d(x,y) \text{ is even,} \\ n-d(x,y)-1, & \text{otherwise.} \end{cases}$$

Corollary 4. [10] *Suppose G is a simple connected graph on n vertices. Then*

$$\eta(G) \leqslant \begin{cases} n-\mathrm{diam}(G), & \text{if } \mathrm{diam}(G) \text{ is even,} \\ n-\mathrm{diam}(G)-1, & \text{otherwise.} \end{cases}$$

3. Relations between nullity and graph structure

In the general case, the problem of finding connections between the structure of a graph G and its nullity seems to be difficult. For example, $\eta(G)$ is not determined by the set of vertex degrees of G (see Fig. 1)

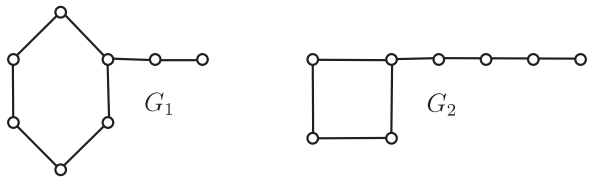

FIGURE 1

In what follows we consider mostly bipartite graphs, although some of the theorems stated below can be extended to non-bipartite graphs (see [8]).

Before proceeding we need some definitions. A matching of G is a collection of independent (mutually non-adjacent) edges of G. A maximum matching is a matching with the maximum possible number of edges. The size of a maximum matching of G, i.e., the maximum number of independent edges of G, is denoted by $m = m(G)$.

Denote by $P_G(\lambda)$ the characteristic polynomial of G. Let

$$P_G(\lambda) = |\lambda I - A| = \lambda^n + a_1\lambda^{n-1} + \cdots + a_n$$

Then [6]

$$a_i = \sum_U (-1)^{p(U)}\, 2^{c(U)} \quad (i = 1, 2, \ldots, n), \tag{2}$$

where the sum is over all subgraphs U of G consisting of disjoint edges and cycles and having exactly i vertices (called "basic figures"). If U is such a subgraph, then $p(U)$ is the number of its components, of which $c(U)$ components are cycles.

For some special classes of bipartite graphs it is possible to find relatively easily the relation between the structure of G and $\eta(G)$. The problem is solved for trees by the following theorem [7].

Theorem 1. [7] *Let T be a tree on $n \geqslant 1$ vertices and let m be the size of its maximum matching. Then its nullity is equal to $\eta(T) = n - 2m$.*

This theorem is an immediate consequence of the statement concerning the coefficients of the characteristic polynomial of the adjacency matrix of a tree (which can be easily deduced from eq. (2)).

Theorem 1 is a special case of one more general theorem that will be formulate in the following.

Theorem 2. [9] *If a bipartite graph G with $n \geqslant 1$ vertices does not contain any cycle of length $4s$ ($s = 1, 2, \ldots$), then $\eta(G) = n - 2m$, where m is the size of its maximum matching.*

Proof. According to the assumption, a bipartite graph G does not contain any basic figure (with an arbitrary number of vertices) with cycles of lengths $4s$ ($s = 1, 2, \ldots$). For a particular basic figure U it holds that $p(U)$ is equal to the total number of cycles of lengths $4s + 2$ ($s = 1, 2, \ldots$) and of graphs K_2. Let $4t_i + 2$ ($i = 1, 2, \ldots, p(U)$) be the numbers of vertices contained in these cycles or graphs K_2. If U is a basic figure with $2q$ ($2q \leqslant n$) vertices we get

$$\sum_{i=1}^{p(U)} (4t_i + 2) = 2q \qquad \text{and} \qquad 2\sum_{i=1}^{p(U)} t_i + p(U) = q.$$

Hence, $p(U) \equiv q \pmod 2$ and all terms (summands) in the expression for the coefficient a_{2q} of the characteristic polynomial have the same sign. Because of this, $a_{2q} \neq 0$ if and only if there is at least one basic figure with $2q$ vertices. Since m is the size of maximum matching of G the statement of the theorem now follows immediately. □

The formula $\eta(G) = n - 2m$ was shown to hold also for all benzenoid graphs (which may contain cycles of the size $4s$) [17]. As a curiosity, we mention that almost twenty years later, Fajtlowicz (using his famous computer system *Grafitty*) conjectured the precisely same result. Although being informed about the existence of the proof of this "conjecture" [17], Sachs and John produced an independent paper on this "discovery" and (together with Fajtlowicz) published it [13].

The problem concerning the relation between the structure of a bipartite graph and its nullity can be reduced to another problem which can be solved in certain special cases. The vertices of a bipartite graph may be numbered so that the adjacency matrix has the following form:

$$A = \begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}.$$

The matrix B is the "incidence matrix" between the two sets X and Y of vertices of the bipartite graph $G = (X, Y, U)$ (U is the set of edges).

Theorem 3. [27] *For the bipartite graph G with n vertices and incidence matrix B, $\eta(G) = n - 2\,r(B)$, where $r(B)$ is the rank of B.*

Since for $G = (X, Y, U)$, we have $r(B) \leqslant \min(|X|, |Y|)$ and Theorem 3 yields the following:

Corollary 5. [7] $\eta(G) \geqslant \max(|X|, |Y|) - \min(|X|, |Y|)$.

If the number of vertices is odd, then $|X| \neq |Y|$ and $\eta(G) > 0$. Thus a necessary condition to have no zeros in the spectrum of a bipartite graph is that the number of vertices is even (what is also in accordance with Theorem 2).

The following three theorems ([7], [9]) enable, in special cases, the reduction of the problem of determining $\eta(G)$ for some graphs to the same problem for simpler graphs.

Theorem 4. [7] *Let $G_1 = (X_1, Y_1, U_1)$ and $G_2 = (X_2, Y_2, U_2)$, where $|X_1| = n_1$, $|Y_1| = n_2$, $n_1 \leqslant n_2$, and $\eta(G_1) = n_2 - n_1$. If the graph G is obtained from G_1 and G_2 by joining (any) vertices from X_1 to vertices in Y_2 (or X_2), then the relation $\eta(G) = \eta(G_1) + \eta(G_2)$ holds.*

Proof. Let B_1, B_2, B be the incidence matrices of the graphs G_1, G_2, G. We may assume that

$$B = \begin{pmatrix} B_1 & M \\ \mathbf{0} & B_2 \end{pmatrix}$$

where B_1 is an $n_1 \times n_2$ matrix, $\mathbf{0}$ is a zero matrix, and M is an arbitrary matrix with entries from the set $\{0, 1\}$.

From $\eta(G_1) = n_2 - n_1$ we have $r(B_1) = n_1$. Thus B_1 contains n_1 linearly independent columns. Consequently, each column of the matrix M can be expressed as a linear combination of the aforementioned columns of B_1. Hence, the matrix B can be reduced by operations not changing the rank to the form

$$B' = \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}.$$

whence $r(B) = r(B_1) + r(B_2)$. Theorem 3 gives $\eta(G) = \eta(G_1) + \eta(G_2)$. □

Corollary 6. [7] *If the bipartite graph G contains a pendent vertex, and if the induced subgraph H of G is obtained by deleting this vertex together with the vertex adjacent to it, then $\eta(G) = \eta(H)$.*

This corollary of Theorem 4 is proved in the following way: we take the complete graph with two vertices as G_1 and the graph H as G_2.

Corollary 7. [7] *Let G_1 and G_2 be bipartite graphs. If $\eta(G_1) = 0$, and if the graph G is obtained by joining an arbitrary vertex of G_1 by an edge to an arbitrary vertex of G_2, then $\eta(G) = \eta(G_2)$.*

Example 1. See Fig. 2.

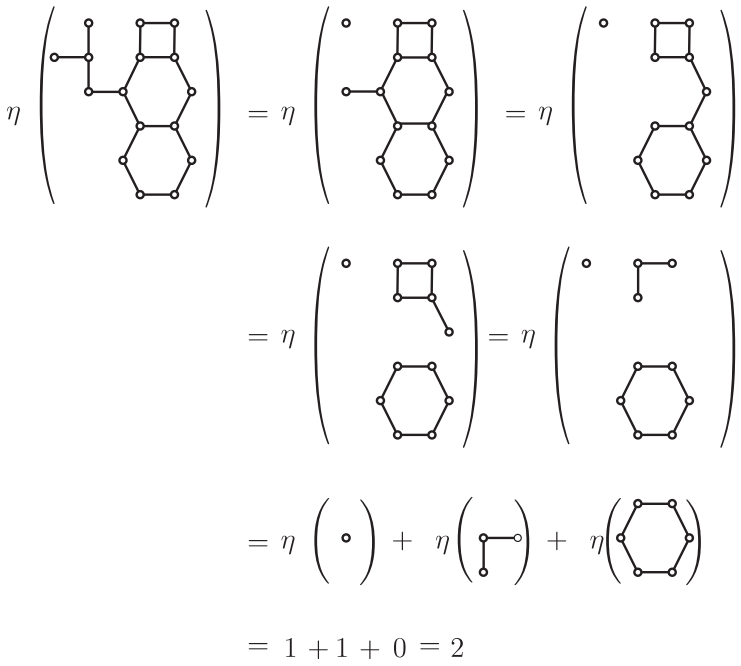

FIGURE 2

Theorem 5. [9] *A path with four vertices of degree 2 in a bipartite graph G can be replaced by an edge* (see Fig. 3) *without changing the value of $\eta(G)$.*

Theorem 6. [9] *Two vertices and the four edges of a cycle of length 4, which are positioned in a bipartite graph G as shown in Fig. 4, can be removed without changing the value of $\eta(G)$.*

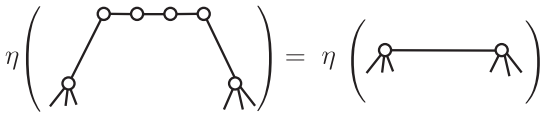

FIGURE 3

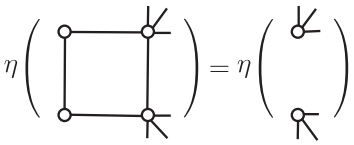

FIGURE 4

Remark. Corollary 6 of Theorem 4, as well as Theorems 5 and 6 hold also in the case when the graph G is non-bipartite [8].

