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SELECTED TOPICS ON APPLICATIONS OF GRAPH SPECTRA

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PREFACE

The volume 13(21) of the *Collection of Papers* (*Zbornik radova*) with the title *Applications of Graph Spectra* appeared in 2009 and was soon out of print. We proposed to the Mathematical Institute of the Serbian Academy of Sciences and Arts to publish a second edition, but the Editorial Board decided to publish a new volume on the same subject with a similar title and with the same guest editors. We have chosen the title **Selected Topics on Applications of Graph Spectra** for the new volume.

The purpose of this volume and of the previous volume is to draw the attention of the mathematical community to the 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 part of the Preface to volume 13(21) is reproduced below.

The new volume contains improved, modified, and extended versions of all chapters from volume 13(21) as well as the following two new chapters:

Spectral Techniques in Complex Networks (S. Gago),
Applications of Graph Spectra in Quantum Physics (D. Stevanović).

The old chapters have been technically improved including the correction of noticed typos and other mistakes. In addition the following changes have been made.

Applications of Graph Spectra: An Introduction to the Literature (D. Cvetković). Some new references have been added and the presentation of some parts is improved.

Multiprocessor Interconnection Networks (D. Cvetković, T. Davidović). New proofs of main theorems are given and the data for some interesting multiprocessor interconnection networks are better presented.

Hyperenergetic and Hypoenergetic Graphs (I. Gutman). This is a new text, with a slight overlap to the chapter *Selected Topics from the Theory of Graph Energy: Hypoenergetic Graphs*, (S. Majstorović, A. Klobučar, I. Gutman), that appeared in volume 13(21).

Nullity Of Graphs: An Updated Survey (I. Gutman, B. Borovićanin). The chapter *Nullity of Graphs*, (I. Gutman, B. Borovićanin), is extended by surveying a number of recently published results, and by updating the bibliography.

The Estrada Index: An Updated Survey (I. Gutman, H. Deng, S. Radenković). The chapter *The Estrada Index*, (H. Deng, S. Radenković, I. Gutman), is extended by surveying a number of recently published results, and by updating the bibliography.

For some more information on these Chapters see Preface to volume 13(21).

The new chapter by S. Gago is about networks with a great number of vertices called *complex networks*. Most physical, biological, chemical, technological, and social systems have a network structure. Examples of complex networks range

from cell biology to epidemiology or to the Internet. The rich information about the topological structure and diffusion processes can be extracted from the spectral analysis of the corresponding networks.

The new chapter by D. Stevanović explains that graph spectra are closely related to many applications in quantum physics: a network of quantum particles with fixed couplings can be modelled by an underlying graph, the Hamiltonian of such system can be approximated either by the adjacency or the Laplacian matrix of that graph, and then quite a few problems can be posed in terms of the eigenvalues of the graph. One particular problem of interest to quantum physicists is addressed: the existence of *perfect state transfer in networks of spin* $-1/2$ *particles*.

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Belgrade and Kragujevac, 2010

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FROM PREFACE TO VOLUME 13(21)

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.

Manuscripts have been submitted in January 2009 and revised in April 2009.

Belgrade and Kragujevac, 2009

Guest Editors:
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Contents

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 (2010): 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).

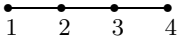
The *adjacency matrix* A is used to represent the adjacency relation, and so the graph G itself. The element a_{ij} of the adjacency matrix A is equal to 1 if vertices i and j are adjacent, and 0 otherwise.

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 $S_5=K_{1,4}$.

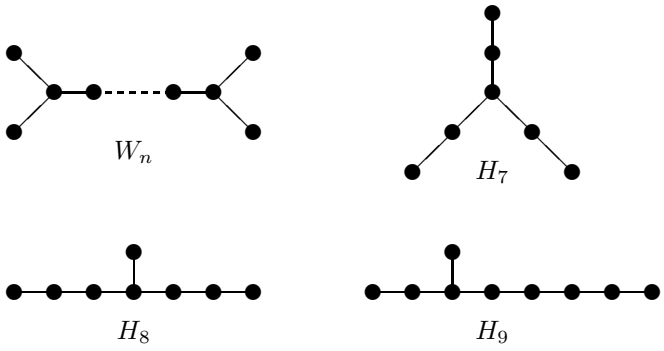


FIGURE 2. Some Smith graphs

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.

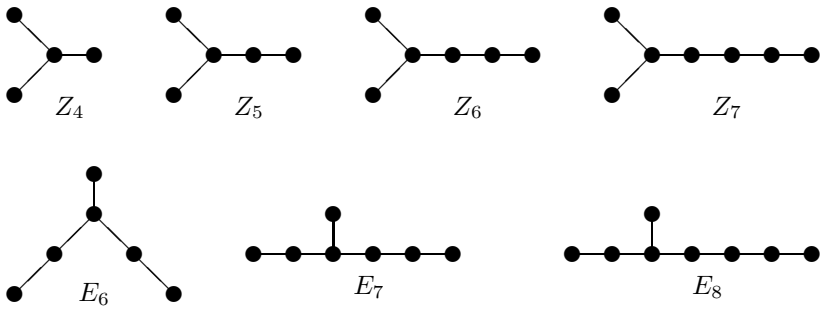


FIGURE 3. Subgraphs of some Smith graphs

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.

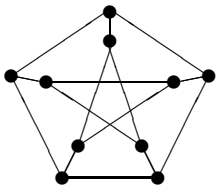


FIGURE 4. The Petersen graph

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 "Selected Topics from the Theory of 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.

See also Chapter *Applications of Graph Spectra in Quantum Physics*.

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 and Chapter *Spectral Techniques in Complex Networks* for applications on Internet).

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 [CvSi1] 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].

Additional information on applications of graph spectra to Computer Science can be found in [CvSi2]. These applications are classified there in the following way:

1. Expanders and combinatorial optimization,
2. Complex networks and the Internet,
3. Data mining,
4. Computer vision and pattern recognition,
5. Internet search,
6. Load balancing and multiprocessor interconnection networks,
7. Anti-virus protection versus spread of knowledge,
8. Statistical databases and social networks,
9. Quantum computing.

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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4.2. Physics. This section contains a list of papers published in scientific journals in the area of Physics in the period 2003–2007 which cite books and papers on graph spectra.

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 (2010): 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 [20] are (undirected, connected) graphs [31, 33]. 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, 35], 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 [14] has been recognized [19]. The general idea of using graph eigenvalues in multiprocessor interconnection networks can be also found in [30]. The main conclusion of [19] 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. 13), known to be a very good interconnection network (see, for example, [37]), 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, [19] 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 [19] 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 [5, 9]).

See references [17, 18, 23, 26, 27] 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 [19] related to the design of multiprocessor topologies. The main conclusion of [19] 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 [19]. 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 [14] 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 [11] for the application in chemical context and [10] 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 [12].

According to the well-known inequality $d_{\min} \leqslant \bar{d} \leqslant \lambda_1 \leqslant d_{\max} = \Delta$, [14, 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 [14]). 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 [14, 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 graphs $\mathrm{spt}(G)$ 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.

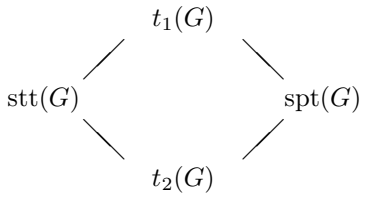

FIGURE 2. Partial order relation between different types of graph tightness

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 [19] 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 labeled 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. □

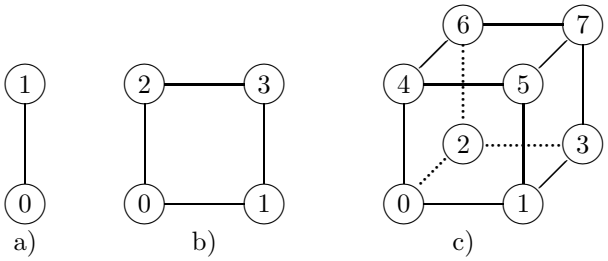

FIGURE 3. The examples of hypercube multiprocessor topologies

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 [19, 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 [28]. We shall describe these structures in some details.

3. *Stars* $S_n = K_{1,n-1}$ are considered as ill-suited topologies in [19], 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.

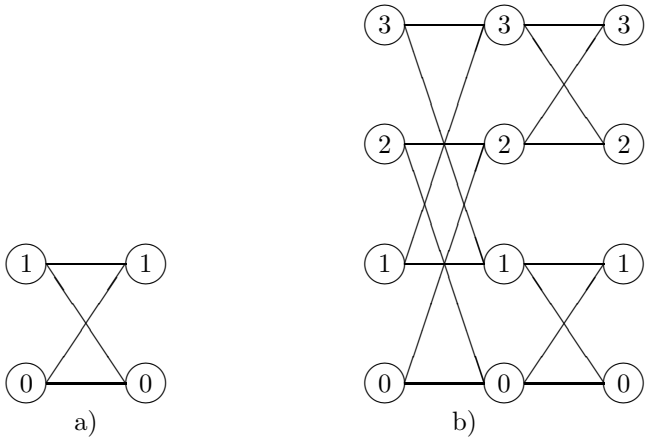

FIGURE 4. The examples of butterfly multiprocessor topologies

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 [14, 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 [14, 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 [19]. Other topologies are called *ill-suited*. Therefore, according to [19], 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. 2, 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.

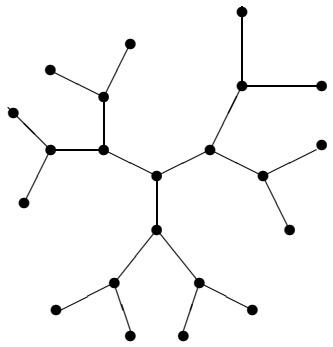

FIGURE 6. Quasi-regular tree $T(3,3)$

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 [25]). 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 [34]. 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 [19]. 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.

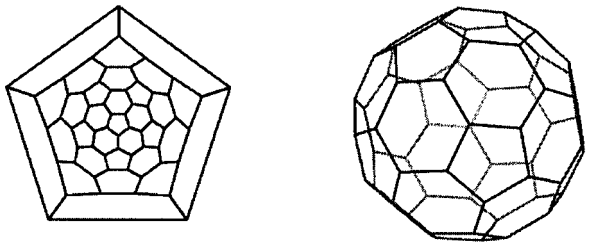

FIGURE 7. a) Planar and b) 3D visualization of the icosahedral fullerene C_{60}

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 [21]), $m = 15$ (see [22]), $\Delta = \lambda_1 = 3$. 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 [22].

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 [22]).

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 $a = 9$.

As explained in Introduction, 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 (see [5, 9]). 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].

We are interested in the 69 graphs given in Figs. 8–13 under names $\Omega_{n,k}$, where n ($2 \leqslant n \leqslant 10$) denotes the number of vertices and $k \geqslant 1$ (being a counter).

In Appendix, we give in Table 3 some data on these 69 graphs.