Example 2. See Fig. 5.

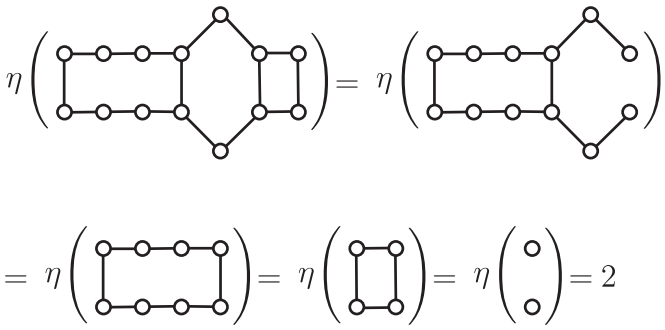

FIGURE 5

4. Graphs with maximum nullity

If we bear in mind Lemmas 1 and 4, it is obvious that $0 \leqslant \eta(G) \leqslant n-2$ if G is a simple non-empty graph on n vertices.

A natural problem is to characterize the extremal graphs whose nullities attain the upper bound $n-2$ and the second upper bound $n-3$.

Theorem 7. [10] *Suppose that G is a simple graph on n vertices and G has no isolated vertices. Then*

(i) $\eta(G) = n-2$ *if and only if G is isomorphic to a complete bipartite graph K_{n_1,n_2}, where $n_1+n_2=n$, $n_1,n_2>0$.*

(ii) $\eta(G) = n-3$ *if and only if G is isomorphic to a complete tripartite graph K_{n_1,n_2,n_3}, where $n_1+n_2+n_3=n$, $n_1,n_2,n_3>0$.*

Several results on the extremal graphs attaining the third and the fourth upper bound were obtained. Before stating them we give some necessary definitions.

Let $\mathcal{G}_n$ be the set of all n-vertex graphs, and let $[0,n] = \{0,1,\ldots,n\}$. A subset N of $[0,n]$ is said to be the *nullity set* of $\mathcal{G}_n$ provided that for any $k \in N$, there exists at least one graph $G \in \mathcal{G}_n$ such that $\eta(G) = k$.

A connected simple graph on n vertices is said to be *unicyclic* if it has n edges and *bicyclic* if it has $n+1$ edges. Denote by $\mathcal{U}_n$ and $\mathcal{B}_n$ the set of all n-vertex unicyclic and bicyclic graphs, respectively. For convenience, let $\mathcal{T}_n$ denote the set of n-vertex trees.

First we determine all graphs with pendent vertices that attain the third-maximum nullity $n-4$ and the fourth-maximum nullity $n-5$, using the results of Li [25]. Then we proceed recursively, as in [25], to construct all graphs having pendent vertices with $\eta(G) > 0$.

Let G_1^* be an n-vertex graph obtained from a complete bipartite graph $K_{r,s}$ and a star $K_{1,t}$ by identifying a vertex of $K_{r,s}$ with the center of $K_{1,t}$, where $r,s,t \geqslant 1$ and $r+s+t = n$. Let $K_{1,l,m}$ be a complete tripartite graph with the maximum-degree vertex v, where $l,m > 0$. Then let G_2 be the n-vertex graph created from $K_{1,l,m}$ and a star $K_{1,p}$ by identifying the vertex v with the center of $K_{1,p}$, where $l,m,p \geqslant 1$ and $l+m+p+1 = n$.

Theorem 8. [25] *Let G be a connected n-vertex graph with pendent vertices. Then $\eta(G) = n-4$ if and only if G is isomorphic to the graph G_1^* or G_2^*, where G_1^* is depicted in Fig. 6, and G_2^* is a connected spanning subgraph of G_2 (see Fig. 6) and contains $K_{l,m}$ as its subgraph.*

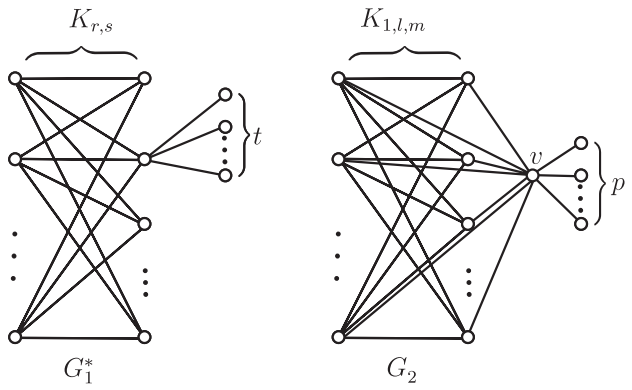

FIGURE 6

Let G_3^* be an n-vertex graph obtained from a complete tripartite graph $K_{r,s,t}$ and a star $K_{1,q}$ by identifying a vertex of $K_{r,s,t}$ with the center of $K_{1,q}$, where $r,s,t,q > 0$ and $r+s+t+q = n$. Let $K_{1,l,m,p}$ be a tetrapartite graph with the maximum-degree vertex v, where $l,m,p > 0$. Then let G_4 be the n-vertex graph

created from $K_{1,l,m,p}$ and a star $K_{1,d}$ by identifying the vertex v and the center of $K_{1,d}$, where $l, m, p, d > 0$ and $l + m + p + d + 1 = n$.

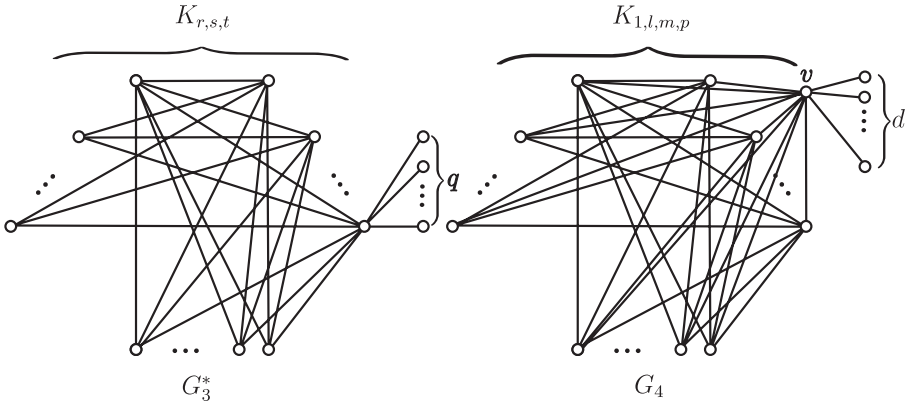

FIGURE 7

Theorem 9. [25] *Let G be a connected graph on n vertices and assume that G has no isolated vertex. Then $\eta(G) = n - 5$ if and only if G is isomorphic to the graph G_3^* or G_4^*, where G_3^* is depicted in Fig. 7, G_4^* is a connected spanning subgraph of G_4 (see e.g. Fig. 7) and contains $K_{l,m,p}$ as its subgraph.*

Using similar reasoning as in Theorems 8 and 9, we may proceed recursively to construct all n-vertex graphs having pendent vertices with $\eta(G) = n-6, n-7, n-8$, and so on. In that way, all n-vertex graphs with pendent vertices satisfying $\eta(G) > 0$ can be determined [25]. In the sequel we formulate some results on the extremal nullity of trees, unicyclic and bicyclic graphs. We also give the characterization of their nullity sets.

For an n-vertex tree, if it is a complete bipartite graph, then the tree should be the star. Since any complete tripartite graph is cyclic, there does not exist a tree that is a complete tripartite graph. Therefore, the following result is a direct consequence of Theorems 7, 8, and 9.

Theorem 10. [12, 25] *Let $\mathcal{T}_n$ be the set of all n-vertex trees.*

(i) *Let $T \in \mathcal{T}_n$. Then $\eta(T) \leqslant n - 2$, and the equality holds if and only if $T \cong S_n$* [12].

(ii) *Let $T \in \mathcal{T}_n \setminus \{S_n\}$. Then $\eta(T) \leqslant n - 4$, and the equality holds if and only if $T \cong T_1$ or $T \cong T_2$, where T_1 and T_2 are depicted in Fig. 8* [25].

(iii) *Let $T \in \mathcal{T}_n \setminus \{S_n, T_1, T_2\}$. Then $\eta(T) \leqslant n - 6$, and the equality holds if and only if $T \cong T_3$ or $T \cong T_4$ or $T \cong T_5$, where trees T_3, T_4, T_5 are shown in Fig. 8* [25].

Just as in Theorem 10, we can use graphs in $\mathcal{T}_n$ (see [25]) whose nullity is $n - 6$ to determine n-vertex trees whose nullity is $n - 8$, and so on. This implies:

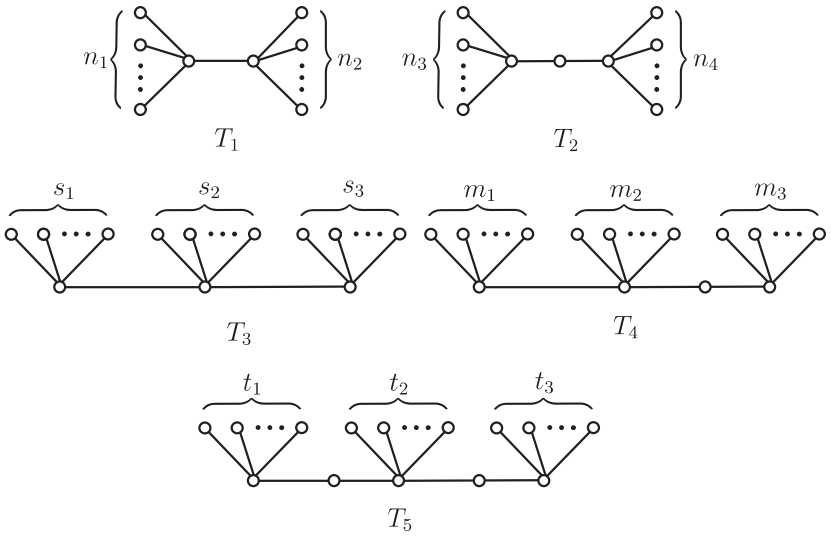

FIGURE 8

Corollary 8. [25] *The nullity set of $\mathcal{T}_n$ is $\{0, 2, 4, \ldots, n-4, n-2\}$ if n is even and $\{1, 3, 5, \ldots, n-4, n-2\}$, otherwise.*

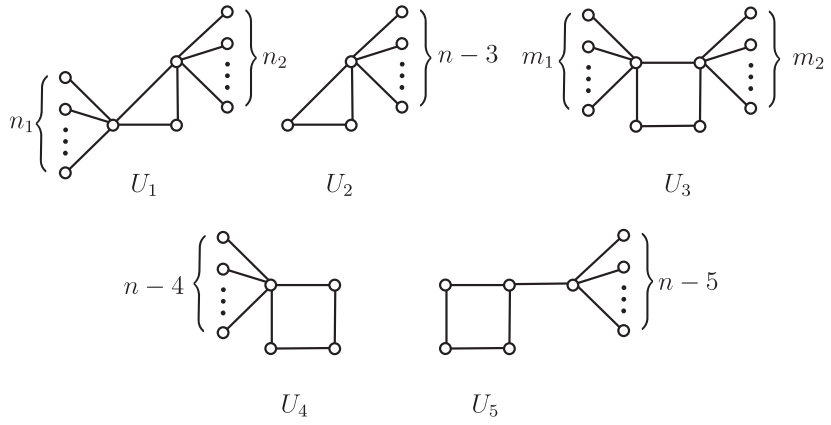

FIGURE 9

As already mentioned, for the cycle C_n, if $n \equiv 0 \pmod 4$, then $\eta(C_n) = 2$ and $\eta(C_n) = 0$, otherwise. Therefore, unicyclic graphs with maximum nullity must contain pendent vertices. On the other hand, the cycle C_4 is the only cycle which is also a complete bipartite graph and the cycle C_3 is the only cycle which is also

a complete tripartite graph. So, for the unicyclic graphs with maximum nullity we have:

Theorem 11. [34] *Let $U \in \mathcal{U}_n$ $(n \geqslant 5)$. Then $\eta(U) \leqslant n-4$ and the equality holds if and only if G is isomorphic to some of the graphs U_1, U_2, U_3, U_4 and U_5, depicted in Fig.* 9.

The nullity set of unicyclic graphs is also determined in [34].

Theorem 12. [34] *The nullity set of $\mathcal{U}_n$ $(n \geqslant 5)$ is $[0, n-4]$.*

In the set of bicyclic graphs, the graph $K_{2,3}$ is the only complete bipartite graph and the graph $K_4 - e$ is the only complete tripartite graph [21, 26]. Thus, the following results are proved.

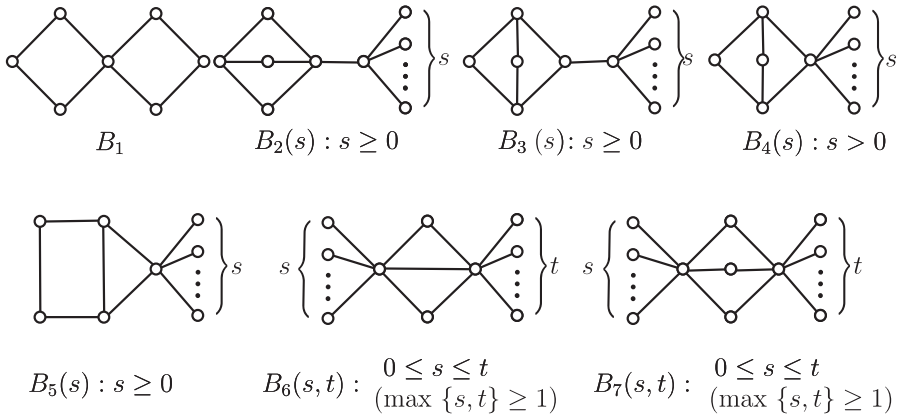

FIGURE 10

Theorem 13. [21, 26] *Let $B \in \mathcal{B}_n$. Then*

(i) *$\eta(B) = n-2$ if and only if $B \cong K_{2,3}$.*
(ii) *$\eta(B) = n-3$ if and only if $B \cong K_4 - e$.*
(iii) *If $B \in \mathcal{B}_n \setminus \{K_{2,3}, K_4 - e\}$, then $\eta(B) \leqslant n-4$ and the equality holds if and only if $B \cong B_i$ $(1 \leqslant i \leqslant 7)$* (Fig. 10)

Theorem 14. [21, 26] *The nullity set of $\mathcal{B}_n$ is $[0, n-2]$.*

From previous considerations it is clear that the problem of finding trees with maximum nullity is easily solved. In the sequel we are concerned with a related problem: namely, determining the greatest nullity among n-vertex trees in which no vertex has degree greater than a fixed value Δ [14].

Let Δ be a positive integer. Denote by $\mathcal{T}(n, \Delta)$ the set of all n-vertex trees in which all vertex degrees are less than or equal to Δ. Furthermore, let $\mathcal{T}(\Delta) = \bigcup_{n \geqslant 1} \mathcal{T}(n, \Delta)$.

For $\Delta = 1$ and $n \geqslant 3$, $\mathcal{T}(n, \Delta) = \emptyset$. For $\Delta = 2$ and $n \geqslant 3$, each set $\mathcal{T}(n, \Delta)$ consists of a single element (the n-vertex path P_n for which $\eta(P_n) \leqslant 1$). Therefore in what follows we assume that $\Delta \geqslant 3$.

Theorem 15. [14] *For all $n \geqslant 1$ and $\Delta \geqslant 3$, if $T \in \mathcal{T}(n, \Delta)$, then $\eta(T) \leqslant n - 2\lceil (n-1)/\Delta \rceil$. For all $n \geqslant 1$ and $\Delta \geqslant 3$ there exist trees $T \in \mathcal{T}(n, \Delta)$ such that $\eta(T) = n - 2\lceil (n-1)/\Delta \rceil$.*

Let $\mathcal{T}(n, \Delta, \max)$ be the set of trees from $\mathcal{T}(n, \Delta)$ with maximum nullity (equal to $n - 2\lceil (n-1)/\Delta \rceil$).

In [14] a method for constructing the trees in $\mathcal{T}(n, \Delta, max)$ was given, and it is conjectured that these trees are all of maximum nullity. Li and Chang [24] gave a counter-example, showing that there exist additional trees with maximum nullity. Furthermore, they slightly modified way in which the elements of $\mathcal{T}(n, \Delta, max)$ are constructed.

Before presenting the Li–Chang method, we need some preparation.

An edge belonging to a matching of a graph G is said to cover its two end vertices. A vertex is said to be perfectly covered (PC) if it is covered in all maximum matchings of G. Obviously, any vertex adjacent to a pendent vertex is a PC-vertex, and there is at most one vertex between any consecutive PC-vertices. However, there may exist PC-vertices that are not adjacent to pendent vertices.

A subset of $\mathcal{T}(n, \Delta, \max)$, denoted by $\mathcal{T}_1^*(n, \Delta, \max)$ is constructed as follows. For $n = 1, 2, \ldots, \Delta$, the unique element of $\mathcal{T}_1^*(n, \Delta, \max)$ is the n-vertex star. For $n = k\Delta + i$, $k \geqslant 1$, $i = 1, 2, \ldots, \Delta$, any tree in $\mathcal{T}_1^*(n, \Delta, \max)$ is obtained from tree $T' \in \mathcal{T}_1^*(n - \Delta, \Delta, \max) \cup \mathcal{T}_2^*(n - \Delta, \Delta, \max)$ and a copy of a Δ-vertex star, by joining one vertex of T' with degree less than Δ to the center of S_Δ, where $\mathcal{T}_2^*(n - \Delta, \Delta, \max)$ is obtained by moving (one-by-one) some pendent vertices of $T \in \mathcal{T}_1^*(n - \Delta, \Delta, \max)$ to some other PC-vertices, taking care that

(i) the vertex degrees do not exceed Δ, and that

(ii) in each step the vertex to which a pendent vertex is added is PC.