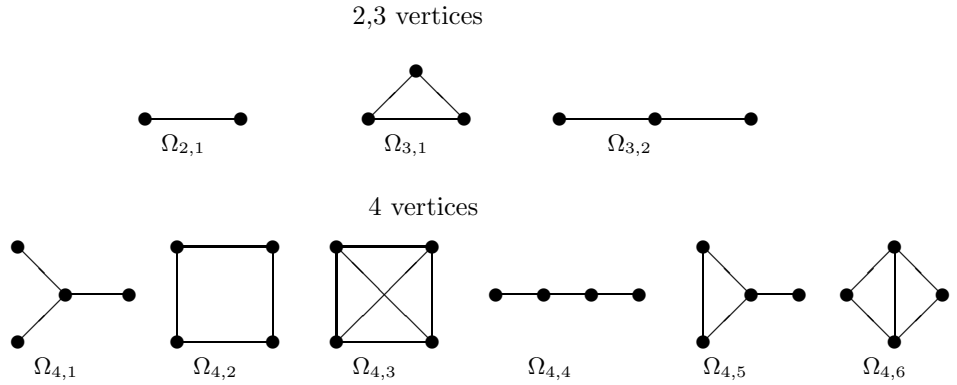

FIGURE 8. Graphs up to 4 vertices with small tightness

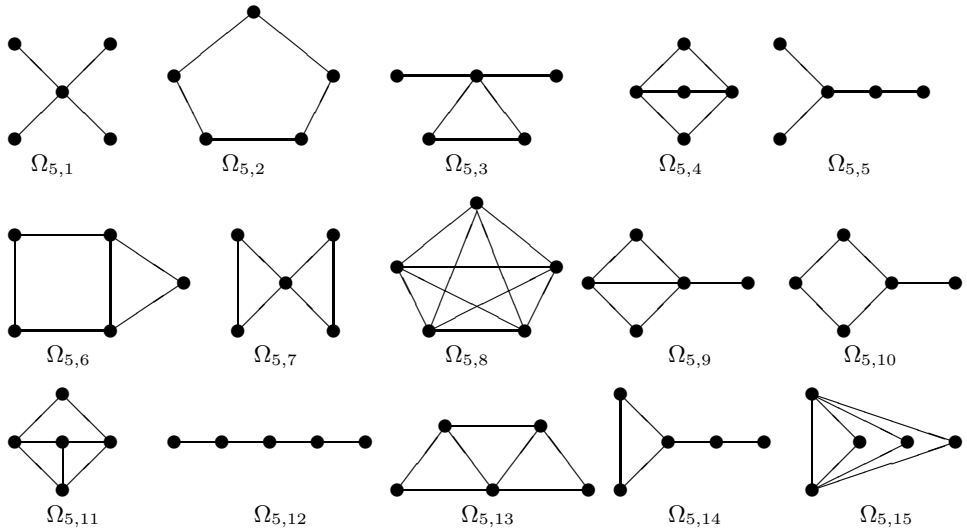

FIGURE 9. Graphs on 5 vertices with small tightness

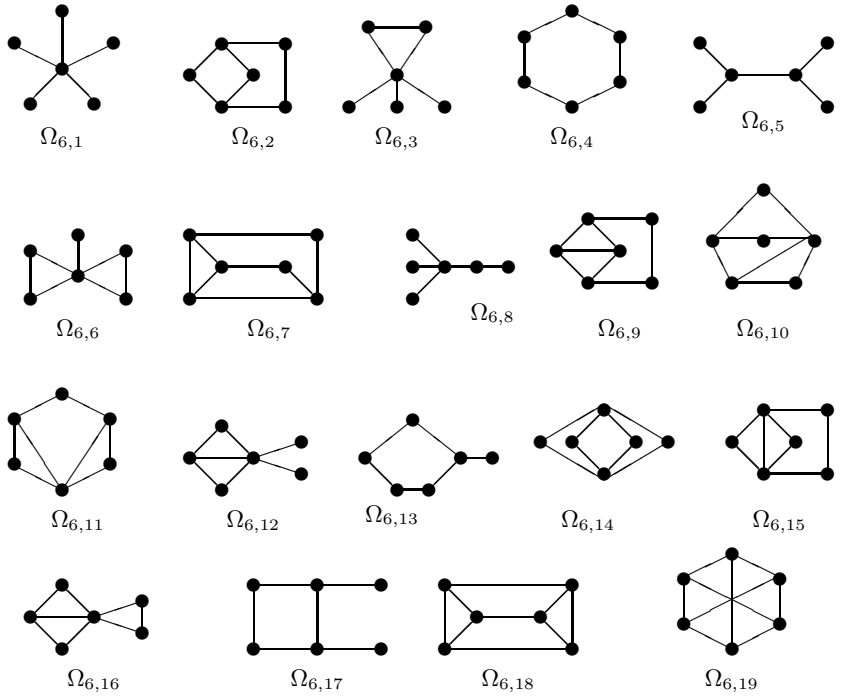

FIGURE 10. Graphs on 6 vertices with small tightness

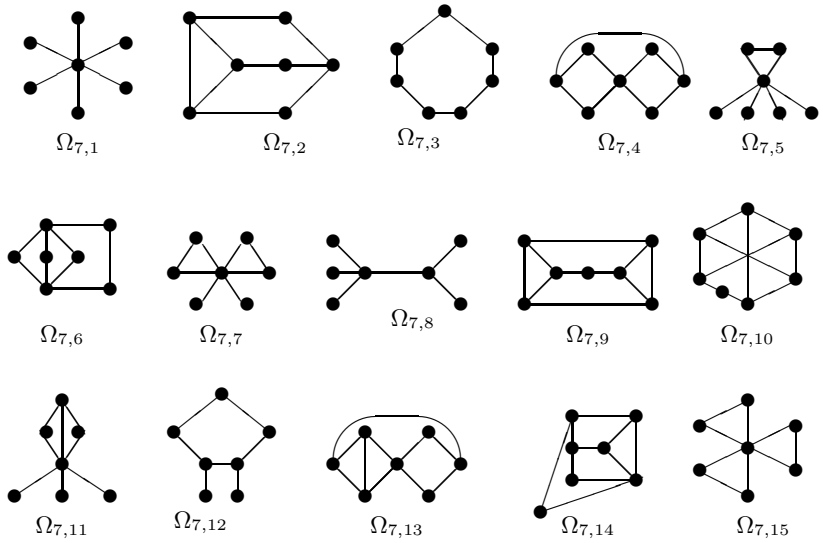

FIGURE 11. Graphs on 7 vertices with small tightness

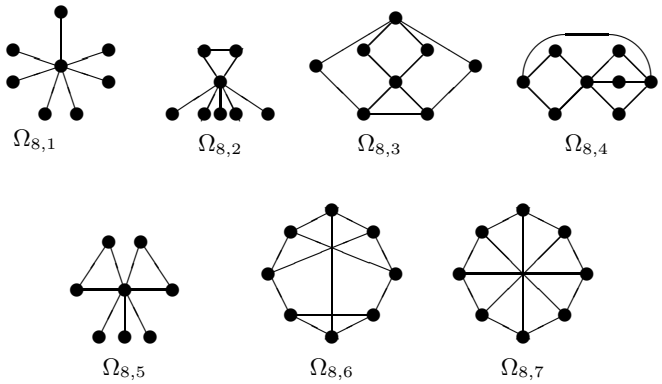

FIGURE 12. Graphs on 8 vertices with small tightness

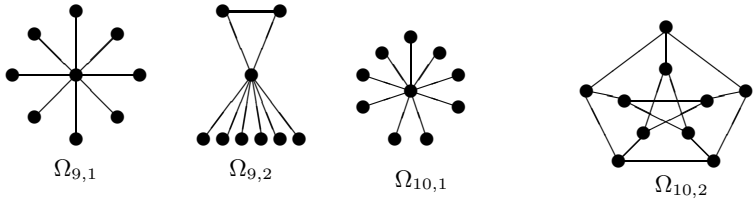

FIGURE 13. Graphs on 9 and 10 vertices with small tightness

The main result of [5] is the next theorem. In [5] only a sketch of a proof is given. The proof is completed in [9].

Theorem 2. *The only non-trivial connected graphs G such that $t_2(G) \leqslant 9$ are the* 69 *graphs $\Omega_{n,k}$, depicted on Figs.* 8–13.

Proof of Theorem 2. We have the following cases:

- a°**:** $D = 1$, $\lambda_1 \leqslant 4.5$. We have complete graphs $\Omega_{2,1}$, $\Omega_{3,1}$, $\Omega_{4,3}$, $\Omega_{5,8}$.
- b°**:** $D = 2$, $\lambda_1 \leqslant 3$. Denote the set of graphs satisfying these conditions by $\mathcal{A}_1$. According to (2) from the introductory chapter we have $\Delta \leqslant \lambda_1^2 \leqslant 9$ and by formula (3) we get $n \leqslant 1 + 9 + 9 \cdot 8 = 82$. For example, the star $\Omega_{10,1} \in \mathcal{A}_1$. The set $\mathcal{A}_1$ is completely determined in Lemma 2.
- c°**:** $D = 3$, $\lambda_1 \leqslant 2.25$. Denote the set of graphs satisfying these conditions by $\mathcal{A}_2$. Now, $\Delta \leqslant 5$ 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 $\mathcal{A}_2$ are listed in Lemma 3.
- d°**:** $D = 4$, $\lambda_1 \leqslant 1.8$. It is easy to see that the only graph in this case is the path $\Omega_{5,12}$ (see information on Smith graphs in Section 2 of the introductory chapter).
- e°**:** $D \geqslant 5$, $\lambda_1 \leqslant 1.5$. There are no graphs satisfying these conditions.

To treat the cases b° and c° in Lemmas 2 and 3 we need an auxiliary result. Let R be the set of graphs satisfying the conditions $D = 2$, $\Delta = 3$.

Lemma 1. *The set R consists of the following* 17 *graphs:* $\Omega_{4,1}$, $\Omega_{4,5}$, $\Omega_{4,6}$, $\Omega_{5,4}$, $\Omega_{5,6}$, $\Omega_{5,11}$, $\Omega_{6,2}$, $\Omega_{6,7}$, $\Omega_{6,9}$, $\Omega_{6,18}$, $\Omega_{6,19}$, $\Omega_{7,2}$, $\Omega_{7,9}$, $\Omega_{7,10}$, $\Omega_{8,6}$, $\Omega_{8,7}$ *and* $\Omega_{10,2}$.

Proof. By formula (3) graphs from R have at most 10 vertices. Consider a graph $G \in R$. It has a vertex v of degree 3. Let f be the number of edges in the subgraph of G induced by the three neighbours of v. We have the following possibilities:

If $f = 3$, we have $G = \Omega_{4,3}$ which is excluded since $D = 1$.

Consider $f = 2$. Now we start from vertex v and its neighbours and add new vertices and edges in such a way that conditions $D = 2$, $\Delta = 3$ are not violated. We readily get $G = \Omega_{4,6}$, or $G = \Omega_{5,11}$ given on Fig. 9, or G is isomorphic to $\Omega_{6,9}$ from Fig. 10.

In the case $f = 1$ the obtained graphs up to 7 vertices are presented on Fig. 14. Finally, we get the graph $\Omega_{8,6}$ from Fig. 12 on $n = 8$ vertices.

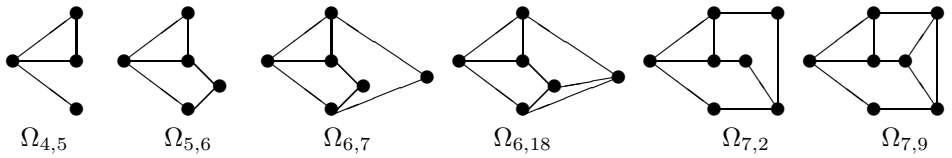

FIGURE 14. Some graphs from the set R

If $f = 0$, we first have complete bipartite graphs $\Omega_{4,1}$, $\Omega_{5,4}$, and $\Omega_{6,19}$, and $\Omega_{6,2}$. For $n = 7$ we again come across graph $\Omega_{7,2}$, and the graph $\Omega_{7,10}$. For $n = 8$ the graphs $\Omega_{8,6}$, $\Omega_{8,7}$ from Fig. 12 appear. The Petersen graph $\Omega_{10,2}$ on 10 vertices belongs here. There are no graphs on 9 vertices. □

Lemma 2. *The set $\mathcal{A}_1$ consists of* 52 *graphs given below.*

$n = 3$: $\Omega_{3,2}$;

$n = 4$: $\Omega_{4,1}$, $\Omega_{4,2}$, $\Omega_{4,6}$, $\Omega_{4,5}$;

$n = 5$: $\Omega_{5,1}$, $\Omega_{5,2}$, $\Omega_{5,3}$, $\Omega_{5,4}$, $\Omega_{5,6}$, $\Omega_{5,7}$, $\Omega_{5,9}$, $\Omega_{5,11}$, $\Omega_{5,13}$, $\Omega_{5,15}$;

$n = 6$: $\Omega_{6,1}$, $\Omega_{6,2}$, $\Omega_{6,3}$, $\Omega_{6,6}$, $\Omega_{6,7}$, $\Omega_{6,9}$, $\Omega_{6,10}$, $\Omega_{6,11}$, $\Omega_{6,12}$, $\Omega_{6,14}$, $\Omega_{6,15}$, $\Omega_{6,16}$, $\Omega_{6,18}$, $\Omega_{6,19}$;

$n = 7$: $\Omega_{7,1}$, $\Omega_{7,2}$, $\Omega_{7,4}$, $\Omega_{7,5}$, $\Omega_{7,6}$, $\Omega_{7,7}$, $\Omega_{7,9}$, $\Omega_{7,10}$, $\Omega_{7,11}$, $\Omega_{7,13}$; $\Omega_{7,14}$, $\Omega_{7,15}$;

$n = 8$: $\Omega_{8,1}$, $\Omega_{8,2}$, $\Omega_{8,3}$, $\Omega_{8,4}$, $\Omega_{8,5}$, $\Omega_{8,6}$, $\Omega_{8,7}$;

$n = 9$: $\Omega_{9,1}$, $\Omega_{9,2}$;

$n = 10$: $\Omega_{10,1}$, $\Omega_{10,2}$ (*the Petersen graph*).

Proof. We shall first prove that there are no graphs on $n > 10$ vertices with diameter 2 and index less than or equal to 3.

Assume to the contrary that G is a graph on $n > 10$ vertices such that $\mathrm{diam}(G) = 2$ and $\lambda_1(G) \leqslant 3$.

We first claim that $\Delta(G) \leqslant 8$. Otherwise, if $\Delta(G) \geqslant 9$ then $\lambda_1(G) > \lambda_1(S_{\Delta+1}) = \sqrt{\Delta} \geqslant 3$, a contradiction. If $\delta(G) = 1$, let v be a pendant vertex G, and w its neighbour. Since the eccentricity of v is at most 2, w must be adjacent to all vertices of G, but then $n \leqslant 10$, a contradiction.

Therefore, we can assume further on that $\delta(G) > 1$ and $\Delta(G) < 9$. Let e be the number of edges of G. Then,

$$3 \geqslant \lambda_1(G) \geqslant \frac{2e}{n} = \bar{d}$$

and the average vertex degree is less than or equal to 3, with equality if and only if G is regular. If G is 3-regular graph with diameter 2, by (4) G can have at most $1 + 3 + 3 \cdot 2 = 10$ vertices, a contradiction.

So the average vertex degree of G is less than 3, and since none of them is of degree 1, nor all are of degree 3, there exists at least one vertex in G, say u, of degree 2. Denote with v and w its neighbours. Let the remaining vertices ($n - 3$ in total) be partitioned as follows: A contains the vertices that are adjacent only to v; B contains the vertices that are adjacent only to w; C contains the vertices that are adjacent to both, v and w. If so

$$|A| + |C| \leqslant 7 \qquad \text{and} \qquad |B| + |C| \leqslant 7.$$

Since $|A| + |B| + |C| = n - 3$ and $n > 10$, we have $|A| > 0$ and $|B| > 0$.

Let all edges incident to v or w be coloured in blue, while the other edges, non-incident to v or w (incident only to vertices from $A \cup B \cup C$) be coloured in red. Let e_b and e_r be the number of blue and red edges in G, respectively. Clearly, $e_b \geqslant n - 1 + |C|$.

We now claim that $e_r \geqslant |A| + |B| - 1$. To see this, assume first that $H = \langle A \cup B \cup C \rangle$ (the subgraph induced by the vertex set $A \cup B \cup C$) is connected. Then, $e_r \geqslant |A| + |B| + |C| - 1 \geqslant |A| + |B| - 1$ and we are done. Let x and y be the vertices belonging to different components of H. Since G is of diameter 2, there is a vertex z adjacent to both vertices x and y. Clearly, $z \neq u$ (otherwise, if $z = u$ then $x = v$ and $y = w$, a contradiction). If $z \in A \cup B \cup C$, then x and y are not in different components of H. So $z = v$ or $z = w$. If $z = v$ then $x, y \in A \cup C$; while if $z = w$ then $x, y \in B \cup C$. It follows that all vertices from the sets A and B are in the same component of H (since x and y cannot belong to $A \cup B$), and therefore $e_r \geqslant |A| + |B| - 1$, as required.

Consequently, we have

$$\frac{3n}{2} \geqslant e = e_b + e_r \geqslant (n - 1 + |C|) + (|A| + |B| - 1) = 2n - 5.$$

But this is equivalent to $n \leqslant 10$, a contradiction.

Hence, there are no graphs on $n > 10$ vertices with diameter 2 and index less than or equal to 3.

By an exhaustive search of connected graphs up to ten vertices one can verify that only the 52 graphs, quoted in the statement of the lemma fulfill the requirements. □

Remark 1. (i) The exhaustive search in [5] was performed by the program **nauty**.

We used publicly available library of programs **nauty** [29] 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.

(ii) Another possibility to find the 52 graphs from Lemma 2 is to use computer assisted reasoning.

Graphs up to 7 vertices can be found using existing graph tables [15, 16] (up to 6 vertices), [13] (7 vertices).

Using an interactive graph package we follow the effect of adding vertices and edges to the largest eigenvalue λ_1. (We have used the package newGRAPH available at the address `http://www.mi.sanu.ac.rs/newgraph/`.)

If $\Delta = k$, then there exists a subgraph in the form of the star S_{k+1}.

If $\Delta = 9$, the only solution is $\Omega_{10,1} = S_{10}$, in all other cases $\lambda_1 > 3$.

If $\Delta = 8$, only one edge can be added and we get $\Omega_{9,1} = S_9$ and $\Omega_{9,2}$. Adding a vertex yields $\lambda_1 > 3$.

If $\Delta = 7$, at most two edges can be added and we get $\Omega_{8,1} = S_8$, $\Omega_{8,2}$ and $\Omega_{8,5}$.

If $\Delta = 6$, addition of at most three edges is possible and we get $\Omega_{7,1} = S_7$, $\Omega_{7,5}$, $\Omega_{7,7}$, $\Omega_{7,11}$, $\Omega_{7,15}$.