Theorem 16. [24] $\mathcal{T}(n, \Delta, \max) = \mathcal{T}_1^*(n, \Delta, \max) \cup \mathcal{T}_2^*(n, \Delta, \max)$.

A result analogous to Theorem 15 has recently been proved for bipartite graphs:

Theorem 17. [29] *Let G be a bipartite graph with $n \geqslant 1$ vertices, e edges and maximum vertex degree Δ. If G does not have as subgraph any cycle whose size is divisible by 4, then $\eta(G) \leqslant n - 2\lceil e/\Delta \rceil$.*

Finally, we mention another family of graphs where the nullity problem has been solved [20]. It is the class of line graphs of trees.

We first observe that the nullity of line graphs may assume any positive integer value. A trivial example for this is $L(pK_2)$, whose nullity is p (see Fig. 11).

If we restrict ourselves to connected graphs then the nullity of the line graph may still be any positive integer. For instance [20], for the graph G_r depicted in Fig. 12, $\eta(L(G_r)) = r + 1$.

With the line graphs of trees the situation is different:

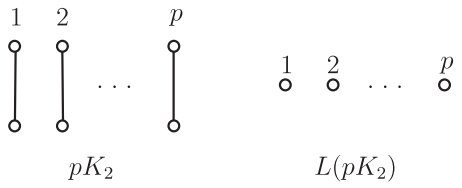

FIGURE 11

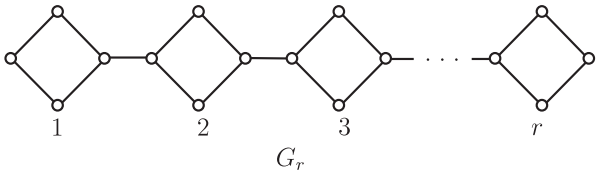

FIGURE 12

Theorem 18. [20] *If T is a tree, then $L(T)$ is either non-singular or has nullity one.*

Remark. It is easy to find examples of trees with $\eta(L(T)) = 0$ and with $\eta(L(T)) = 1$. For instance, $\eta(L(P_n)) = 0$ and $\eta(L(P_n)) = 1$ for, respectively, odd and even value of n.

More results on graphs whose nullity is one can be found in the papers [32, 33].

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THE ESTRADA INDEX

Abstract. If λ_i, $i = 1, 2, \ldots, n$, are the eigenvalues of the graph G, then the Estrada index EE of G is the sum of the terms e^{λ_i}. This graph invariant appeared for the first time in year 2000, in a paper by Ernesto Estrada, dealing with the folding of protein molecules. Since then a remarkable variety of other chemical and non-chemical applications of EE were communicated.

The mathematical studies of the Estrada index started only a few years ago. Until now a number of lower and upper bounds were obtained, and the problem of extremal EE for trees solved. Also, approximations and correlations for EE were put forward, valid for chemically interesting molecular graphs.

In this paper the relevant results on the Estrada index are surveyed.

Mathematics Subject Classification (2000): 05C50; 05C90; 92E10

Keywords: Estrada index; spectrum (of graph); chemistry

Contents

1. Introduction: the Estrada index and its various applications

Let G be a graph without loops and multiple edges. Let n and m be, respectively, the number of vertices and edges of G. Such a graph will be referred to as an (n, m)-graph.

The eigenvalues of the adjacency matrix of G are said to be [1] the eigenvalues of G and to form the spectrum of G. A graph of order n has n (not necessarily distinct, but necessarily real-valued) eigenvalues; we denote these by $\lambda_1, \lambda_2, \ldots, \lambda_n$, and assume to be labelled in a non-increasing manner: $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. The basic properties of graph eigenvalues can be found in the book [1].

A graph-spectrum-based invariant, recently put forward by Estrada is defined as

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}. \tag{1}$$

We proposed [2] to call it the *Estrada index*, a name that in the meantime has been commonly accepted.

Although invented in year 2000 [3], the Estrada index has already found a remarkable variety of applications. Initially it was used to quantify the degree of folding of long-chain molecules, especially proteins [3, 4, 5]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (this time of simple graphs, like those studied in the present paper) was put forward by Estrada and Rodríguez-Velázquez [6, 7]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc) networks; these ideas were recently further elaborated and extended [8]. In [9] a connection between EE and the concept of extended atomic branching was established, which was an attempt to apply EE in quantum chemistry. Another such application, this time in statistical thermodynamics, was proposed by Estrada and Hatano [10] and later further extended in [11]. Recently,

Carbó-Dorca [12] endeavored to find connections between EE and the Shannon entropy.

The proposed biochemical [3, 4, 5], physico–chemical [9, 10], network–theoretical [6, 7, 8], and infomation–theoretical [12] applications of the Estrada index are nowadays widely accepted and used by other members of the scientific community; see, for example [13–20]. In addition, this graph invariant is worth attention of mathematicians. Indeed, in the last few years quite a few mathematicians became interested in the Estrada index and communicated mathematical results on EE in mathematical journals. In what follows we briefly survey the most significant of these results.

2. Elementary properties of the Estrada index

Directly from the definition of the Estrada index, Eq. (1) we conclude the following [7, 21].

1° Denoting by $M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k$ the k-th spectral moment of the graph G, and bearing in mind the power–series expansion of e^x, we have

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \tag{2}$$

At this point one should recall [1] that $M_k(G)$ is equal to the number of self-returning walks of length k of the graph G. The first few spectral moments of an (n, m)-graph satisfy the following relations [1]:

$$M_0 = n; \quad M_1 = 0; \quad M_2 = 2m; \quad M_3 = 6t$$

where t is the number of triangles.

2° As a direct consequence of (2), for any graph G of order n, different from the complete graph K_n and from its (edgeless) complement $\bar{K}_n$,

$$EE(\bar{K}_n) < EE(G) < EE(K_n).$$

3° If G is a graph on n vertices, then $EE(G) \geqslant n$; equality holds if and only if $G \cong \bar{K}_n$ [22].

4° The eigenvalues of a bipartite graph satisfy the pairing property [1]: $\lambda_{n-i+1} = -\lambda_i$, $i = 1, 2, \ldots, n$. Therefore, if the graph G is bipartite, and if n_0 is nullity (= the multiplicity of its eigenvalue zero), then

$$EE(G) = n_0 + 2 \sum_{+} \cosh(\lambda_i) \tag{3}$$

where cosh stands for the hyperbolic cosine [$\cosh(x) = (e^x + e^{-x})/2$], whereas $\sum_+$ denotes summation over all positive eigenvalues of the corresponding graph.

5° If $\mathbf{A}(G)$ is the adjacency matrix of the graph G, then $EE(G) = \operatorname{tr} e^{\mathbf{A}(G)}$, with tr standing for the trace of the respective matrix.

3. Bounds for the Estrada index

Numerous lower and upper bounds for the Estrada index have been communicated. In what follows we first state the simplest and earliest such bounds (as Theorem 3.1), and provide them with complete proofs. The other bounds will only be stated, and their proofs skipped.

Theorem 3.1. [2] *Let G be an (n, m)-graph. Then the Estrada index of G is bounded as*

$$\sqrt{n^2 + 4m} \leqslant EE(G) \leqslant n - 1 + e^{\sqrt{2m}}. \tag{4}$$

Equality on both sides of (4) *is attained if and only if $G \cong \bar{K}_n$.*

Proof of the lower bound (4). From the definition of the Estrada index, Eq. (1), we get

$$EE^2 = \sum_{i=1}^{n} e^{2\lambda_i} + 2 \sum_{i<j} e^{\lambda_i}\, e^{\lambda_j}. \tag{5}$$

In view of the inequality between the arithmetic and geometric means,

$$\begin{aligned} 2 \sum_{i<j} e^{\lambda_i}\, e^{\lambda_j} &\geqslant n(n-1) \left(\prod_{i<j} e^{\lambda_i}\, e^{\lambda_j} \right)^{2/[n(n-1)]} \\ &= n(n-1) \left[\left(\prod_{i=1}^{n} e^{\lambda_i} \right)^{n-1} \right]^{2/[n(n-1)]} \\ &= n(n-1) \left(e^{M_1} \right)^{2/n} = n(n-1). \end{aligned} \tag{6}$$

By means of a power–series expansion, and bearing in mind the properties of M_0, M_1, and M_2, we get

$$\sum_{i=1}^{n} e^{2\lambda_i} = \sum_{i=1}^{n} \sum_{k \geqslant 0} \frac{(2\lambda_i)^k}{k!} = n + 4m + \sum_{i=1}^{n} \sum_{k \geqslant 3} \frac{(2\lambda_i)^k}{k!}. \tag{7}$$

Because we are aiming at an (as good as possible) lower bound, it may look plausible to replace $\sum_{k \geqslant 3} \frac{(2\lambda_i)^k}{k!}$ by $8 \sum_{k \geqslant 3} \frac{(\lambda_i)^k}{k!}$. However, instead of $8 = 2^3$ we shall use a multiplier $\gamma \in [0, 8]$, so as to arrive at:

$$\begin{aligned} \sum_{i=1}^{n} e^{2\lambda_i} &\geqslant n + 4m + \gamma \sum_{i=1}^{n} \sum_{k \geqslant 3} \frac{(\lambda_i)^k}{k!} \\ &= n + 4m - \gamma n - \gamma m + \gamma \sum_{i=1}^{n} \sum_{k \geqslant 0} \frac{(\lambda_i)^k}{k!} \end{aligned}$$

i.e.,

$$\sum_{i=1}^{n} e^{2\lambda_i} \geqslant (1 - \gamma)n + (4 - \gamma)m + \gamma EE. \tag{8}$$

By substituting (6) and (8) back into (5), and solving for EE we obtain

$$EE \geqslant \frac{\gamma}{2} + \sqrt{\left(n - \frac{\gamma}{2}\right)^2 + (4-\gamma)m}. \tag{9}$$

It is elementary to show that for $n \geqslant 2$ and $m \geqslant 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4-x)m}$$

monotonically decreases in the interval $[0, 8]$. Consequently, the best lower bound for EE is attained not for $\gamma = 8$, but for $\gamma = 0$.

Setting $\gamma = 0$ into (9) we arrive at the first half of Theorem 3.1.

Remark. If in Eq. (7) we utilize also the properties of the third spectral moment, we get

$$\sum_{i=1}^{n} e^{2\lambda_i} = n + 4m + 8t + \sum_{i=1}^{n} \sum_{k \geqslant 4} \frac{(2\lambda_i)^k}{k!}$$

which, in a fully analogous manner, results in

$$EE \geqslant \sqrt{n^2 + 4m + 8t}. \tag{10}$$

Proof of the upper bound (4). Starting with Eq. (2) we get

$$\begin{aligned} EE &= n + \sum_{i=1}^{n} \sum_{k \geqslant 1} \frac{(\lambda_i)^k}{k!} \leqslant n + \sum_{i=1}^{n} \sum_{k \geqslant 1} \frac{|\lambda_i|^k}{k!} \\ &= n + \sum_{k \geqslant 1} \frac{1}{k!} \sum_{i=1}^{n} \left[(\lambda_i)^2\right]^{k/2} \leqslant n + \sum_{k \geqslant 1} \frac{1}{k!} \left[\sum_{i=1}^{n} (\lambda_i)^2\right]^{k/2} \\ &= n + \sum_{k \geqslant 1} \frac{1}{k!} (2m)^{k/2} = n - 1 + \sum_{k \geqslant 0} \frac{(\sqrt{2m})^k}{k!} \end{aligned}$$

which directly leads to the right–hand side inequality in (4).

From the derivation of (4) it is evident that equality will be attained if and only if the graph G has no non-zero eigenvalues. This, in turn, happens only in the case of the edgeless graph $\bar{K}_n$ [1].

By this the proof of Theorem 3.1 is completed. □

Recently Zhou [23] arrived at the following generalizations of Theorem 3.1:

Theorem 3.2. [23] *If G is a graph on n vertices and k_0 is an integer, $k_0 \geqslant 2$, then*

$$EE(G) \geqslant \sqrt{n^2 + \sum_{k=2}^{k_0} \frac{2^k\, M_k(G)}{k!}} \tag{11}$$

with equality if and only if $G \cong \bar{K}_n$.

For $k_0 = 2$ and $k_0 = 3$, the right–hand side of (11) reduces to the lower bounds (4) and (10), respectively.

Theorem 3.3. [23] *Let G be an (n, m)-graph and k_0 same as in Theorem 3.2. Then*

$$EE(G) \leqslant n - 1 - \sqrt{2m} + e^{\sqrt{2m}} + \sum_{k=2}^{k_0} \frac{M_k - \left(\sqrt{2m}\right)^k}{k!}$$

with equality if and only if $G \cong \bar{K}_n$.

Note that for $k_0 = 2$, Theorem 3.3 yields $EE \leqslant n - 1 + e^{\sqrt{2m}} - \sqrt{2mm}$, which is better than the right-hand side of (4).

If graph parameters other than n and m are included into consideration, then further bounds for the Estrada index could be deduced.

Theorem 3.4. [23] *Let G be a graph on n vertices, and d_i, $i = 1, 2, \ldots, n$, the degrees of its vertices. Let $D = \sum_{i=1}^{n} (d_i)^2$. Then*

$$EE(G) \geqslant e^{\sqrt{D/n}} + (n-1)\, e^{-\frac{1}{n-1}\sqrt{D/n}}$$

with equality if and only if either $G \cong K_n$ or $G \cong \bar{K}_n$.

Theorem 3.5. [23] *Let λ_1 be the greatest eigenvalue of an (n, m)-graph G. Let k_0 be the same as in Theorems* 3.2 *and* 3.3. *Then*

$$EE(G) \leqslant n - 2 - \lambda_1 - \sqrt{2m - (\lambda_1)^2} + e^{\sqrt{2m-(\lambda_1)^2}} + \sum_{k=2}^{k_0} \frac{M_k - (\lambda_1)^k - \left(\sqrt{2m - (\lambda_1)^2}\right)^k}{k!}$$

with equality if and only if $G \cong \bar{K}_n$.

The special cases of Theorem 3.5 for $k_0 = 2$ and $k_0 = 3$ read:

$$EE \leqslant n - 2 - \lambda_1 - \sqrt{2m - (\lambda_1)^2} + e^{\lambda_1} + e^{\sqrt{2m-(\lambda_1)^2}} \quad \text{and}$$

$$EE \leqslant n - 2 - \lambda_1 - \sqrt{2m - (\lambda_1)^2} + e^{\lambda_1} + e^{\sqrt{2m-(\lambda_1)^2}} + t - \frac{(\lambda_1)^3}{6} - \frac{\left(\sqrt{2m - (\lambda_1)^2}\right)^3}{6}$$

respectively.

Theorem 3.6. [24] *If G is an (n, m)-graph either without isolated vertices or having the property $2m/n \geqslant 1$, then $EE(G) \geqslant n \cosh\left(\sqrt{2m/n}\right)$ with equality if and only if G is a regular graph of degree* 1.

Recall that $2m/n$ is equal to the average vertex degree. Thus, if G is connected, then necessarily $2m/n \geqslant 1$, and the 2-vertex complete graph (K_2) is the only graph for which equality holds.

Theorem 3.7. [24] *If G is an (n, m)-graph, such that $2m/n < 1$, then*

$$EE(G) \geqslant n - 2m + 2m\cosh(1).$$

Equality holds if and only if G consists of $n - 2m$ isolated vertices and m copies of K_2.

Theorem 3.8. [24, 25] *If G is an (n, m)-graph with at least one edge, and if n_0 is its nullity, then*

$$EE(G) \geqslant n_0 + (n - n_0)\cosh\left(\sqrt{\frac{2m}{n - n_0}}\right).$$

Equality holds if and only if $n - n_0$ is even, and if G consists of copies of complete bipartite graphs K_{r_i,s_i}, $i = 1, \ldots, (n - n_0)/2$, such that all products $r_i \cdot s_i$ are mutually equal.

Theorem 3.8 should be compared with inequality (3). It was first proven for bipartite graphs [25] and eventually extended to all graphs. The same result was later communicated also in [23].

If the graph G is regular of degree r, then its greatest eigenvalue is equal to r. If, in addition, G is bipartite, then its smallest eigenvalue is equal to $-r$ [1]. Bearing these facts in mind, some of the above bounds could have been simplified [2]:

Theorem 3.9. [2] *Let G be a regular graph of degree r and of order n. Then*

$$e^r + \sqrt{n + 2nr - (2r^2 + 2r + 1) + (n - 1)(n - 2)\, e^{-2r/(n-1)}} \leqslant EE(G) \leqslant n - 2 + e^r + e^{\sqrt{r(n-r)}}.$$

The lower bound is improved by including into the consideration also the third spectral moment:

$$EE(G) \geqslant e^r + \sqrt{n + 2nr - (2r^2 + 2r + 1) + (n - 1)(n - 2)\, e^{-2r/(n-1)} - \tfrac{4}{3}\,(r^3 - 6t)}.$$

Theorem 3.10. [2] *Let G be a bipartite regular graph of degree r and of order n. Then*

$$2\cosh(r) + \sqrt{(n - 2)^2 + 2nr - 4\,r^2} \leqslant EE(G) \leqslant n - 4 + 2\cosh(r) + 2\cosh\left(\sqrt{nr/2 - r^2}\right).$$

4. Estrada indices of some graphs

For graphs whose spectra are known [1], by Eq. (1) one gets explicit expressions for their Estrada index. In particular:

$$EE(K_n) = e^{n-1} + (n - 1)\, e^{-1}$$

$$EE(K_{a,n}) = a + b - 2 + 2\cosh\left(\sqrt{ab}\right).$$

If S_n is the n-vertex star, then $EE(S_n) = n - 2 + 2\cosh\left(\sqrt{n - 1}\right)$. If Q_n is the hypercube on 2^n vertices, then $EE(Q_n) = [2\cosh(1)]^n$ [22].

The $(n+1)$-vertex wheel W_{n+1} is obtained by joining a new vertex to each vertex of the n-vertex cycle C_n. Then $EE(W_{n+1}) = EE(C_n) - e^2 + 2e\cosh\left(\sqrt{n-1}\right)$ [22].