If $\Delta = 5$, again by adding at most three edges we get $\Omega_{6,1} = S_6$, $\Omega_{6,3}$, $\Omega_{6,6}$, $\Omega_{6,12}$, $\Omega_{6,15}$. Now adding vertices in a specific way is possible and we get $\Omega_{8,4}$.

If $\Delta = 4$, we get $\Omega_{8,3}$ and graphs with less than 8 vertices can be found by graph tables.

The case $\Delta = 3$ is covered by Lemma 1, while the cases $\Delta < 3$ are trivial.

Lemma 3. *The set $\mathcal{A}_2$ consists of* 12 *graphs listed below.*

$n = 4:\ \ \Omega_{4,4}$; $\qquad n = 5:\ \ \Omega_{5,5},\ \Omega_{5,10},\ \Omega_{5,14}$;

$n = 6:\ \ \Omega_{6,4},\ \Omega_{6,5},\ \Omega_{6,8},\ \Omega_{6,13},\ \Omega_{6,17}$; $\qquad n = 7:\ \ \Omega_{7,3},\ \Omega_{7,8},\ \Omega_{7,12}$.

Proof. By Table 3 given in Appendix the above 12 graphs clearly belong to the set $\mathcal{A}_2$. We shall show that no other graphs H belong to $\mathcal{A}_2$.

Maximal degree of H cannot be at least 5 since in this case H would contain S_6 with an additional vertex (since $D = 3$). Such a subgraph would have $\lambda_1 > 2.25$ which is forbidden.

If $\Delta = 4$, H contains a subgraph isomorphic to S_5. We cannot add an edge to S_5, since then we obtain $\Omega_{5,3}$ with $\lambda_1 > 2.25$ (see Table 3). However, S_5 can be

extended with new vertices to graphs $\Omega_{6,8}$ and $\Omega_{7,8}$. 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 using Lemma 1. □

This completes the proof of Theorem 2.

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

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

It is obvious that $T_1^a \subseteq T_{\text{stt}}^a \subseteq T_2^a$ and $T_1^a \subseteq T_{\text{spt}}^a \subseteq T_2^a$ because of the partial order between tightness values given on Fig. 2.

Using Table 3 from Appendix we can immediately verify the following corollaries of Theorem 2.

Corollary 3. *The only non-trivial connected graphs G such that $t_1(G) \leqslant 9$ are* 14 *graphs $\Omega_{i,j}$, where (i,j) is:*

$$(2,1),\ (3,1),\ (3,2),\ (4,j)\ (j \in \{1,\dots,4\}),$$
$$(5,j)\ (j \in \{2,4,8\}),\ (6,4),\ (6,19),\ (7,3),\ (10,2).$$

Corollary 4. *The only non-trivial connected graphs G such that $\text{stt}(G) \leqslant 9$ are* 27 *graphs $\Omega_{i,j}$, where (i,j) is:*

$$(2,1),(3,1),(3,2),\ (4,j)\ (j \in \{1,\dots,6\}),\ (5,j)\ (j \in \{2,4,6,8,11\},$$
$$(6,j)\ (j \in \{2,4,7,9,18,19\}),\ (7,j)\ (j \in \{2,3,9,10\}),\ (8,6),(8,7),(10,2).$$

Corollary 5. *The only non-trivial connected graphs G such that $\text{spt}(G) \leqslant 9$ are* 21 *graphs $\Omega_{i,j}$, where (i,j) is:*

$$(2,1),\ (3,1),\ (3,2),\ (4,j)\ (j \in \{1,\dots,5\}),\ (5,j)\ (j \in \{1,2,4,8,\}),$$
$$(6,j)\ (j \in \{1,4,14,19\}),\ (7,1),\ (7,3),\ (8,1),\ (10,2).$$

Corollaries 1–3 have been proved in [5] in another way.

Remark 2. In fact in [5] we have 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

$$Q = \{K_2, K_3, K_4, K_5, P_3, P_4, C_4, C_5, C_6, C_7, K_{1,3}, K_{2,3}, K_{3,3}, PG\},$$
$$S' = \{P_5, K_{1,4}, K_{1,5}, K_{1,6}, K_{1,7}, K_{1,8}, K_{1,9}\},$$
$$R' = \{\Omega_{4,5}, \Omega_{4,6}, \Omega_{5,6}, \Omega_{5,11}, \Omega_{6,2}, \Omega_{6,7}, \Omega_{6,9}, \Omega_{6,18}, \Omega_{7,2}, \Omega_{7,9}, \Omega_{7,10}, \Omega_{8,6}, \Omega_{8,7}\}$$

and V' consists of the remaining 35 graphs. Here, PG denotes the Petersen graph. We see that the sets Q and S' (related to tightness t_1 and spt) contain only the standard graphs. When considering stt and t_2, the graphs with non-standard names occur.

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 Corollary 1 of Theorem 2 we are in a position to find the best configurations w.r.t. t_1 up to 10 vertices.

Theorem 3. *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 2. Together with extremal graphs, the corresponding tightness values are given in parentheses.

TABLE 2. 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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Appendix

The Table 3 given below contains some relevant data about 69 graphs with second type mixed tightness not exceeding 9.

Graphs are ordered first by n (the number of vertices), and within the groups with fixed n, by t_2. Columns of the table provide graph name, the number of vertices n, the number of edges e, the name(s) under which the graph appeared in [5], diameter D, maximum vertex degree Δ, the number of distinct eigenvalues m, the spectrum starting with the largest eigenvalue λ_1. Last four columns contain the values of the four types of tightness $t_1, \mathrm{stt}, \mathrm{spt}, t_2$.

As "the old names" we used different notation. First we distinguish the well known graphs such as complete graphs, circuits, stars, complete bipartite graphs, and so on. For graphs up to 5 vertices we used the notation from [14], while graphs on $n = 6$ vertices are marked primarily as in [15]. $N(n, j)$ denotes the j-th graph on n vertices generated by program **nauty**. PG denotes the well known Petersen graph.

TABLE 3. Graphs on up to 10 vertices with small tightness

graph	n	e	old name(s)	D	Δ	m	$\lambda_1, \lambda_2, \ldots, \lambda_n$	t_1	stt	spt	t_2
$\Omega_{2,1}$	2	1	$G_1 = K_2 = P_2$	1	1	2	**1**, -1	2	2	2	2
$\Omega_{3,1}$	3	3	$G_2 = K_3 = C_3$	1	2	2	**2**, -1, -1	4	4	4	4
$\Omega_{3,2}$		2	$G_3 = P_3 = S_3 = K_{1,2}$	2	2	3	**1.41**, 0, -1.41	6	6	4.23	4.23
$\Omega_{4,1}$	4	3	$G_8 = S_4 = K_{1,3}$	2	3	3	**1.73**, 0, 0, -1.73	9	9	5.19	5.19
$\Omega_{4,2}$		4	$G_7 = C_4 = K_{2,2}$	2	2	3	**2**, 0, 0, -2	6	6	6	6
$\Omega_{4,3}$		6	$G_4 = K_4$	1	3	2	**3**, -1, -1, -1	6	6	6	6
$\Omega_{4,4}$		3	$G_9 = P_4$	3	2	4	**1.62**, 1.62, 0.62, -0.62, -1.62	8	8	6.47	6.47
$\Omega_{4,5}$		4	G_6	2	3	4	**2.17**, 0.31, -1, -1.48	12	9	8.68	6.51
$\Omega_{4,6}$		5	G_5	2	3	4	**2.56**, 0, -1, -1.56	12	9	10.24	7.68
$\Omega_{5,1}$	5	5	$G_{28} = S_5 = K_{1,4}$	2	4	3	**2**, 0, 0, 0, -2	12	12	6	6
$\Omega_{5,2}$		5	$G_{27} = C_5$	2	2	3	**2**, 0.62, 0.62, -1.62, -1.62	6	6	6	6
$\Omega_{5,3}$		5	G_{23}	2	4	5	**2.34**, 0.47, 0, -1, -1.81	20	12	11.71	7.03
$\Omega_{5,4}$		6	$G_{22} = K_{2,3}$	2	3	3	**2.45**, 0, 0, 0, -2.45	9	9	7.35	7.35
$\Omega_{5,5}$		4	G_{29}	3	3	5	**1.85**, 0.77, 0, -0.77, -1.85	15	12	9.24	7.39
$\Omega_{5,6}$		6	G_{21}	2	3	5	**2.48**, 0.69, 0, -1.17, -2	15	9	12.41	7.44
$\Omega_{5,7}$		6	G_{20}	2	4	4	**2.56**, 1, -1, -1, -1.46	16	12	10.25	7.68
$\Omega_{5,8}$		10	$G_{10} = K_5$	1	4	2	**4**, -1, -1, -1, -1	8	8	8	8
$\Omega_{5,9}$		6	G_{18}	2	4	5	**2.69**, 0.33, 0, -1.27, -1.75	20	12	13.43	8.06
$\Omega_{5,10}$		5	G_{26}	3	3	5	**2.14**, 0.66, 0, -0.66, -2.14	15	12	10.68	8.54
$\Omega_{5,11}$		7	G_{17}	2	3	5	**2.86**, 0.32, 0, -1, -2.18	15	9	14.28	8.57
$\Omega_{5,12}$		4	$G_{30} = P_5$	4	2	5	**1.73**, 1, 0, -1, -1.73	10	10	8.66	8.66
$\Omega_{5,13}$		7	G_{16}	2	4	5	**2.94**, 0.62, -0.46, -1.47, -1.62	20	12	14.68	8.81
$\Omega_{5,14}$		5	G_{25}	3	3	5	**2.21**, 1, -0.54, -1, -1.67	15	12	11.07	8.86
$\Omega_{5,15}$		7	G_{15}	2	4	4	**3**, 0, 0, -1, -2	16	12	12	9

Table 3: Graphs on up to 10 vertices with small tightness (cont.)

graph	n	e	old name(s)	D	Δ	m	$\lambda_1, \lambda_2, \ldots, \lambda_n$	t_1	stt	spt	t_2
$\Omega_{6,1}$	6	5	$S_6 = K_{1,5} = CP(107) = N(6,1)$	2	5	3	**2.24**, 0, 0, 0, 0, -2.24	15	15	6.71	6.71
$\Omega_{6,2}$		7	$CP(93) = N(6,35)$	2	3	6	**2.39**, 0.77, 0.62, 0, -1.62, -2.16	18	9	14.35	7.17
$\Omega_{6,3}$		6	$CP(94) = N(6,3)$	2	5	5	**2.51**, 0.57, 0, 0, -1, -2.09	25	15	12.57	7.54
$\Omega_{6,4}$		6	$C_6 = CP(106) = N(6,49)$	3	2	4	**2**, 1, 1, -1, -1, -2	8	8	8	8
$\Omega_{6,5}$		5	$CP(109) = N(6,5)$	3	3	5	**2**, 1, 0, 0, -1, -2	15	12	10	8
$\Omega_{6,6}$		7	$CP(79) = N(6,17)$	2	5	5	**2.71**, 1, 0.19, -1, -1, -1.90	25	15	13.55	8.13
$\Omega_{6,7}$		8	$CP(72) = N(6,89)$	2	3	6	**2.74**, 0.71, 0.62, -0.23, -1.62, -2.22	18	9	16.45	8.22
$\Omega_{6,8}$		5	$CP(108) = N(6,2)$	3	4	5	**2.07** , 0.84, 0, 0, -0.84, -2.07	20	16	10.37	8.30
$\Omega_{6,9}$		8	$CP(69) = N(6,90)$	2	3	6	**2.79**, 1, 0.62, -1, -1.62, -1.79	18	9	16.75	8.37
$\Omega_{6,10}$		8	$CP(71) = N(6,36)$	2	4	5	**2.80**, 0.85, 0, 0, -1.20, -2.45	20	12	13.98	8.39
$\Omega_{6,11}$		8	$CP(68) = N(6,57)$	2	4	6	**2.81**, 1, 0.53, -1, -1.34, -2	24	12	16.88	8.44
$\Omega_{6,12}$		7	$CP(75) = N(6,8)$	2	5	5	**2.81**, 0.53, 0, 0, -1.34, -2	25	15	14.07	8.44
$\Omega_{6,13}$		6	$CP(105) = N(6,19)$	3	3	6	**2.11**, 1, 0.62, -0.25, -1.62, -1.86	18	12	12.69	8.46
$\Omega_{6,14}$		8	$K_{2,4} = CP(73) = N(6,13)$	2	4	3	**2.83**, 0, 0, 0, 0, -2.83	12	12	8.49	8.49
$\Omega_{6,15}$		8	$CP(66) = N(6,39)$	2	4	5	**2.90**, 0.81, 0, 0, -1.71, -2	20	12	14.52	8.71
$\Omega_{6,16}$		8	$CP(61) = N(6,32)$	2	5	6	**2.95**, 1.16, 0, -1, -1.29, -1.82	30	15	17.68	8.84
$\Omega_{6,17}$		6	$CP(102) = N(6,18)$	3	3	6	**2.25**, 0.80, 0.55, -0.55, -0.80, -2.25	18	12	13.48	8.99
$\Omega_{6,18}$		9	$CP(51) = N(6,93)$	2	3	4	**3**, 1, 0, 0, -2, -2	12	9	12	9
$\Omega_{6,19}$		9	$K_{3,3} = CP(52) = N(6,71)$	2	3	3	**3**, 0, 0, 0, 0, -3	9	9	9	9
$\Omega_{7,1}$	7	6	$S_7 = K_{1,6} = N(7,1)$	2	6	3	**2.45**, 0, 0, 0, 0, 0, -2.45	18	18	7.35	7.35
$\Omega_{7,2}$		9	$N(7,337)$	2	3	5	**2.66**, 1.21, 0.62, 0.62, -1.62, -1.62, -1.87	15	9	13.28	7.97
$\Omega_{7,3}$		7	$C_7 = N(7,292)$	3	2	4	**2**, 1.255, 1.25, -0.45, -0.45, -1.80, -1.80	8	8	8	8
$\Omega_{7,4}$		9	$N(7,156)$	2	4	6	**2.68**, 1, 0.64, 0, 0, -2, -2.32	24	12	16.09	8.04
$\Omega_{7,5}$		7	$N(7,3)$	2	6	5	**2.68**, 0.64, 0, 0, 0 ,-1, -2.32	30	18	13.41	8.04

Table 3: Graphs on up to 10 vertices with small tightness (cont.)