The Estrada index of the cycle C_n can be approximated as $EE(C_n) \approx n\, I_0$, [26] where

$$I_0 = \frac{1}{\pi}\int_0^{\pi} e^{2\cos x}\, dx = \sum_{k=0}^{\infty} \frac{1}{(k!)^2} = 2.27958530\cdots .$$

In an analogous manner [26, 27]

$$EE(P_n) \approx (n+1)\, I_0 - \cosh(2)$$
$$EE(Z_n) \approx (n+2)\, I_0$$
$$EE(ZZ_n) \approx (n+1)\, I_0 + 2 + \cosh(2)$$

where P_n is the n-vertex path, Z_n is the $(n+2)$-vertex tree obtained by attaching two pendent vertices to a terminal vertex of P_n, whereas ZZ_n is the $(n+4)$-vertex tree obtained by attaching two pendent vertices to each of the two terminal vertices of P_n.

For positive integers n and m, the tree $P_{n,m}$ on $(m+1)n$ vertices is obtained by attaching m pendent vertices to each vertex of P_n. Then [27]

$$EE(P_{n,m}) \approx (m-1)n + 2(n+1)\, J_m$$

where

$$J_m = \frac{1}{\pi}\int_0^{\pi} e^{\cos x}\, \cosh\left(\sqrt{m+\cos^2 x}\,\right)\, dx.$$

Approximations for the Estrada index of Bethe and double-Bethe trees were reported in [28]. Expressions and approximate expressions for EE of several other graphs can be found in [22].

In [29] the following approximate expression for the Estrada index of an (n, m)-graph was deduced using a Monte Carlo technique:

$$n\left(\sqrt{6m/n}\right)^{-1} \sinh\left(\sqrt{6m/n}\right)$$

where sinh stands for the hyperbolic sine [$\sinh(x) = (e^x - e^{-x})/2$]. In [29] also some more complicated approximations for EE of (n, m)-graphs were proposed.

4.1. Estrada index of line graphs.

Theorem 4.1. [30] *If G is an r-regular graph with n vertices and $m = rn/2$ edges, and $L(G)$ is its line graph, then $EE(L(G)) = e^{r-2}EE(G) + (m-n)e^{-2}$.*

By Theorem 4.1, if G is a connected r-regular graph, then $EE(L(G)) = EE(G)$ holds if and only if $r = 1, 2$, i.e., if and only if either $G \cong K_2$ or $G \cong C_n$ [22]. To see this, suppose that $EE(L(G)) = EE(G)$ and $r \geqslant 3$. Then $m > n$ and $EE(G) = (n-m)/[e^2\,(e^{r-2}-1)]$. This would imply that $EE(G) < 0$, a contradiction.

The k-th iterated line graph $L^k(G)$ of a graph G is defined recursively by $L^k(G) = L(L^{k-1}(G))$ where $L^0(G) \equiv G$ and $L^1(G) \equiv L(G)$.

Theorem 4.2. [30] *If G is an r-regular graph with n vertices, and $k \geqslant 1$, then*

$$EE(L^k(G)) = a_k(r)\, EE(G) + b_k(r)\, n$$

where $a_k(r)$ and $b_k(r)$ are functions depending solely on the variable r and parameter k.

In [30] it was shown that $a_k(r) = e^{(r-2)(2^k-1)}$, which implies $a_k(r) = O\big(e^{(r-2)2^k}\big)$. An explicit expression for $b_k(r)$ could not be determined, but it was established [30] that $b_k(r)$ has the same asymptotic behavior as $a_k(r)$, viz., $b_k(r) = O\big(e^{(r-2)2^k}\big)$.

4.2. Estrada index of some graph products.

Let G and H be two graphs with disjoint vertex sets. The join $G+H$ of G and H is the graph obtained by connecting all vertices of G with all vertices of H. If $G_1, G_2, \ldots, G_n$ are graphs with mutually disjoint vertex sets, then we denote $G_1 + G_2 + \cdots + G_n$ by $\sum_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\sum_{i=1}^{n} G_i$ by $n\,G$.

Theorem 4.3. [22] *Let G and H be r- and s-regular graphs with p and q vertices, respectively. Then*

$$EE(G+H) = EE(G) + EE(H) - (e^r + e^s) + 2e^{(r+s)/2} \cosh\left(\tfrac{1}{2}\sqrt{(r-s)^2 + 4pq}\right).$$

Corollary 4.4. [22] *If G is an r-regular n-vertex graph then*

$$EE(2G) = 2EE(G) - 2e^r + 2e^r \cosh(n)$$

$$EE(3G) = 3EE(G) - 3e^r + 2e^r \cosh(n) + 2e^{(2r+n)/2} \cosh(3n/2) - e^{r+n}.$$

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If $G_1, G_2, \ldots, G_n$ are graphs with mutually disjoint vertex sets, then we denote $G_1 \times G_2 \times \cdots \times G_n$ by $\prod_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\prod_{i=1}^{n} G_i$ by G^n.

Theorem 4.5. [22] $EE(G \times H) = EE(G)\, EE(H)$. *More generally,*

$$EE\left(\prod_{i=1}^{r} G_i\right) = \prod_{i=1}^{r} EE(G_i).$$

In particular, $EE(G^r) = EE(G)^r$.

5. Graphs with extremal Estrada indices

In [2] de la Peña, Gutman and Rada put forward two conjectures:

Conjecture A. Among n-vertex trees, the path P_n has the minimum and the star S_n the maximum Estrada index, i.e., $EE(P_n) < EE(T_n) < EE(S_n)$, where T_n is any n-vertex tree different from S_n and P_n.

Conjecture B. Among connected graphs of order n, the path P_n has the minimum Estrada index.

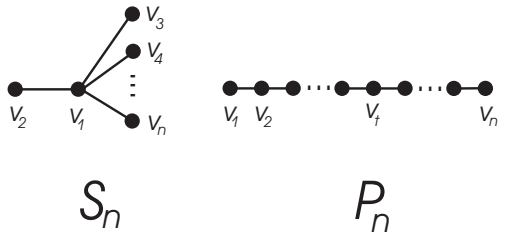

FIGURE 1. The star S_n and the path P_n, and the labelling of their vertices.

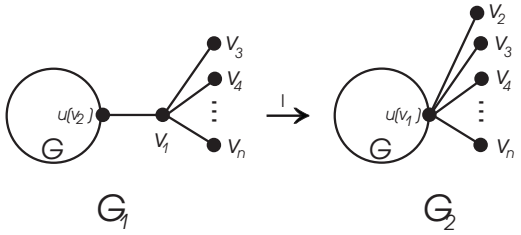

FIGURE 2. Transformation I.

In what follows we first state some transformations of graphs and establish the respective change in the spectral moments, and then provide a complete proof of these conjectures.

Lemma 5.1. [31] *Let S_n be the n-vertex star with vertices $v_1, v_2, \ldots, v_n$, and center v_1, as shown in Figure* 1. *Then there is an injection ξ_1 from $W_{2k}(v_2)$ to $W_{2k}(v_1)$, and ξ_1 is not surjective for $n \geqslant 3$ and $k \geqslant 1$, where $W_{2k}(v_1)$ and $W_{2k}(v_2)$ are the sets of self-returning walks of length $2k$ of v_1 and v_2 in S_n, respectively.*

Proof. Let $\xi_1 : W_{2k}(v_2) \to W_{2k}(v_1)$, $\forall w \in W_{2k}(v_2)$, if $w = v_2 v_1 v_{i_1} \ldots v_{i_{2k-3}} v_1 v_2$, then $\xi_1(w) = v_1 v_2 v_1 v_{i_1} \ldots v_{i_{2k-3}} v_1$.

Obviously, ξ_1 is injective. However, there is no $w \in W_{2k}(v_2)$ such that

$$\xi_1(w) = v_1 v_3 v_1 v_3 v_1 \ldots v_3 v_1 \in W_{2k}(v_1)$$

and ξ_1 is not surjective for $n \geqslant 3$ and $k \geqslant 1$. □

Lemma 5.2. [31] *Consider the Transformation I shown in Figure* 2. *Let u be a non-isolated vertex of a simple graph G. Let G_1 and G_2 be the graphs obtained from G by, respectively, identifying a leaf v_2 and the center v_1 of the n-vertex star S_n with the vertex u, cf. Figure* 2. *Then $M_{2k}(G_1) < M_{2k}(G_2)$ for $n \geqslant 3$ and $k \geqslant 2$.*

Proof. Let $W_{2k}(G)$ denote the set of self-returning walks of length $2k$ of G. Then $W_{2k}(G_i) = W_{2k}(G) \cup W_{2k}(S_n) \cup A_i$ is a partition, where A_i is the set of self-returning walks of length $2k$ of G_i, each of them containing both at least one edge in $E(G)$ and at least one edge in $E(S_n)$, $i = 1, 2$. So, $M_{2k}(G_i) = |W_{2k}(G)| + |W_{2k}(S_n)| + |A_i| = M_{2k}(G) + M_{2k}(S_n) + |A_i|$. Obviously, it is enough to show that $|A_1| < |A_2|$.

Let $\eta_1 : A_1 \to A_2$, $\forall w \in A_1$, $\eta_1(w) = (w - w \cap S_n) \cup \xi_1(w \cap S_n)$, i.e., $\eta_1(w)$ is the self-returning walk of length $2k$ in A_2 obtained from w by replacing its every maximal (v_2, v_2)-section in S_n (which is a self-returning walk of v_2 in S_n) with its image under the map ξ_1.

By Lemma 5.1, ξ_1 is injective. It is easily shown that η_1 is also injective. However, there is no $w \in A_1$ such that $\eta_1(w) \in A_2$ and $\eta_1(w)$ does not pass the edge v_1v_2 in G_2. So, η_1 is not surjective. Consequently, $|A_1| < |A_2|$ and $M_{2k}(G_1) < M_{2k}(G_2)$. □

Lemma 5.3. [31] *Let $P_n = v_1v_2 \dots v_n$ be the n-vertex path, depicted in Figure 1. Then there is an injection ξ_2 from $W'_{2k}(v_1)$ to $W'_{2k}(v_t)$, and ξ_2 is not a surjection for $n \geqslant 3$, $1 < t < n$ and $k \geqslant 1$, where $W'_{2k}(v_1)$ and $W'_{2k}(v_t)$ are the sets of self-returning walks of length $2k$ of v_1 and v_t in P_n, respectively.*

Proof. First, let $f : \{v_1, v_2, \dots, v_t\} \to \{v_1, v_2, \dots, v_t\}$, $f(v_i) = v_{t-i+1}$ for $i = 1, 2, \dots, t$. Then we can induce a bijection by f from the set of self-returning walks of length $2k$ of v_1 in the sub-path $P_t = v_1v_2 \dots v_t$ and the set of self-returning walks of length $2k$ of v_t in P_t.

Secondly, let $\xi_2 : W'_{2k}(v_1) \to W'_{2k}(v_t)$, $\forall w \in W'_{2k}(v_1)$.

(i) If w is a walk of $P_t = v_1v_2 \dots v_t$, i.e., w does not pass the edge v_tv_{t+1}, then $\xi_2(w) = f(w)$.

(ii) If w passes the edge v_tv_{t+1}, we can decompose w into $w = w_1 \cup w_2 \cup w_3$, where w_1 is the first (v_1, v_t)-section of w, w_3 is the last (v_t, v_1)-section of w, and the rest w_2 is the internal maximal (v_t, v_t)-section of w, i.e., w is a self-returning walk of v_1, first passing the walk w_1 from v_1 to v_t, next passing the walk w_2 from v_t to v_t, and last passing the walk w_3 from v_t to v_1; then $\xi_2(w) = w_1^{-1} \cup w_3^{-1} \cup w_2$, that is, $\xi_2(w)$ is a self-returning walk v_t, first passing the reverse of w_1 from v_t to v_1, next passing the reverse of w_3 from v_1 to v_t, and last passing the walk w_2 from v_t to v_t.

Obviously, ξ_2 is injective. And ξ_2 is not surjective since there is no $w \in W'_{2k}(v_1)$ such that $\xi_2(w)$ is a self-returning walk not passing the edge v_tv_{t-1} in P_n of length $2k$ of v_t. □

Lemma 5.4. [31] *Let u be a non-isolated vertex of a simple graph H. If H_1 and H_2 are the graphs obtained from H by identifying, respectively, an end vertex v_1 and an internal vertex v_t of the n-vertex path P_n to u, cf. Figure 3, then $M_{2k}(H_1) < M_{2k}(H_2)$ for $n \geqslant 3$ and $k \geqslant 2$.*

Proof. Let B_i be the set of self-returning walks of length $2k$ of H_i, each of them containing both at least one edge in $E(H)$ and at least one edge in $E(P_n)$, $i = 1, 2$. Similarly to the proof of Lemma 5.2, it is enough to show that $|B_1| < |B_2|$.

Let $\eta_2 : B_1 \to B_2$, $\forall w \in B_1$, $\eta_2(w) = (w - w \cap P_n) \cup \xi_2(w \cap P_n)$, i.e., $\eta_2(w)$ is the self-returning walk of length $2k$ in B_2 obtained from w by replacing its every section in P_n (which is a self-returning walk of v_1 in P_n) with its image under the map ξ_2.

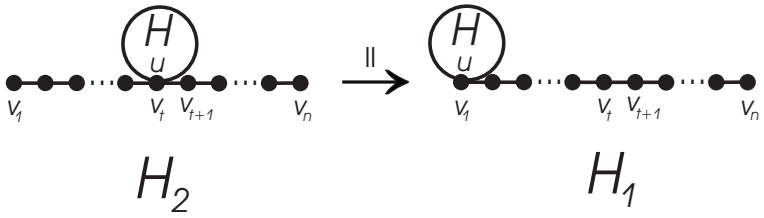

FIGURE 3. Transformation II.

By Lemma 5.3, ξ_2 is injective. It follows that η_2 is also injective. But, η_2 is not surjective since there is no $w \in B_1$ with $\eta_2(w) \in B_2$ not passing the edges $v_t v_{t-1}$ in H_2. So, $|B_1| < |B_2|$. □

Theorem 5.5. [31] *If T_n is a n-vertex tree different from S_n and P_n, then*

$$EE(P_n) < EE(T_n) < EE(S_n). \tag{12}$$

Proof. Repeating Transformation I, as shown in Figure 2, any n-vertex tree T can be changed into the n-vertex star S_n. By Lemma 5.2, we have $M_{2k}(T) < M_{2k}(S_n)$ for $k \geqslant 2$. This implies

$$EE(T) = \sum_{k\geqslant 0} \frac{M_{2k}(T)}{(2k)!} < \sum_{k\geqslant 0} \frac{M_{2k}(S_n)}{(2k)!} = EE(S_n).$$

On the other hand, repeating Transformation II, as shown in Figure 3, any n-vertex tree T can be changed into the n-vertex path P_n. By Lemma 5.4, we have $M_{2k}(T) > M_{2k}(P_n)$ for $k \geqslant 2$. Consequently,

$$EE(T) = \sum_{k\geqslant 0} \frac{M_{2k}(T)}{(2k)!} > \sum_{k\geqslant 0} \frac{M_{2k}(P_n)}{(2k)!} = EE(P_n).$$

So the inequalities (12) hold. □

Theorem 5.5 shows that the path P_n and the star S_n have the minimum and the maximum Estrada indices among n-vertex trees, i.e., Conjecture A is true.

Zhao and Jia [32] have determined also the trees with the second and the third greatest Estrada index. In fact, they proved:

Theorem 5.6. [32] *Let $S_n^1 \cong S_n$ be the n-vertex star, cf. Figure 1, and let the n-vertex trees S_n^i, $i = 2, 3, 4, 5, 6$, be those shown in Figure 4. Let T_1 and T_2 be n-vertex trees, such that $T_1 \notin \{S_n^i \mid i = 1, 2, 3, 4, 5, 6\}$ and $T_2 \notin \{S_n^i \mid i = 1, 2, 3\}$. Then for $n \geqslant 6$,*

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(S_n^5) > EE(S_n^6) > EE(T_1)$$

and

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(T_2).$$

Consequently, among n-vertex trees, the first three trees with the greatest Estrada indices are S_n, S_n^2 and S_n^3, respectively.

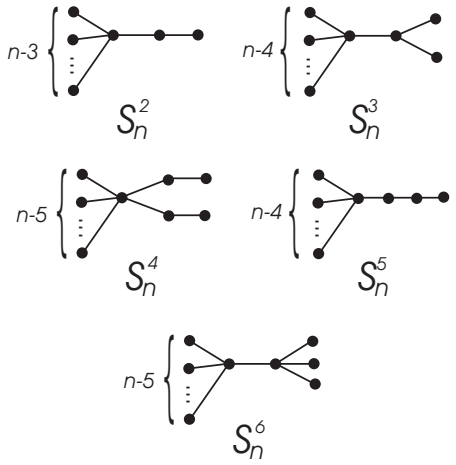

FIGURE 4. The graphs S_n^i, $i = 2, 3, 4, 5, 6$, having the second, third, fourth, fifth, and sixth greatest Estrada indices among n-vertex trees [32, 33].

Recently it was demonstrated [33] that $EE(S_n^3) > EE(S_n^4) > EE(S_n^5)$, from which follows:

Theorem 5.7. [33] *Among n-vertex trees, $n \geqslant 6$, the first six trees with the greatest Estrada indices are S_n, S_n^2, S_n^3, S_n^4, S_n^5, S_n^6, respectively, cf. Figure* 4.

Let G be a connected graph of order n and let e be an edge of G. The graph $G' = G - e$ is obtained from G by deleting the edge e. Obviously, any self-returning walk of length k of G' is also a self-returning walk of length k of G. Thus,

$$M_k(G') \leqslant M_k(G) \quad \text{and} \quad EE(G') \leqslant EE(G).$$

In particular, if T is a spanning tree of G, then

$$M_k(T) \leqslant M_k(G) \quad \text{and} \quad EE(T) \leqslant EE(G).$$

From Theorem 5.5 it follows that $EE(P_n) \leqslant EE(G)$. So, we have:

Theorem 5.8. [31] *If G is a simple connected graph of order n different from the complete graph K_n and the path P_n, then*

$$EE(P_n) < EE(G) < EE(K_n).$$

Theorem 5.7 shows that the path P_n and the complete graph K_n have the minimum and the maximum Estrada indices among connected graphs of order n, i.e., Conjecture B is true.