graph	n	e	old name(s)	D	Δ	m	$\lambda_1, \lambda_2, \ldots, \lambda_n$	t_1	stt	spt	t_2
$\Omega_{7,6}$	7	9	$N(7,75)$	2	4	6	**2.75**, 0.84, 0.62, 0, 0, -1.62, -2.59	24	12	16.51	8.25
$\Omega_{7,7}$		8	$N(7,23)$	2	6	6	**2.86**, 1, 0.32, 0, -1, -1, -2.18	36	18	17.13	8.57
$\Omega_{7,8}$		6	$N(7,5)$	3	4	5	**2.18**, 1.13, 0, 0, 0, -1.13, -2.18	20	16	10.88	8.70
$\Omega_{7,9}$		10	$N(7,624)$	2	3	7	**2.90**, 1.41, 0.81, 0, -1.41, -1.71, -2	21	9	20.32	8.71
$\Omega_{7,10}$		10	$N(7,514)$	2	3	6	**2.90**, 0.81, 0.73, 0, 0, -1.71, -2.73	18	9	17.42	8.71
$\Omega_{7,11}$		8	$N(7,8)$	2	6	5	**2.94**, 0.66, 0, 0, 0, -1.37, -2.24	30	18	14.72	8.83
$\Omega_{7,12}$		7	$N(7,92)$	3	3	6	**2.21**, 1, 1, 0, -0.54, -1.68, -2	18	12	13.29	8.86
$\Omega_{7,13}$		10	$N(7,448)$	2	4	7	**2.98**, 1.33, 0.65, 0, -1, -1.77, -2.19	28	12	20.86	8.94
$\Omega_{7,14}$		9	$N(7,324)$	2	4	7	**2.97**, 0.80, 0.70, 0.45, -0.55, -2.12, -2.25	28	12	20.77	8.90
$\Omega_{7,15}$		9	$N(7,219)$	2	6	4	**3**, 1, 1, -1, -1, -1, -2	24	18	12	9
$\Omega_{8,1}$	8	7	$S_8 = K_{1,7} = N(8,1)$	2	7	3	**2.65**, 0, 0, 0, 0, 0, 0, -2.65	21	21	7.94	7.94
$\Omega_{8,2}$		8	$N(8,3)$	2	7	5	**2.54** , 0.69, 0, 0, 0, 0, -1, -2.84	35	21	14.22	8.53
$\Omega_{8,3}$		11	$N(8,1039)$	2	4	8	**2.90**, 1.30, 0.81, 0.62, 0, -1.62, -1.71, -2.30	32	12	23.23	8.71
$\Omega_{8,4}$		11	$N(8,342)$	2	5	6	**2.98**, 1.13, 0.65, 0, 0, 0, -2.07, -2.68	30	15	17.86	8.93
$\Omega_{8,5}$		9	$N(8,30)$	2	7	6	**3**, 1, 0.41, 0, 0, -1, -1, -2.41	42	21	18	9
$\Omega_{8,6}$		12	$N(8,8469)$	2	3	6	**3**, 1.56, 0.62, 0.62, 0, -1.62, -1.62, -2.56	18	9	18	9
$\Omega_{8,7}$		12	$N(8,6660)$	2	3	5	**3**, 1, 1, 0.41, 0.41, -1, -2.41,-2.41	15	9	15	9
$\Omega_{9,1}$	9	8	$S_9 = K_{1,8} = N(9,1)$	2	8	3	**2.83**, 0, 0, 0, 0, 0, 0, 0, -2.83	24	24	8.49	8.49
$\Omega_{9,2}$		9	$N(9,3)$	2	8	5	**3**, 0.73, 0, 0, 0, 0, 0, -1, -2.73	40	24	15	9
$\Omega_{10,1}$	10	9	$S_{10} = K_{1,9} = N(10,1)$	2	9	3	**3**, 0, 0, 0, 0, 0, 0, 0, 0, -3	27	27	9	9
$\Omega_{10,2}$		15	$PG = N(10,8027956)$	2	3	3	**3**, 1, 1, 1, 1, 1, -2, -2, -2, -2	9	9	9	9

Silvia Gago

SPECTRAL TECHNIQUES IN COMPLEX NETWORKS

Abstract. Most physical, biological, chemical, technological and social systems have a network structure. Examples of complex networks range from cell biology to epidemiology or to the Internet. In the recent years, several models of complex networks have been proposed, as the random graph of Erdős and Rényi, the small-world model of Watts and Strogatz or the scale-free networks of Barabási and Albert.

The topological structure of such networks can be fully described by the associated adjacency matrices and their spectral density. The rich information about the topological structure and diffusion processes can be extracted from the spectral analysis of the networks. For instance, the power-law behavior of the density of eigenvalues is a notable feature of the spectrum of scale-free networks. Dynamical network processes, like synchronization can be determined by the study of their Laplacian eigenvalues. Furthermore, the eigenvalues are related to many basic topological invariants of networks such as diameter, mean distance, betweenness centrality, etc.

Spectral techniques are also used for the study of several network properties: community detection, bipartition, clustering, design of highly synchronizable networks, etc.

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Contents

1. Introduction

Complex networks are everywhere. They are formed by a large set of vertices representing the entities of the system, and a set of edges, representing the interactions between their elements. Examples of complex networks include the Internet, World Wide Web, social networks of acquaintances or other connections between individuals, distribution networks such as postal delivery routes, neural networks, food webs, metabolic networks, networks of citations between papers, organizational networks and networks of business relations between companies, and many others (see Fig. 1). In the recent last years, two classes of complex networks have aroused a great deal of interest in the literature: small-world networks and scale-free networks, as many real networks exhibit characteristics of both classes.

The spectrum of the adjacency and *Laplacian* matrices provide a great deal of information about the structure of a network. As usual, the eigenvalues of the adjacency matrix are denoted by λ_i, $1 \leqslant i \leqslant n$. Recall that the *Laplacian* matrix of a graph is a symmetric matrix L whose diagonal elements l_{ii} are the degrees of the vertices, and whose off-diagonal elements l_{ij} are -1 if the vertex v_i is connected to v_j, and 0 otherwise. More precisely, if D is the diagonal matrix of vertex degrees d_i and A is the adjacency matrix of the graph, $L = D - A$. Note that L is semi-positive definite, $x^T Lx \geqslant 0$ for any vector x, its first eigenvector is $j = (1, \ldots, 1)^T$ corresponding to the first eigenvalue $\theta_1 = 0$, and the second largest eigenvalue θ_2 is called the *algebraic connectivity* or*Fiedler value*, because its proximity to 0 reveals whether the graph can be easily disconnected. Its corresponding eigenvector v_2 is also known as the *Fiedler vector*, and is essential for the bisection method. The *Laplacian spectrum* is denoted by

$$\mathrm{sp}(L) = \{0 \leqslant \theta_2 \leqslant \ldots \leqslant \theta_n\}.$$

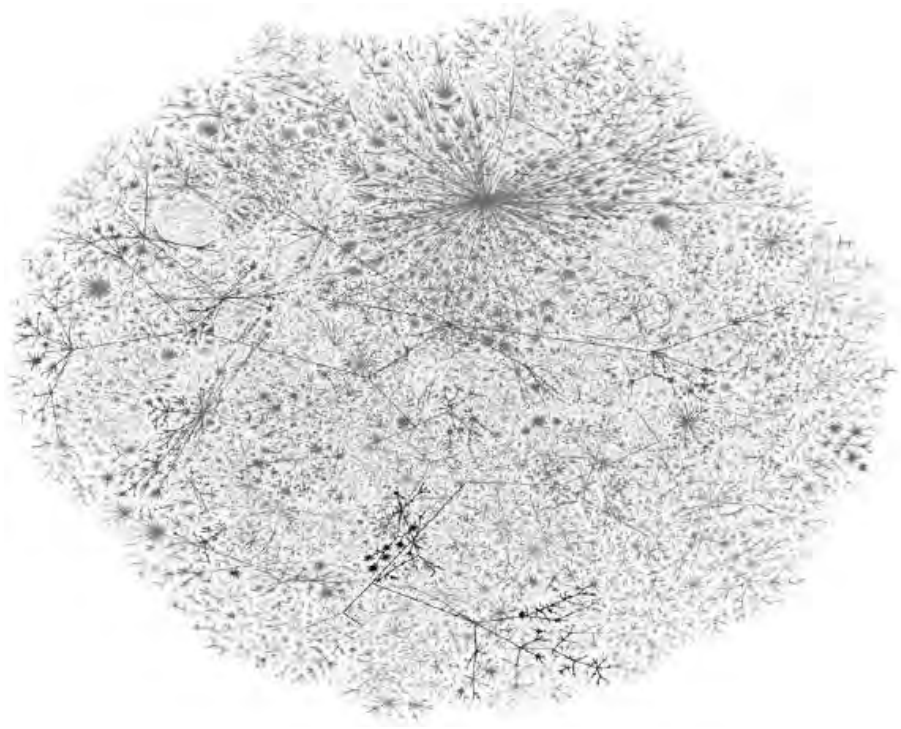

FIGURE 1. A complex network: a picture of the World Wide Web, from Hal Burch and Bill Cheswick, Lumeta Corp.

The *normalized Laplacian* matrix is introduced by Chung and defined as the symmetric matrix $\mathcal{L}$ whose diagonal elements l_{ii} are 1, and whose off-diagonal elements $l_{ij} = -1/\sqrt{d_i d_j}$ if the vertex v_i is connected to v_j, and 0 otherwise. Its relation with the Laplacian is given by $\mathcal{L} = D^{-1/2} L D^{-1/2}$.

Several topological parameters are considered for the study of complex networks. Some of them are well known in graph theory, like the *diameter*, *mean distance*, *isoperimetric number*, *maximum and minimum degree* and *edge connectivity*.

The *edge connectivity*, $e(G)$, of a graph G is the minimum number of edges which must be deleted in G to disconnect it. The *minimum and maximum degree* of the graph are denoted by δ and Δ respectively. Denoting by $d(u, v)$ the distance between two vertices $u, v \in V(G)$ (the length of the shortest path), the *diameter* is $D = \max_{u,v \in V} d(u, v)$, and the *mean distance* or *average path length* is

$$\overline{l} = \frac{2}{n(n-1)} \sum_{(u,v) \in V(G)} d(u, v).$$

The graph diameter provides an inverse measure of the vertex connectivity. Intuitively, we can say that two vertices in a network are weakly connected if their

shortest connection passes through many other vertices. When this happens for all pairs of nodes, the diameter D of the graph is large.

The *isoperimetric number* of a graph is introduced by Mohar in [42] as the number $i(G) = \min_{|X| \leqslant \frac{n}{2}} |\delta X|/|X|$, where X is a subset of vertices, δX is the boundary of X, i.e., the set of edges in G between vertices in X and vertices not in X. It is a measure of whether or not a graph can be split in two subgraphs of the same cardinality. In the same paper there are two different bounds for the isoperimetric number.

New parameters and tools are also considered to characterize properties of these new networks, like the degree distribution, eigenvalue distribution, spectral density, clustering parameter and betweenness centrality.

Clustering parameter. Let e_i be the number of edges connecting the neighbors of a vertex u_i of degree δ_i, then the clustering coefficient of u_i is $C_i = 2e_i/\delta_i(\delta_i - 1)$, for any $1 \leqslant i \leqslant n$, and the clustering coefficient or parameter of the graph G is defined as

$$C = \frac{1}{n} \sum_{i=1}^{n} C_i.$$

Power-laws distributions. A power-law function follows the polynomial form $f(x) = ax^{-\gamma}$, where a, γ are constants and γ is called the power-law exponent. This kind of distribution was previously known as Pareto distribution or Zipfs law. The main property of power laws is their scale invariance, i.e., any scaling of the argument x by a constant factor causes only a proportionate scaling of the function itself, i.e., $f(cx) = a(cx)^{-\gamma} = c^{-\gamma} f(x) \propto f(x)$, which means that they are proportional and therefore it preserves the shape of the function itself. Moreover, by taking logarithms a linear relation is obtained $\log f(x) = \log a - \gamma \log x$. A network with degree power law distribution is called *scale-free*.

Spectral density. Given a graph G of order n, and adjacency matrix eigenvalues λ_i, $1 \leqslant i \leqslant n$, the spectral density of the graph is defined as

$$\rho(x) = \frac{1}{n} \sum_{j=1}^{n} \delta(x - \lambda_j), \quad \text{where} \quad \delta(x) = \begin{cases} 1, & \text{if } x = 0, \\ 0, & \text{if } x \neq 0. \end{cases}$$

is the Kronecker or delta function.

Betweenness centrality. Vertex betweenness centrality was introduced by a sociologist Freeman [29] in 1977, as a measure of the importance of a vertex in a network. Since the appearance of complex networks it has become an important parameter to study networks features [45], generalizing the concept for edge betweenness centrality. Spectral bounds for either the vertex betweenness and edge betweennes of a graph are studied in [15], and more general properties can be found in [32]. The *maximum betweenness centrality*, $B_{\max}$, is also considered for studying several aspects of the network, as its synchronization capability (Section 3), or used for performance of bisection methods (Section 4).

To be more precise, if $\sigma_{uv}(w)$ denotes the number of shortest paths from vertex u to vertex v that go through w, and σ_{uv} is the total number of shortest paths from u to v, then $b_w(u, v) = \sigma_{uv}(w)/\sigma_{uv}$. The betweenness of a vertex w is

$B_w = \sum_{u,v \neq w} b_w(u,v)$. The betweenness centrality of a graph G of order n is

$$\overline{B} = \frac{1}{n} \sum_{u \in V} B_u,$$

and the maximum betweenness of the graph G is $B_{\max} = \max\{B_u \mid u \in V\}$. The mean betweenness $\overline{B}$ is closely related with the mean distance $\overline{l}$ of the graph as $\overline{B} = (n-1)(\overline{l}-1)$ [15]. The same parameters can be defined for edges, and the most used one is the maximum edge betweenness centrality, $\mathcal{B}^E$.

2. Internet graph models and their spectra

Traditionally networks have been described by either regular graphs or random models like the classical model of Erdős–Rényi [22]. The later consists of a graph on n vertices, $G(n,p)$, where the vertices are connected between them with probability p. In particular the distribution of the degree of any particular vertex v is binomial

$$P(d_v = k) = \binom{n}{k} p^k (1-p)^{n-k}.$$

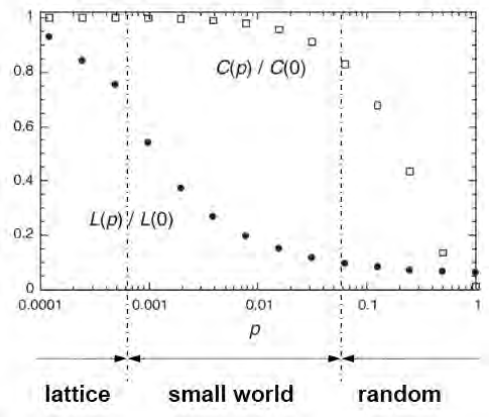

FIGURE 2. Watts and Strogatz small-world model. The diagram represents the rewiring probability p versus normalized mean distance $\overline{l}$ and clustering parameter C. Observe that as p increases, both $\overline{l}$ and C decrease. However, $\overline{l}$ decays faster than C, which allows a probability region, $0.01 \leqslant p \leqslant 0.1$, where $\overline{l}$ is a small and C is still high.

However, the appearance of new networks like the Internet graph, which could not be reproduced by these classical models, motivated Watts and Strogatz to introduce a new model for describing them [60]. They observed that such networks have a small diameter or mean distance as the former, and a large clustering parameter, as the later. Sparse random graphs have a small clustering coefficient while real world networks often have a coefficient significantly larger.