6. Estrada indices of molecular graphs

In view of the chemical origin of the Estrada index, it is natural than molecular graphs [34], especially acyclic and benzenoid, were among the first whose structure–dependence was systematically examined.

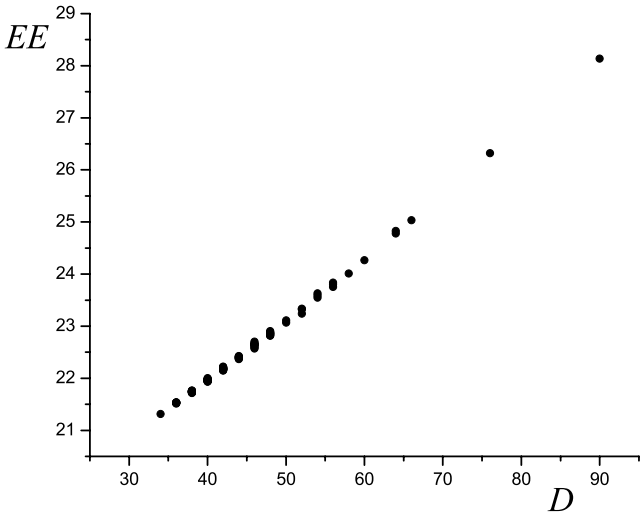

FIGURE 5. Correlation between the Estrada indices and the parameter D (= sum of squares of vertex degrees) for the 106 trees on 10 vertices.

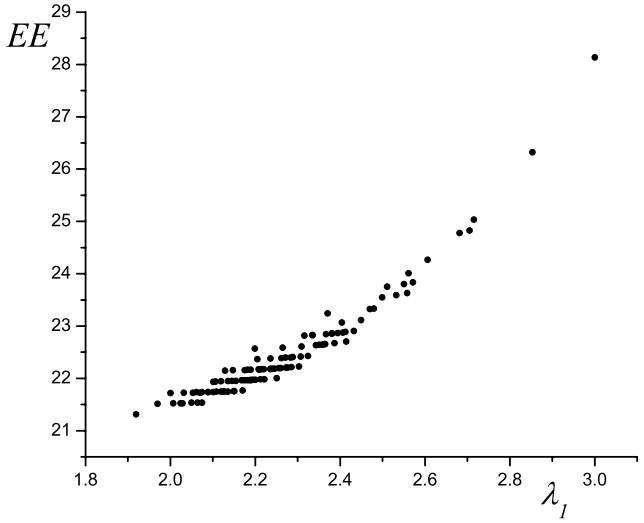

FIGURE 6. Correlation between the Estrada index (EE) and the greatest graph eigenvalue λ_1 for the 106 trees on 10 vertices.

A chemical tree is a tree in which no vertex has degree greater than four [34]. Among the n-vertex chemical trees, P_n has minimum Estrada index. For the

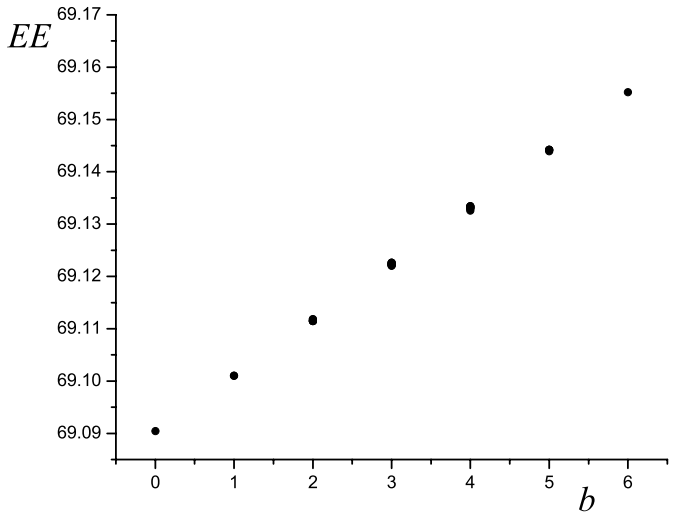

FIGURE 7. Correlation between the Estrada indices (EE) of the 36 catacondensed benzenoid systems with 6 hexagons and the number b of their bay regions.

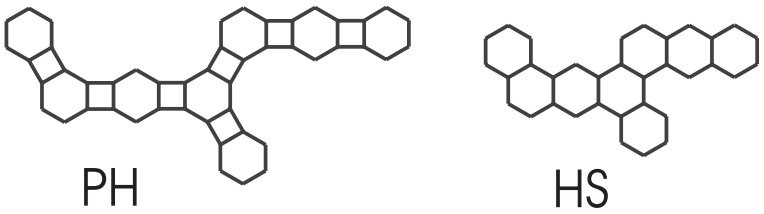

FIGURE 8. A phenylene (PH) and its hexagonal squeeze (HS).

Estrada index of chemical trees it was concluded [35] that the n-vertex chemical tree with the greatest Estrada index might be the Volkmann tree $VT_n(4)$. However, this assertion cannot be considered as proven in a rigorous mathematical manner. Such a proof awaits to be achieved in the future.

In the case of trees with a fixed number of vertices (including both chemical and non-chemical trees) it was found that EE increases with the increasing extent of branching [36]. This fact motivated investigations of the relation between EE and other branching indices. It was established that there is a linear correlation between EE and the quantity $D = \sum_{i=1}^{n} (d_i)^2$, earlier encountered in Theorem 3.4, see Figure 5.

The quantitative analysis of these correlations resulted in the following approximate expression:

$$EE \approx 1.735\, n - 0.13 + 0.11\, D.$$

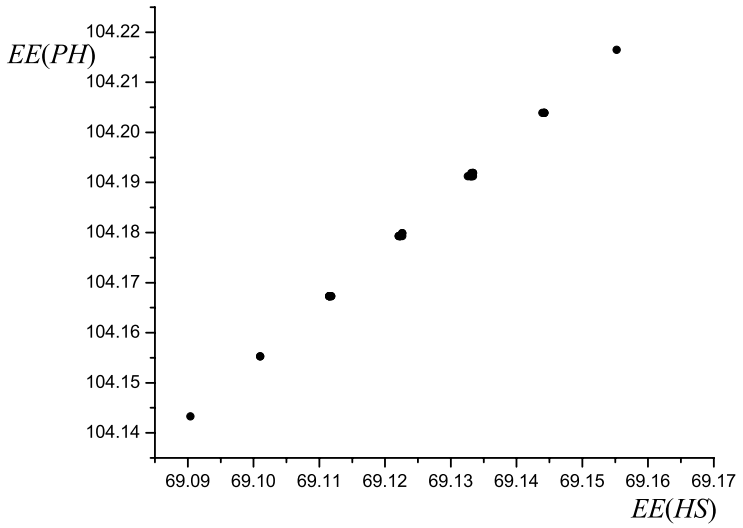

FIGURE 9. Correlation between the Estrada indices of phenylenes, $EE(PH)$, and the Estrada indices of the corresponding hexagonal squeezes, $EE(HS)$. The data points shown in this figure pertain to phenylenes with 6 hexagons; there are 37 species of this kind.

This formula is capable of reproducing EE with an error less than 0.1%.

The Estrada index of trees was also correlated with the greatest graph eigenvalue [35, 37]; a characteristic example of such correlations is shown in Figure 6. One can see that the EE/λ_1 relation is not simple. The fact that the (EE, λ_1) data points are grouped on several (almost) horizontal lines indicates that EE is much less sensitive to structural features than λ_1.

Empirical studies revealed that the number of vertices n and number of edges m are the main factors influencing EE-value of molecular graphs [29, 36, 38]. For benzenoid systems, (m, n)-type approximations are capable of reproducing over 99.8% of EE-value [29, 38]. In order to find some finer structural details on which EE depends, series of isomeric benzenoid systems (having equal n and m) were examined. The Estrada indices of benzenoid isomers vary only to a very limited extent. The main structural feature influencing these variations is the number of bay regions, b. (The quantity b is equal to the number of edges on the boundary of a benzenoid graph, connecting two vertices of degree 3; for details see [39].) Within sets of benzenoid isomers, EE is an increasing linear function of b, see Figure 7.

Phenylenes are molecular graphs consisting of hexagons and squares, joined in a manner that should be evident from the example depicted in Figure 8. To each phenylene a so-called "hexagonal squeeze" can be associated, containing only hexagons, cf. Figure 8.

The Estrada index of phenylenes was studied in [40]. Within sets of isomers (having equal number of hexagons) a good linear correlation exists between the Estrada index of phenylenes, $EE(PH)$ and of the corresponding hexagonal squeezes, $EE(HS)$, see Figure 9. Bearing in mind that the hexagonal squeezes are benzenoid systems, and that the structure-dependence of EE of benzenoids is almost completely understood, the good linear correlation between $EE(PH)$ and $EE(HS)$ resolves also the problem of structure–dependence of the Estrada index of phenylenes.

Concluding this section we wish to clearly emphasize that the relations established for molecular graphs, in particular those illustrated in Figures 5, 6, 7, and 9, are empirical findings that have not (yet) been proven in a rigorous mathematical manner. It should be a challenge for the reader of this article to accomplish the needed proofs.

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