The model proposed by Watts and Strogatz starts from a regular graph with a large clustering parameter, which is transformed into a small world graph by the random reconnection of only a small number of edges, as the diameter is drastically reduced while the clustering coefficient of the regular graph remains large (see Fig. 2).

Since the appearance of this breakthrough a large number of stochastic and deterministic models have been appearing in the literature. For more information about them we refer the reader to the surveys [6] and [14].

In 1999 Faloutsos, Faloutsos and Faloutsos [25] made an experimental study of one part of the Internet graph, obtaining power laws in the distribution of many of the different parameters of the network, as the vertex degrees or the adjacency matrix eigenvalues. A typical value for the degree power-law exponent in real networks is $2 \leqslant \gamma \leqslant 3$. For obtaining the eigenvalue power-law, the eigenvalues λ_i of the adjacency matrix are sorted in decreasing order and plotted versus the associated increasing sequence of numbers i representing the order of the eigenvalue (see Fig. 3). A similar relation has been recently obtained for the normalized Laplacian eigenvalues in [53] and for the weighted Laplacian and the weighted adjacency matrix in [38]. Former experimental studies indicate that the power law exponents have not changed over the years in spite of the exponential network growth [34, 52].

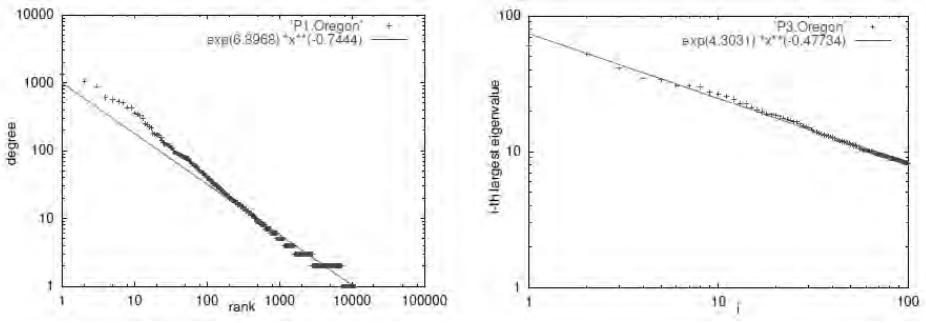

FIGURE 3. Power law distributions at the AS level Oregon Internet network, from [25]. On the left it is represented the histogram of 10000 highest vertex degrees and on the right the 100 largest eigenvalues versus their order, both in a log-log scale.

Mihail et al. in [41] found a surprising relationship between the degree and the eigenvalue exponents: the eigenvalue exponent is approximately half of the degree exponent. This fact indicates that the first largest eigenvalues are the square root of the first largest degrees. They also claimed that the eigenvalue distribution is a consequence of the degree distribution. However, in [31] it is proved by the construction of a deterministic model based on direct products of star graphs that the eigenvalue power-law is not a consequence of the degree power-law.

Among the scale-free models the most studied one is proposed by Barabási and Albert in 1999 [2]. The model is based on two observed facts in real networks: networks expand continuously by the addition of new vertices, and new vertices attach preferentially to sites that are already well connected. They used the so-called preferential attachment model. The model starts with a small number of vertices m_0 at step $t = 0$, and at every time step a new vertex u is connected to $m \leqslant m_0$ vertices of the existing graph. The probability of the new vertex u of being connected to an existing vertex u_i depends on its degree d_i, i.e.,

$$p(u \text{ is connected to } u_i) = p_i = \frac{d_i}{\sum_j d_j}, \text{ for } 1 \leqslant i \leqslant m.$$

The Barabási–Albert model produces a degree power-law distribution with exponent $\gamma = -3$, meanwhile the Watts and Strogatz and the Erdős-Rényi follow a Poisson distribution. This means that vertices with higher degree have stronger ability to grab links added to the network.

The main tool used for studying the spectra of large complex networks is the spectral density $\rho(\lambda)$. For a uncorrelated random graph, a graph where the probability for any pair of its vertices being connected is the same, p, and where these probabilities are independent variables, the adjacency matrix A is a real symmetric $n \times n$ uncorrelated random matrix, i.e., $EA_{ij} = 0$ and $EA_{ij}^2 = \sigma$. For this matrix, the limit of the spectral density when $n \to \infty$ converges to a semicircular distribution (if rescaled as $\lambda' = \lambda[np(1-p)]^{-1/2} \propto \lambda n^{-1/2}$)

$$\rho(\lambda') = \begin{cases} (2\pi)^{-1}\sqrt{4-\lambda'^2}, & \text{if } |\lambda'| < 2\sigma, \\ 0, & \text{otherwhise.} \end{cases}$$

This theorem is known as Wigner's semicircular law [61]. Surprisingly, the semicircular spectral density is not valid for any realistic graph models.

The spectrum and the corresponding eigenvectors of the Barabási and Albert model have been studied by Goh et al. in [35] obtaining that the distribution of the spectra is quite far from a semicircle. The eigenvalues decay exponentially around the center and have power-law long tails at both edges. The same result was obtained by Farkas et al. in [26], where the spectral density of both Watts and Strogatz and Barabási and Albert models are studied, finding that they have a special shape. In particular, scale-free graphs develop a triangle-like spectral density with a power-law tail when plotted in log-log scale (see Fig. 4), while small-world graphs have a complex spectral density consisting of several sharp peaks (Fig. 5). They also found that the eigenvalues λ_1 and $|\lambda_n|$ depend on n as $n^{1/4}$ for large n, and that the eigenvector corresponding to the largest eigenvalue is strongly localized at the vertex with the largest degree and is independent of the system size n.

Nevertheless, Chung et al. [11] showed that, depending on the matrix, under a certain mild condition (that the minimum expected degree is significantly larger than the square root of the expected average degree), the eigenvalues of the normalized Laplacian of a random power-law graph follow the semicircle law, whereas the spectrum of the adjacency matrix of a power-law graph obeys the power law.

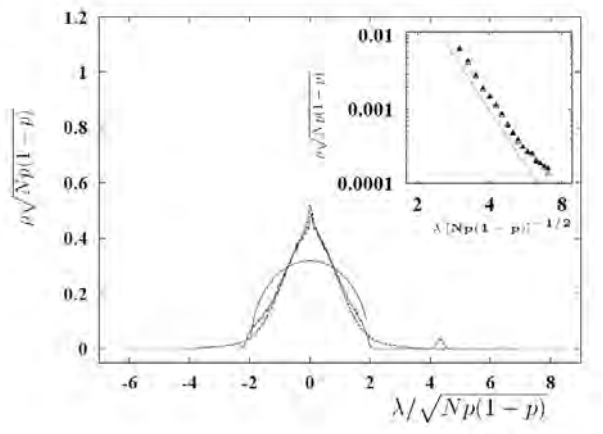

FIGURE 4. The spectral density of a Barabási-Albert graph with $m = 5$, and $n = 7000$ has a triangle-like shape compared with the semicircle, with a power-law decay in both sides. The isolated peak corresponds to the principal eigenvalue. In the upper corner the power-law decay is represented in a log-log scale. (from [26])

Furthermore, it has been reported that the k largest eigenvalues of the adjacency matrix of random power-law graphs have a power-law distribution (provided that the largest k degrees are large in the terms of the second-order average degree) [11, 26, 35, 41]. The k largest eigenvalues and eigenvectors have several applications in complex networks, as the search of clusters or communities (Section 4). For instance, Gkantsidis et al. [34] performed a comparison of clustering coefficients using the eigenvectors of the k largest eigenvalues of the adjacency matrices of Autonomous Systems (AS) topologies, where k is chosen to retain the strongest eigenvectors discarding most of the others. These and further results indicate that the spectra of correlated graphs represent a practical tool for graph classification and can provide useful insight into the relevant structural properties of real networks.

The spectra of the normalized Laplacian matrix of complex networks have been also studied, as its reflects global properties of the graph whereas the spectrum of the adjacency matrix contains information about local properties of the graph [11, 12]. Vukadinović et al. [57] were the first to investigate the properties of the AS topology based on the normalized Laplacian spectrum. They observed that it can be used to distinguish between synthetic topologies generated by graph generators like Inet and BGP. The eigenvectors corresponding to the largest eigenvalues of the Laplacian matrix can also be used to find clusters of AS with certain characteristics [34]

Other feature studied in [26] is the relation between the largest eigenvalue λ_1 and the "bulk" part of the spectrum $\lambda_2, \ldots, \lambda_n$. It is showed that in the case

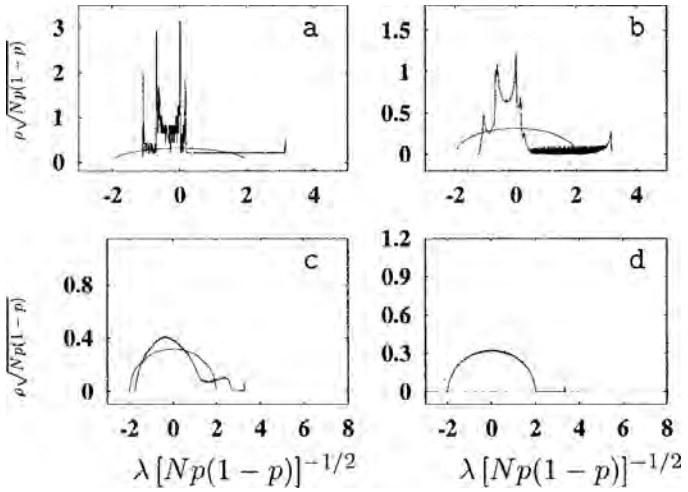

FIGURE 5. Spectral densities of several Watts and Strogatz small world models. The solid line shows the semicircular distribution for comparison: (a) with $p = 0$, $k = 10$ and $n = 1000$, the regular ring density is composed by a great deal of singularities, (b) with $p = 0.01$ the small-world graph density still has important singularities, (c) with $p = 0.3$ the small-world graph density is different from the semicircle shape, (d) and finally with $p = 1$ the uncorrelated random graph density has the semicircle shape. (from [26])

of random networks the largest adjacency eigenvalue grows much faster than the second largest one: $\lim_{n\to\infty}(\lambda_1/n) = p$ with probability 1, while for any $\epsilon > 1/2$, $\lim_{n\to\infty}(\lambda_2/n^\epsilon) = 0$. A similar relation holds for the smallest eigenvalue as well. This means that the spectral gap $g(A) = \lambda_1 - \lambda_2$ grows very fast, while the bulk of the spectrum is concentrated in a semi-circle denoted by $w(A) = \lambda_2 - \lambda_n$ (see Fig. 4). Similar situations have been observed for small-world graphs as well as for scale-free graphs. The bulk part of the scale-free graphs the spectral density is triangle-like instead of semi-circular in the scale-free case. For this reason, the quantity $R = (\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_n)$ has been proposed as a measure of the distance of the first eigenvalue from the main part of the distribution of eigenvalues normalized by the extension of the main part (see Fig. 6). This ratio is intimate-related to some dynamical properties of the graph, as its synchronizability (Section 3).

Finally, the second largest eigenvalue of the Laplacian matrix or algebraic connectivity, has been also studied for either the Watts and Strogatz small-world model and the Barabási and Albert scale-free model in [58, 59]. For the former, they find a linear dependency between $-\theta_2$ and the rewiring probability p for a fixed n, that is, for any given value of n, $-\theta_2$ decreases to $-n$ as p increases from 0 to 1. And for the later they find that for any given value of $p \in (0, 1]$, $-\theta_2$ decreases to $-\infty$ as n increases to $+\infty$ (see Fig. 7 and Fig. 8)

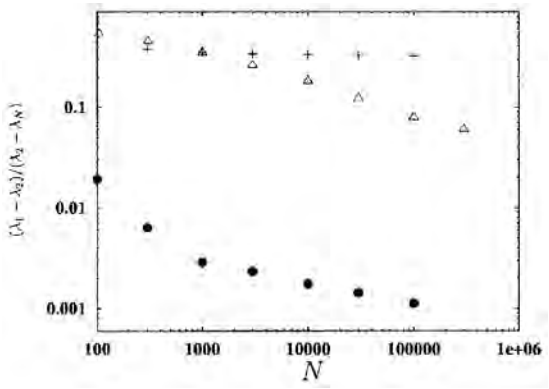

FIGURE 6. The ratio $R = (\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_n)$ for a sparse uncorrelated random graph (+), small-world graph with $p = 0.01$ (•) and scale-free network (△), versus the size of the graph n. Observe that for the first R converges to a constant, whereas for the others decays rapidly as $n \to \infty$. (from [26])

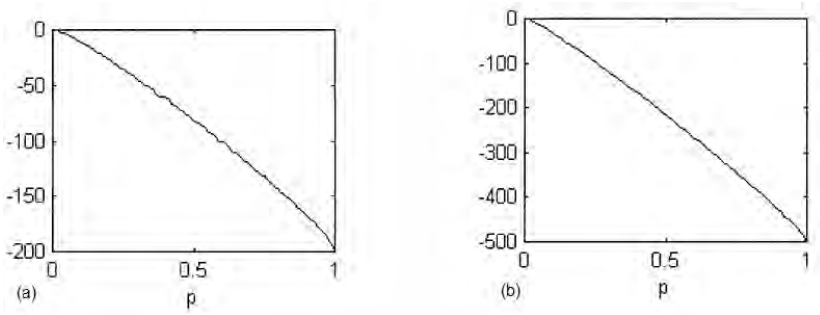

FIGURE 7. The opposite of the algebraic connectivity, $-\theta_2$, at two Watts and Strogatz models as a function of the probability, for (a) $n = 200$ and (b) $n = 500$. (from [59])

The opposite of the algebraic connectivity at the Barabási and Albert model is studied in [58] for three cases, obtaining in all of them that $-\theta_2$ bounded function as n increases to ∞ (Fig. 9). Observe that it has a small value, which implies that scale-free networks have poor synchronizability (Section 3).

3. Synchronization

Synchronization is the process where two or more systems interact with each other and come to move together. Synchronization processes are ubiquitous in nature and are present in many different contexts such as biology, technology, sociology, climatology, etc. The dynamics e.g., of the human cardiorespiratory system, of

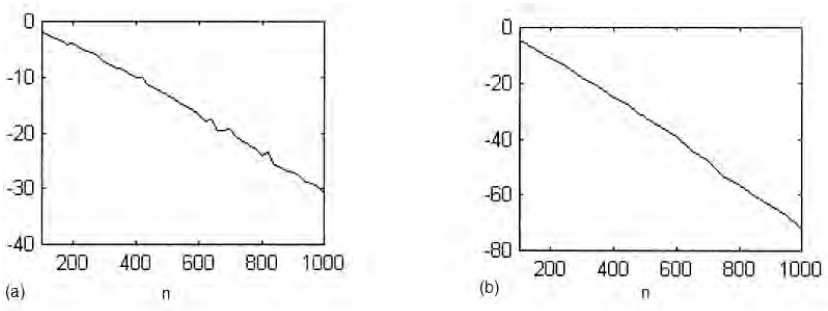

FIGURE 8. The opposite of the algebraic connectivity, $-\theta_2$, at two Watts and Strogatz models as a function of the size of the network n, for (a) $p = 0.05$ and (b) $p = 0.1$. (from [59])

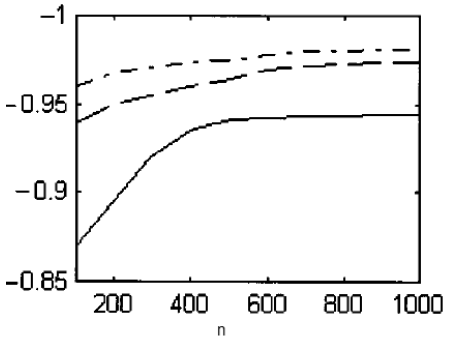

FIGURE 9. The opposite of the algebraic connectivity, $-\theta_2$, at the Barabási and Albert model with $m_0 = m = 3$ (lower), $m_0 = m = 5$ (middle) and $m_0 = m = 7$ (upper). (from [58])

an extended ecological system, of the magnetoencephalographic activity of Parkinsonian patients, and of electrosensitive cells of the paddlefish, have been shown to display synchronization features.

Historically, in 1667 Huygens observed the first synchronization phenomenon between two pendulum metronomes: putting them side by side oscillating at the same frequency with a 180° out of phase, after a small perturbation the clocks ended up synchronizing and persisted indefinitely. The synchronization of a few interacting oscillators has been widely studied in physics and mathematics literature, and also other aspects like the stability of the synchronization state against small perturbations. Initially, the attention was mainly focused to synchronization of periodic systems, while recently the interest for synchronization has moved to chaotic systems, as they are bound to be more common in nature. A dynamical system is called chaotic whenever its evolution sensitively depends on the initial

conditions. There are several types of synchronization features in chaotic systems: complete synchronization, lag synchronization, generalized synchronization, phase and imperfect phase synchronization. The most studied is the complete synchronization, which consists of the perfect hooking of the trajectories of a system of identical chaotic oscillators in the course of the time.

From different theoretical frameworks considered to study the synchronization of complex networks, their topology has turned out to play a crucial role in determining their dynamical behavior. Several models for real networks associated with complex systems are used to study relationships between the system synchronization and graph invariants, as well as some of the system relevant topological parameters. To be more precise, the Laplacian spectra and the algebraic connectivity or second smallest eigenvalue of the Laplacian matrix are important factors for obtaining the synchronization state or the stability of the synchronization state for some of these theoretical models. Their relation with other topological parameters of the network, as the diameter or the mean distance, provides some interesting conditions for existence of the synchronization. Besides, the recent appearance of large complex networks and the study of their dynamical characteristics, has become a new challenge for the scientific community. Synchronization in small-world and scale-free networks have aroused a great deal of interest. For more information about synchronization theory in dynamical systems we refer the reader to review papers [1, 5].

Therefore in this section we first study two of these theoretical frameworks relating synchronization with Laplacian eigenvalues. By using known bounds for the algebraic connectivity θ_2 and the largest Laplacian eigenvalue θ_n we derive bounds for the synchronization ratio θ_n/θ_2. And finally we take advantage of the classical techniques from the spectral graph theory [17] to construct a large family of highly synchronizable networks.

Coupled identical oscillators. In the work [50] of Pecora and Caroll the stability of the synchronized state of a network of coupled identical oscillators is studied by using the so-called Master Stability Function. When all the oscillators are initially synchronized it is a crucial question to know whether this state is stable in the presence of small perturbations. The motion of a system is described by the general equation

$$\dot{x} = F(x), \quad x \in \mathbb{R}^n.$$

Considering linear time-continuous systems, this equation turns out into:

$$\dot{x}_i(t) = F(x_i(t)) + \sigma \sum_{j=1}^{n} L_{ij} H(x_j(t)), \quad i = 1, \ldots, n, \tag{3.1}$$

where $x_i(t) = (x_{i_1}(t), \ldots, x_{i_n}(t))^T \in \mathbb{R}^n$ represents the state variables at each oscillator i. The first part of the equation, $\dot{x}(t) = F(x(t))$ explains the dynamics of each node, and the function $H(x(t))$ is the output function (the same at each node), which represents the influence of network in the oscillator i. The parameter σ is the coupling strength, and L is the Laplacian matrix. There is a completely

synchronized state if

$$x_1(t) = x_2(t) = \cdots = x_n(t) = s(t),$$

where $s(t)$ is the desired synchronized state. When all the oscillators are initially synchronized, they remain synchronized until the presence of small perturbation interferes. Now the question is whether the synchronization state is stable in the presence of small perturbations δx_i. In this case $x_i(t) = s(t) + \delta x_i$, and expanding the functions F and H to first order in a Taylor series, i.e., $F(x_i) = F(s)+DF(s)\delta x_i$ and $H(x_i) = H(s)+DH(s)\delta x_i$, where $DF(s)$ and $DH(s)$ are the Jacobian matrices of L and H on s respectively, we obtain the following variational linear equations for δx_i

$$\delta x_i = DF(s) + \sigma DH(s) \sum_{j=1}^{n} L_{ij}\delta x_j, \quad i = 1, \ldots, n.$$

By projecting $\delta f x_i$ into the eigenspaces spanned by the eigenvectors v_i of the Laplacian matrix L, the former equations that can be diagonalized into blocks as

$$\dot{y}(t) = [DF(s) + \theta DH(s)]y(t),$$

where y represents the different perturbation modes from the synchronized state, $\theta = \sigma\theta_i$ for each i-block, with θ_i the i-th eigenvalue of the Laplacian matrix, $i = 1, \ldots, n$. The idea is to project δx_i into the eigenspace spanned by the eigenvectors v_i of the coupling matrix L.

The linear stability of the synchronized state for any linear coupling is provided by the largest Lyapunov exponent of this equation $\Delta(\theta)$. In [50] it is shown that the synchronization state is stable if $\Delta(\sigma\theta_i) < 0$ for $i = 2, \ldots, n$. Moreover, it has been found [3] that for many chaotic oscillators there exists a range of values in the interval (α_1, α_2) where this condition is satisfied. In this case, there exists a value of the coupling strength σ such that the synchronization state is linearly stable if and only if

$$\theta_n/\theta_2 < \alpha_2/\alpha_1 \equiv \beta,$$

where β is a constant independent of the Laplacian matrix L. The values for β depend on the different kind of oscillator, but for many chaotic oscillators they use to be between 5 and 100 [50]. Therefore, for large values of θ_n/θ_2 it is not possible to obtain synchronization, independently of the value of the coupling strength and the kind of oscillator.

Furthermore, Wang and Chen in a former paper [58], study the asymptotical synchronization of a dynamical network model characterized by Equation 3.1 with $H(x_j(t)) = -x_j(t)$. It is said that the dynamical system reaches a state of asymptotical synchronization if

$$x_1(t) = \cdots = x_n(t) = s(t),$$

when $t \to \infty$, where $s(t)$ can be an equilibrium point, a periodic orbit, or a chaotic attractor. They show that the system is exponentially stable if $1/\theta_2$ is bounded by a constant.

In both models we can see that the synchronization of the network depends on algebraic connectivity θ_2. When it is close to 0, $1/\theta_2$ is large, then the network

cannot reach a synchronization state. Besides, in the first model the largest Laplacian eigenvalue θ_n has also a great influence, and more precisely the ratio θ_n/θ_2, should also be small to attain synchronizability. Nevertheless, these two Laplacian eigenvalues by themselves do not provide information about the relationship between the network topology and the dynamics of synchronization. In the following subsection we will study some spectral bounds obtained from the classical spectral graph theory that will provide a connection between the synchronization of a network and several of its main invariants and parameters.

3.1. Synchronization and topological parameters. In order to characterize the synchronization of a network, we study the relationship between the inverse of the second eigenvalue of the Laplacian matrix, $1/\theta_2$, and the ratio θ_n/θ_2, with other graph topological parameters like the minimum and maximum degrees, diameter, mean distance, isoperimetric number, betweenness centrality and clustering parameter. Most of these bounds can be found in [16]. From the bounds that can be obtained for $1/\theta_2$ and by using the classical bound $\Delta < \theta_n \leqslant 2\Delta$ provided by Fiedler [27] we can derive new lower and upper bounds for the synchronization ratio θ_n/θ_2.

Minimum and maximum degrees of the graph. The minimum degree of a graph, δ, is related to the minimum connectivity of the graph. As $\theta_2 \leqslant \delta n/(n-1)$, and $\theta_n \geqslant (\Delta+1)$ (see [36]), one can be obtain

$$\Big(1-\frac{1}{n}\Big)\frac{(\Delta+1)}{\delta} \leqslant \frac{\theta_n}{\theta_2}.$$

When the difference between the maximum and minimum degree is large (hetereogenity), the synchronizability will be not reached. Now considering scale-free networks, for which $\delta = 1$, and Δ, n are large then $1-1/n \simeq 1$, and $(\Delta+1) \leqslant \theta_n/\theta_2$, which means that the network has a very low synchronization capability.

Edge connectivity. From a bound in [27] it can be easily obtained:

$$\frac{\theta_n}{\theta_2} \leqslant \frac{\Delta}{e(G)\big(1-\cos\frac{\pi}{n}\big)}.$$

Observe that when n is large the bound becomes independent of the value of $e(G)$, which does not provide much information.

Diameter. One of the bounds relating the algebraic connectivity with the diameter was given by Mohar in [43] as $D \geqslant 4/(n\theta_2)$ and so we obtain:

$$\frac{\theta_n}{\theta_2} \leqslant \frac{nD\Delta}{2}.$$

For graphs with a large D or n, this equation provides a large upper bound. However, if both values are small then the network will be easy to synchronize. A lower bound for the inverse algebraic connectivity can be obtained from the diameter bound $D \leqslant 2\big\lceil \frac{\Delta+\theta_2}{4\theta_2}\ln(n-1)\big\rceil$ from [43], where Δ is the maximum degree of the graph:

$$\Big(\frac{4}{\ln(n-1)}\Big\lfloor\frac{D}{2}\Big\rfloor - 1\Big)\frac{(\Delta+1)}{\Delta} \leqslant \frac{\theta_n}{\theta_2}.$$

From the former equation, note that if $D \gg \ln(n-1)$, then the bound is greater than 1, and it will be difficult to reach a synchronization state provided that the maximum degree Δ is very large.

Now, consider the following bound in [43]: if there are two subsets of vertices, B and C, at distance $r+1$:

$$4(r-1)^2 \frac{|B||C|}{(n-|B|-|C|)\cdot(|B|+|C|)} < \frac{\theta_n}{\theta_2},$$

where $|B|$ are $|C|$ are the cardinalities of the subsets. If both subsets have only one vertex and they are at maximum distance D, the bound results

$$\frac{2(D-2)^2}{(n-2)} < \frac{\theta_n}{\theta_2}.$$

For large n and a small D the bound will tend to 0 and synchronization is possible. Also, for graphs with a diameter close to n would lead to large lower bound and the networks will not synchronize.

Studies about the diameter in small-world networks show that many real networks associated with complex systems have a logarithmic diameter $D \sim \ln n$ (similar to). In this case, the lower bound can be written approximately as $1/\Delta \leqslant 1/\theta_2$. Since the maximum degree Δ is also large, in scale-free networks the lower bound will approach 0 and synchronization is possible.

Mean distance. In [43] several bounds relating the mean distance with the algebraic connectivity can be found. Firstly we find this bound relating the mean distance with Q:

$$\bar{l} < \frac{n}{n-1}\left[1+\sqrt{\frac{\theta_n}{\theta_2}}\sqrt{\frac{\alpha^2-1}{4\alpha}}\right]\left(\frac{1}{2}+\left\lceil \log_\alpha \frac{n}{2}\right\rceil\right),$$

where $\alpha > 1$ is a parameter. A large mean distance hinders the network synchronization. A lower bound can be obtained from

$$\bar{l} \leqslant \frac{n}{n-1}\left(\left\lceil \frac{\Delta+\theta_2}{4\theta_2}\ln(n-1)\right\rceil + \frac{1}{2}\right),$$

$$\left(\left\lfloor \frac{2\bar{l}(n-1)-n}{2n\ln(n-1)}\right\rfloor - \frac{1}{4}\right)\frac{4(\Delta+1)}{\Delta} \leqslant \frac{\theta_n}{\theta_2}.$$

Note that as n becomes large, the bound takes a lower value if the mean distance is also small. However, if n is small and $\bar{l}$ relatively large, the bound is also large and the synchronization of the network would not be possible. The maximum degree also is an influence on the synchronization, larger degrees make it easier.

Isoperimetric number of a graph or Cheeger constant. In [42] we find two different bounds for the isoperimetric number. The lower bound $i(G) \geqslant \theta_2/2$, gives us

$$\frac{\Delta+1}{2i(G)} \leqslant \frac{\theta_n}{\theta_2}.$$

From this bound, if the isoperimetric number is near 0, the network will be easy to disconnect in two parts and by using the previous bound the inverse algebraic connectivity will be large, and the synchronization would not be possible. Cheeger

inequalities relate the isoperimetric number of a graph with its algebraic connectivity θ_2 and its maximum degree Δ. From the upper bound $i(G) \leqslant \sqrt{\theta_2(2\Delta - \theta_2)}$, we have the inequality $\theta_2^2 - 2\Delta\theta_2 + i(G)^2 \leqslant 0$ which leads us to

$$\frac{2}{1+\sqrt{1-(i(G)/\Delta)^2}} \leqslant \frac{\theta_n}{\theta_2} \leqslant \frac{2}{1-\sqrt{1-(i(G)/\Delta)^2}}.$$

In this case, if $i(G) \sim \Delta$, then both bounds in reach 2 and the synchronization should be possible, meanwhile $i(G) \sim 0$ the lower bound goes to infinity and the network cannot synchronize.

Betweenness centrality and maximum betweenness centrality. The maximum betweenness centrality, $B_{\max}$, is larger than $\overline{B}$, so the corresponding lower bounds can also be used to obtain lower bounds. Moreover, in [15] a bound can be found that relates $B_{\max}$ to the isoperimetric number:

$$B_{\max} + 2 \geqslant \frac{n}{\sqrt{\theta_2(2\Delta - \theta_2)}}.$$

Therefore it can be easily deduced that

$$\frac{\Delta}{\Delta+\sqrt{\Delta^2-(n/(B_{\max}+2))^2}} \leqslant \frac{\theta_n}{\theta_2} \leqslant \frac{2\Delta}{\Delta-\sqrt{\Delta^2-(n/(B_{\max}+2))^2}}.$$

Observe that if $(B_{\max}+2)/\Delta \sim n$, then $\theta_n/\theta_2 \leqslant 2$ and synchronization is possible, but if $B_{\max}+2 \sim 2n(n-1)+2$ (as in a star graph), then $1/2\Delta \leqslant 1/\theta_2 \leqslant \infty$ and the bounds are not useful to describe the synchronizability of a network.

The following lower and upper bounds are given in [49]:

$$\Big(1-\frac{1}{n}\Big)\frac{\Delta}{\delta} \leqslant \frac{\theta_n}{\theta_2} \leqslant (n-1)\Delta\mathcal{B}^E_{\max}D\bar{l},$$

where $\mathcal{B}^E_{\max}$ is the maximum edge betweenness of the network [15, 33]. From the lower bound it can be deduced that the heterogeneity of degrees affects the synchronization of the network. A large difference between the maximum and minimum degrees makes the network more difficult to synchronize, which uses to happen in scale-free networks. However, homogeneous networks not always synchronize. Several studies on model networks corroborate this result in [30].

3.2. Design of synchronizable networks.

As seen in previous sections, both scale-free and small-world networks display better synchronization than regular graphs [3]. However, it has also been observed that networks with strong heterogeneity in the degree distribution are much more difficult to synchronize than random homogeneous networks [49]. Donetti et al. in [19, 20] proposed entangled networks, which are extremely homogeneous regular networks, as examples of highly synchronizable networks. These graphs are obtained by using a numerical optimization algorithm, which excludes the possibility of using mathematical tools to generate infinitely many such networks. However, Estrada et al. [24, 7] propose a different approach, introducing a family of graphs (golden spectral graphs) which can be built by using analytical tools from the classical algebraic graph theory [17].

Observe that for a regular graph the synchronization ratio is related with R by

$$Q = \frac{\theta_n}{\theta_2} = \frac{\lambda_1 - \lambda_n}{\lambda_1 - \lambda_2} = \frac{\lambda_2 - \lambda_n}{\lambda_1 - \lambda_2} \cdot \frac{\lambda_1 - \lambda_n}{\lambda_2 - \lambda_n} = \omega_1(G) \cdot \omega_2(G) = \frac{1}{R} \cdot (R+1),$$

where

$$\omega_1(G) = \frac{\lambda_2 - \lambda_n}{\lambda_1 - \lambda_2}, \quad \lambda_1 \neq \lambda_2, \qquad \omega_2(G) = \frac{\lambda_1 - \lambda_n}{\lambda_2 - \lambda_n}, \quad \lambda_2 \neq \lambda_n,$$

are inverse, and therefore it is not easy to find graphs in which their product is small. This fact clearly hampers the synchronization of the network. In the search of graphs with small $Q = \omega_1(G) \cdot \omega_2(G)$, we consider those where both spectral ratios are equal, as it is straightforward to check that in this case $\omega_1(G) = \omega_2(G) = \varphi = (1+\sqrt{5})/2$ and thus $Q = \varphi^2 = \varphi + 1$.

Definition 3.1. A golden spectral graph (GSG) is a graph for which both spectral ratios are identical, that is

$$\omega_1(G) = \omega_2(G) = \varphi,$$

where $\varphi = (1+\sqrt{5})/2$ is the golden section, golden mean or divine proportion.

The first examples and properties of golden spectral graphs are found by Estrada in [7] and amplified in [24] by using classical spectral techniques, finding infinite families of such graphs (see Fig. 10).

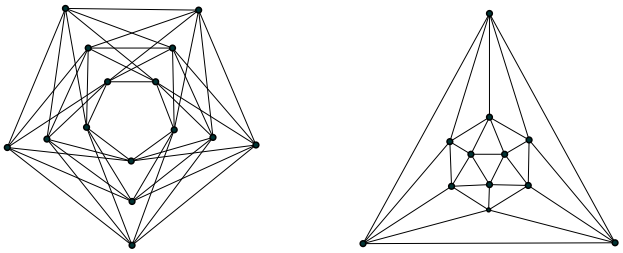

FIGURE 10. Two examples of highly synchronizable networks: $C_5 \otimes J_3$ and the icosahedral graph.

4. Community detection and spectral bisection

Empirical studies reveal a common property between many networks: community structure, i.e., the division of network vertices into groups with dense connections between them and sparse connections between groups [33, 47]. Communities are important because they often correspond to functional units such as cycles or pathways in metabolic networks or collections of pages on a single topic on the web. Moreover, networks can have properties at the community level that are quite different for the entire network.

A huge variety of community detection techniques have been developed, based on centrality measures, spectral techniques, flow models, random walks, resistor networks, optimization and many other approaches [18, 47]. There is a large literature about finding connections between divisions of networks and matrix spectra, the so-called spectral partition or spectral clustering [56]. The main tools for spectral clustering are graph Laplacian matrices or normalized Laplacian matrices. Most approaches to graph partitioning are based on iterative bisection methods, that is, finding the best division of the graph into two groups and then further subdividing those two into more groups. The spectral bisection method is originally due to Fiedler [27] and popularized by Pothen et al. [51], and is based on the Laplacian matrix eigenvectors. We describe here the simplest form of this method.

For dividing the graph into two subgraphs it is usual to consider the following parameter:

Definition 4.1. Given two subsets A and B of the vertex set $V(G)$ of a graph G and forming a partition of it, the number of edges connecting them is called the cut size

$$R = \frac{1}{2} \sum_{i \in A,\, j \in B} a_{i,j}, \tag{4.1}$$

where the factor $1/2$ compensates for counting each edge twice.

Now consider an index vector s with n elements as

$$s_i = \begin{cases} 1, & \text{if } i \in A, \\ -1, & \text{if } i \in B. \end{cases} \tag{4.2}$$

Observe that $s^T s = n$, and

$$\frac{1}{2}(1 - s_i s_j) = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are in different groups,} \\ 0, & \text{if } i \text{ and } j \text{ are in the same group.} \end{cases}$$

This allows us to rewrite Equation 4.1 as

$$R = \frac{1}{4} \sum_{i,\, j \in V(G)} (1 - s_i s_j) a_{i,j}.$$

Recalling that the degree of a vertex i is $k_i = \sum_j a_{ij}$, then

$$\sum_{i,j \in V(G)} a_{ij} = \sum_{i \in V(G)} k_i = \sum_{i \in V(G)} s_i^2 k_i = \sum_{i,j \in V(G)} s_i s_j k_i \delta_{ij},$$

where $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. Therefore

$$R = \frac{1}{4} \sum_{i,j \in V(G)} s_i s_j (k_i \delta_{ij} - a_{i,j}) = \frac{1}{4} s^T L s.$$

Considering an orthogonal basis of Laplacian eigenvectors v_i, for $1 \leqslant i \leqslant n$, the index vector s can be expressed as a linear combination of the Laplacian eigenvectors,

$s = \sum_{i=1}^{n} \alpha_i v_i$, where $\alpha_i = v_i^T s$. Note that $\sum_{i=1}^{n} \alpha_i^2 = n$, then

$$R = \Big(\sum_{i \in V(G)} \alpha_i v_i^T \Big) L \Big(\sum_{i \in V(G)} \alpha_i v_i \Big) = \sum_{i \in V(G)} \alpha_i^2 \theta_i.$$

Therefore minimizing R implies minimizing α_i^2. So fixing both sizes of the subgraphs $|A| = n_1$ and $|B| = n_2$, observe that $\alpha_1^2 = (v_1^T s)^2 = (n_1 - n_2)^2/n$. As we cannot vary this coefficient, R would be minimized by taking s proportional to v_2 (the Fiedler vector, which is orthogonal to v_i, for $i \geqslant 3$). However, the restriction due to Equation 4.2 implies that this cannot be possible in most of the cases, but a good approximation could be taking s as close to a parallel vector with v_2 as possible. This implies maximizing the quantity

$$|v_2^T s| = \left| \sum_{i=1}^{n} v_i^{(2)} s_i \right| \leqslant \sum_{i=1}^{n} |v_i^{(2)}|,$$

where $v_i^{(2)}$ are the i-components of the Fiedler vector. The maximum of $|v_2^T s|$ is reached when $v_i^{(2)} s_i \geqslant 0$ for all $1 \leqslant i \leqslant n$, that means that s_i must have the same sign as $v_i^{(2)}$. Therefore, the sign of each component $v_i^{(2)}$ of the Fiedler vector determines if the vertex i belongs to either A or B, which very often is against the condition of the desired sizes of the two subgraphs. In such a case, several options can be taken, as assigning either the most positive elements of s to the smaller group or to the larger group, and then taking the option which gives the smallest R.

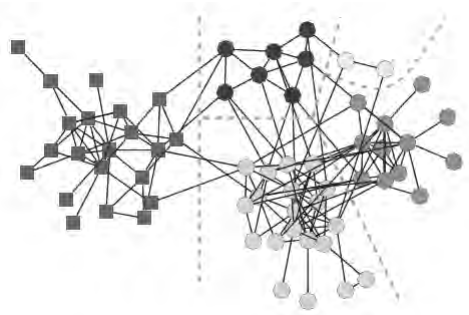

FIGURE 11. Community structure in the social network of bottlenose dolphins assembled by Lusseau et al. extracted using the algorithm of Girvan and Newman. The squares and circles denote the initial split of the network by using the bisection method. (from [47])

Consequently, the method does not guarantee to minimize R, but in many cases (when θ_2 is well separated from the rest of the eigenvalues), it does it very well. Generalizations of this method for a partition of k vertices subsets has been also

studied, and besides using other kinds of Laplacian matrices. For an extensive study about this subject we refer the reader to [56].

However, the method is a poor tool for detecting natural community structure in real-world networks, as the sizes of the groups are fixed from the beginning. Several approaches have been proposed to solve this problem. For this reason, Girvan and Newman [33] implemented an algorithm for calculating the modularity of the network, a new measure of how good is a particular division of the network is (see Fig. 11). That is, for a division with k groups, consider the $k \times k$ matrix E whose component e_{ij} is the fraction of edges in the original network that connect vertices in group i to those in group j. Then the modularity index is defined as

$$Q = \sum_i e_{ii} - \sum_{ijk} e_{ij} e_{ki}.$$

Physically Q is the fraction of all edges that lie within communities minus the expected value of the same quantity in a graph in which the vertices have the same degrees but where edges are placed at random without regard for the communities. If $Q = 0$ the community structure is not stronger than the one that can be expected by random chance. Local peaks in the modularity during the progress of the community structure algorithm indicate particularly good divisions of the network.

Modularity can also be approached by spectral methods. In [48] three spectral techniques can be found for approximating this parameter: the leading eigenvector method, other eigenvectors of the modularity matrix and a vector partitioning algorithm. All of them follow similar spectral techniques to the ones used in the first part of this section.

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APPLICATIONS OF GRAPH SPECTRA IN QUANTUM PHYSICS

Abstract. Graph spectra are closely related to many applications in quantum physics: a network of quantum particles with fixed couplings can be modelled by an underlying graph, with the Hamiltonian of such system approximated by the adjacency matrix of that graph, and the energy levels and states represented by the eigenvalues and eigenvectors of the adjacency matrix. From that viewpoint, quite a few quantum physics problems can be posed in terms of the spectral properties of the graph. In this chapter we survey one particular problem which received a lot of attention recently: the existence of *perfect state transfer* in the network of spin-1/2 particles.

Mathematics Subject Classification (2010): Primary: 05-02, 05C50; Secondary 81P68

Keywords: Quantum spin system; Perfect state transfer.

Contents

1. Introduction

Graph spectra have had a long history of applications in statistical physics, through dimer problem, and in chemistry, through Hückel's theory [31]. Here we survey another, more recent application of graph spectra in sciences, this time in quantum physics, through the problem of establishing perfect transfer of qubit states in the network of spin-1/2 particles. Most of the results we review here were published with last six years.

After necessary initial review in Section 2 of quantum mechanical terms and notions, assembled by a non-physicist for other non-physicists, the notion of perfect state transfer is defined in Section 3. These two sections are the only ones dealing with physical aspects of perfect state transfer, the rest of the survey being devoted to mathematical results. It turns out that it is not easy to find graphs admitting perfect state transfer between a pair of its vertices: in Section 4 it is shown that any automorphism of a graph fixing one vertex must fix the other vertex as well, and that the angles of both vertices have to coincide. Among paths, only those of lengths 2 and 3 admit perfect state transfer, while it does not exist in any longer path (Section 5). Regular, integral graphs turn out to be presently richest source of graphs with perfect state transfer: some particular examples are exhibited in Section 6, while the classes of cubelike and integral circulant graphs are treated in Sections 8 and 9. From known graphs with perfect state transfer it is possible

to construct new graphs admitting perfect state transfer: the Cartesian product of graphs is best suited in this respect (Section 7), while a few more specialized constructions are given in Section 10. In Section 11 we review a concept of routing of quantum states, which further builds upon the concept of perfect state transfer and may present the source of new, interesting mathematical problems. Concluding remarks are given in Section 12.

We review here perfect state transfer in uniformly coupled spin networks (simple graphs) only. Another aspect of perfect state transfer that we do not consider here is its physical implementation. There is a large body of physics literature on this topic, and most of it is listed in references, so that the interested researcher may find the list of references as a useful start point.

2. Basics of quantum mechanics

Bra-ket notation. Bra-ket notation was introduced in 1939 by Paul Dirac, and is also known as Dirac notation [92]. It is used to denote abstract vectors and linear functionals in mathematics, and it is a standard notation for describing quantum states in the theory of quantum mechanics. It is called bra-ket because the inner product of two states (vectors) is denoted by a bracket, $\langle x|y\rangle$, consisting of a left part *bra*, $\langle x|$, and a right part *ket*, $|y\rangle$. The bra $\langle x|$ represents a row vector x^T, while the ket $|y\rangle$ represents a column vector y. Thus, $\langle x|y\rangle$ is same as $x^T y$. If $A\colon H \to H$ is a linear operator, applying A to the ket $|y\rangle$ gives a new ket $A|y\rangle$. Thus, $\langle x|A|y\rangle$ is same as $x^T Ay$.

Classical and quantum description of mechanics A physical system is generally described by three basic ingredients: states; observables; and dynamics (or law of time evolution) or, more generally, a group of physical symmetries. A classical description can be given in a fairly direct way by a phase space model of mechanics: states are points in a symplectic phase space, observables are real-valued functions on it, time evolution is given by a one-parameter group of symplectic transformations of the phase space, and physical symmetries are realized by symplectic transformations [93].

In a quantum description, each physical system is associated with a (topologically) separable complex Hilbert space $\mathcal{H}$ with inner product $\langle x|y\rangle$. Rays (one-dimensional subspaces) in $\mathcal{H}$ are associated with states of the system. In other words, physical states can be identified with equivalence classes of unit vectors in $\mathcal{H}$, where two vectors represent the same state if they differ only by a phase factor. Physical observables are represented by densely-defined self-adjoint operators on $\mathcal{H}$. The expected value of the observable A for the system in state represented by the unit vector $|\psi\rangle \in \mathcal{H}$ is $\langle\psi|A|\psi\rangle$. The possible values of the observable A in any state must belong to the spectrum of A, and in the special case A has only discrete spectrum, the possible outcomes of measuring A are its eigenvalues.

Schrödinger equation and Hamiltonian The time evolution of the state is given by a differentiable function from $\mathbf{R}$, representing instants of time, to the Hilbert space of system states. The *Schrödinger equation* [91] says that, if $|\psi(t)\rangle$

denotes the state of the system at any one time t, then

$$H|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle,$$

where H is a densely-defined self-adjoint operator, called the system Hamiltonian, i is the imaginary unit, and $\hbar$ is reduced Planck's constant. As an observable, H corresponds to the total energy of the system.

The Hamiltonian generates the time evolution of quantum states. Given the state at some initial time ($t = 0$), we can integrate Schrödinger equation to obtain the state at any subsequent time. In particular, if H is independent of time, then

$$|\psi(t)\rangle = e^{-\frac{itH}{\hbar}}|\psi(0)\rangle.$$

As everything in quantum setting is quantized in terms of $\hbar$, it is usual to assume $\hbar = 1$ so that times and energies can be treated as dimensionless. The operators

$$U(t) = e^{-itH} = \sum_{n\geqslant 0}\frac{i^n t^n H^n}{n!}$$

form a one-parameter unitary group $U(t)\colon \mathcal{H} \to \mathcal{H}$, which realize physical symmetries of the closed quantum system.

Spin Experiments show that most subatomic particles have a permanent, built-in angular momentum, which is not due to their motion through space. This quantity is called the *spin* [91], and it has no correspondence at all in conventional physics. The spin σ comes in units of $\hbar/2$ and it belongs to the discrete set of values: $\sigma \in \{-S\hbar, -(S-1)\hbar, \dots, +(S-1)\hbar, +S\hbar\}$, where S is the *spin quantum number* of a particle. All elementary particles of a given kind have the same spin quantum number S. One distinguishes *bosons* ($S = 0, 1, 2, \dots$) and *fermions* ($S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$). Quanta of light are bosons with $S = 1$ and electrons are fermions with $S = 1/2$.

Qubit The unit of quantum information—the quantum analogue of the classical bit—is a quantum bit, or *qubit* [1, 95]. Contrary to a classical bit, the qubit is described by state of a spin-$\frac{1}{2}$ particle (although any two-level quantum system, such as quantum dot, may be used to describe qubit). The qubit has two basis states in which its spin can be measured: $|0\rangle$ corresponding to spin $-\frac{1}{2}$, and $|1\rangle$ corresponding to spin $+\frac{1}{2}$. A pure qubit state is a linear combination of $|0\rangle$ and $|1\rangle$,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where $\alpha, \beta \in \mathbf{C}$ are probability amplitudes. When we measure this qubit in the standard basis, the probability of outcome $|0\rangle$ is $|\alpha|^2$ and the probability of outcome $|1\rangle$ is $|\beta|^2$ (thus, $|\alpha|^2 + |\beta|^2 = 1$). Note, however, that when we measure the state of the qubit we alter the values of α and β: for instance, if the state $|0\rangle$ is measured, α is changed to 1 (up to phase) and β is changed to 0.

Geometrically, the state space of a single qubit can be represented by the Bloch sphere. This is a two-dimensional space which has an underlying geometry of the surface of a sphere, meaning that the single qubit register space has two local degrees of freedom. Represented on such a sphere, a classical bit could only be on

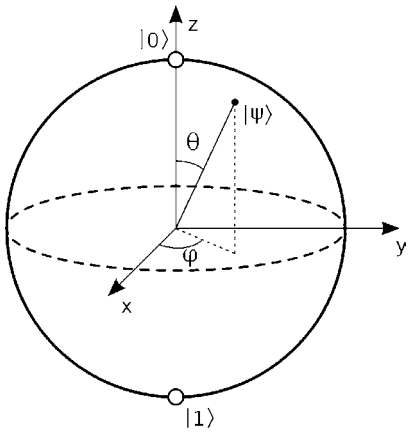

FIGURE 1. Bloch sphere.

the z-axis at the top or bottom of the sphere, in the locations where $|0\rangle$ and $|1\rangle$ are. The rest of the surface is inaccessible to a classical bit.

Unitary transformations that can be performed on pure qubit states correspond to rotations of the Bloch sphere. These rotations can be represented as combinations of rotations about the x-axis (σ_x), the y-axis (σ_y), or the z-axis (σ_z). For spin-$\frac{1}{2}$ particles, these basic rotations are represented by three Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Each Pauli matrix is an observable describing the spin of a particle in the three spatial directions.

Quantum computing A quantum computer is a computation device that makes direct use of quantum mechanical properties, such as superposition and entanglement, to represent data and perform operations on them [94]. Although quantum computing is still in its infancy, experiments have been carried out in which quantum computational operations were executed on a very small number of qubits. If large-scale quantum computers can be built, they will be able to solve certain problems much faster than any current classical computers (for example Shor's algorithm for prime factorization). Quantum computer do not allow the computations of functions that are not theoretically computable by classical computers, i.e., they do not alter the Church-Turing thesis. The gain is only in efficiency.

Quantum computers only run probabilistic algorithms. A quantum computer is said to *solve* a problem if, for every instance, its answer will be right with high probability. In classical randomized computation, the system evolves according to the application of stochastic matrices, which preserve that the probabilities add up to one (i.e., preserve the l_1 norm). In quantum computation, allowed operations are unitary transformations, which are effectively rotations. They preserve that

the sum of the squares add up to one, the Euclidean or l_2 norm). Consequently, since rotations can be undone by rotating backward, quantum computations are reversible.

When algorithm terminates, the result needs to be read off from a memory register. In a classical computer, which has a memory made up of bits, we sample from the probability distribution on the n-bit register to obtain one definite n-bit string. The memory register in a quantum computer is made up of n qubits, such that the state of each qubit is encoded with the state of the corresponding spin-$\frac{1}{2}$ particle. We read the quantum register by measuring qubit states, which is equivalent to collapsing the quantum state down to a classical distribution (with the coefficients in the classical state being the squared magnitudes of the coefficients for the quantum state) followed by sampling from that distribution. Note that n qubits can be in an arbitrary quantum superposition of up to 2^n different states simultaneously—this is a true advantage over classical computer which can only be in *one* of these 2^n states at any one time.

3. Perfect transfer of quantum states

An important task in quantum-information processing is the transfer of quantum states from one location (u) to another location (v). In general, photons are excellent flying qubits as they can be transmitted coherently over very large distances [38, 61], and optical systems, often employed in quantum communication and cryptography applications, transfer quantum states from u to v directly via photons [11, 12]. Thus, one possibility to transfer the quantum state is that it is imprinted onto a photon which is then used as the flying qubit over an optical fiber. However, it is very difficult to realize such transfer in solid-state quantum systems, as it requires perfect interface betwen photons and the main hardware of the quantum computer, and may not be worth it for short-distance communication (e.g., between two quantum processors).

Another way to accomplish quantum state transfer at short distance is by multiple applications of controlled swap operations along the communication line. However, every external manipulation inevitably induces noise in the system. It is therefore desirable to minimize the amount of external control on the system, to the point that it is not needed at all during the transfer. In such case, a *quantum wire*, the most fundamental unit of any quantum processing device, is made out of many interacting components [14, 28]. There are various physical systems that can serve as quantum wires, one of them being a quantum spin system. It is generally defined as a network of interacting qubits, whose dynamics is governed by a suitable Hamiltonian, e.g., the Heisenberg or XY Hamiltonian.

A quantum spin system is obtained by attaching a spin-$\frac{1}{2}$ particle to each vertex of a connected, finite graph $G = (V, E)$. To each vertex $i \in V$, one can associate a Hilbert space $\mathcal{H}_i \cong \mathbf{C}^2$, so that the Hilbert space associated with G is given by

$$\mathcal{H}_G = \bigotimes_{i \in V} \mathcal{H}_i \cong (\mathbf{C}^2)^{\otimes n},$$

where $n = |V|$ is the number of vertices in G. The dynamics of the system is governed by the XY Hamiltonian

$$H_G = \frac{1}{2} \sum_{(i,j)\in E(G)} J_{ij}[\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y],$$

where the symbols σ_i^x, σ_i^y and σ_i^z denote the Pauli matrices acting on the Hilbert space $\mathcal{H}_i$, and J_{ij} is the coupling strength between the vertices i and j of G. The couplings J_{ij} represent the weights of the edges of G, so that its adjacency matrix A_G is given by

$$A_{ij}(G) = \begin{cases} J_{ij}, & \text{if } (i,j) \in E \\ 0, & \text{if } (i,j) \notin E \end{cases}$$

Note that $J_{ij} = J_{ji}$ since H_G is Hermitian.

The total z component of the spin, given by

$$\sigma_{\text{tot}}^z = \sum_{i\in V} \sigma_i^z,$$

is conserved, i.e., $[\sigma_{\text{tot}}^z, H_G] = 0$. The Hilbert space $\mathcal{H}_G$ is then decomposed into invariant subspaces, each of which is a distinct eigenspace of the operator σ_{tot}^z.

For the purpose of quantum state transfer, it suffices to restrict our attention to the single excitation subspace $\mathcal{S}_G$, which is the n-dimensional eigenspace of σ_{tot}^z, corresponding to the eigenvalue $1 - \frac{n}{2}$. The quantum states initially in $\mathcal{S}_G$ will remain there under time evolution. A basis state in $\mathcal{S}_G$ corresponds to a configuration of spins in which all the spins except one are $|0\rangle$ and one spin is $|1\rangle$. Such a basis state can hence be denoted by the ket $|j\rangle$, where $j \in V$ is the vertex at which the spin is $|1\rangle_j$. Thus, $\{|j\rangle \colon j \in V\}$ denotes a complete set of orthonormal basis vectors spanning $\mathcal{S}_G$. When restricted to the subspace $\mathcal{S}_G$, H_G is represented, in this basis, by an $n \times n$ matrix which is *identical* to the adjacency matrix A_G. As known, the spectrum of the adjacency matrix of a graph is, by definition, the spectrum of the graph. In this way we see that the theory of graph spectra is relevant for the problems that we consider, i.e. in quantum computing. Some basic information on the theory of graph spectra can be found in the introductory chapter of this book, while further information may be found in the textbook [33].

The quantum spin system on G has the role of a (noiseless) quantum channel [28]. The process of transmitting a quantum state from u to v proceeds in four steps:

(1) Initialization of the spin system to the state $|\overline{0}\rangle := |0_u 0 \dots 0 0_v\rangle$. This is a zero-energy eigenstate of H_G.

(2) Creation of the quantum state $|\psi\rangle_u \in \mathcal{H}_u$ at vertex u to be transmitted. Let $|\psi\rangle_u = \alpha|0\rangle_u + \beta|1\rangle_u$ with $\alpha, \beta \in \mathbf{C}$ and $|\alpha|^2 + |\beta|^2 = 1$.

(3) Time evolution of the system for an interval of time, say t_0.

(4) Recovery of the state at vertex v.

The state of the entire spin system after step (2) is given by

$$|\Psi(0)\rangle = |\psi_u 0 \dots 0 0_v\rangle = \alpha|0_u 0 \dots 0 0_v\rangle + \beta|1_u 0 \dots 0 0_v\rangle = \alpha|\bar{0}\rangle + \beta|u\rangle.$$

Since the $|\overline{0}\rangle$ component of the state $|\Psi(0)\rangle$, as the zero-energy eigenstate of H_G, is invariant under the evolution, it suffices to focus on the evolution of the $|u\rangle$

component, i.e., to the choice $\alpha = 0$ and $\beta = 1$ above. This state evolves in time t to

$$|\Psi(t)\rangle = e^{-iA_G t}|u\rangle = \sum_{j=1}^{n} \beta_j(t)|j\rangle$$

with complex coefficients $\beta_j(t)$, where $1 = \sum_{j=1}^{n} |\beta_j(t)|^2$. At time t, the spin $|1\rangle_v$ may be measured at vertex v with probability $|\beta_v(t)|^2$, where

$$\beta_v(t) = \langle v|e^{-iA_G t}|u\rangle.$$

Thus, we say that G has *perfect state transfer* from u to v in time t if

$$|\langle v|e^{-iA_G t}|u\rangle| = 1.$$

In such case, $\langle j|e^{-iA_G t}|u\rangle = 0$ for all $j \neq v$. The effect of the modulus above is that the quantum state after transfer is not exactly equal $|v\rangle$, but rather $e^{i\phi}|v\rangle$. However, the phase factor $e^{i\phi}$ is not a problem, because ϕ will be a known quantity for G, and it can be corrected for with an appropriate phase gate.

The *communication distance* of a graph G is the maximum distance between vertices u and v of G for which perfect state transfer is possible. For a fixed number of qubits, the basic question is to find quantum spin systems which maximize the communication distance.

The time evolution of states in $\mathcal{S}_G$ under the action of the Hamiltonian H_G may also be interpreted as a *continuous-time quantum walk* on G, first considered by Farhi and Gutmann in 1998 [35] (see also [25]). The quantum walks are interesting in their own right due to their property of universal quantum computation [26].

Let λ_k and $|\mu_k\rangle$ be the eigenvalues and the unit eigenvectors of A_G, for $k = 1, \ldots, n$. Recall that, if f is a complex function defined on the eigenvalues of A, then

$$f(A_G) = \sum_{i=1}^{n} f(\lambda_i)|\mu_i\rangle\langle\mu_i|.$$

In particular,

$$e^{-iA_G t} = \sum_{i} e^{-i\lambda_i t}|\mu_i\rangle\langle\mu_i|,$$

and

$$\langle v|e^{-iA_G t}|u\rangle = \langle v|\left\{\sum_{k=1}^{n} e^{-i\lambda_k t}|\mu_k\rangle\langle\mu_k|\right\}|u\rangle.$$

One can use this formula to check that paths with two and three vertices have perfect state transfer between their end-vertices:

(a) For path $P_2 = (\{1,2\}, \{\{1,2\}\})$ we have

$$\langle 1|e^{-iA_{P_2} t}|2\rangle = -i\sin t \quad \text{and} \quad |\langle 1|e^{-iA_{P_2}\frac{\pi}{2}}|2\rangle| = 1.$$

(b) For path $P_3 = (\{1,2,3\}, \{\{1,2\},\{2,3\}\})$ we have

$$\langle 1|e^{-iA_{P_3} t}|3\rangle = -\sin^2(t/\sqrt{2}) \quad \text{and} \quad |\langle 1|e^{-iA_{P_3}\frac{\pi}{\sqrt{2}}}|3\rangle| = 1.$$

4. Consequences of perfect state transfer on relations between vertices

Let G be a graph of the quantum spin system with unit couplings and adjacency matrix A. Godsil [40] has recently derived few important lemmas on the relationship between vertices among which perfect state transfer occurs. Let $\mathrm{Aut}(G)_v$ denotes the group of automorphisms of G that fix its vertex v.

Lemma 4.1. [40] *If G admits perfect state transfer from u to v, then* $\mathrm{Aut}(G)_u = \mathrm{Aut}(G)_v$.

Proof. We identify the automorphisms of G with the permutation matrices that commute with A. Since e^{-iAt} is a polynomial in A, any permutation matrix from $\mathrm{Aut}(G)$ commutes with e^{-iAt}. If the automorphism associated with P fixes u, then $P|u\rangle = |u\rangle$. If perfect state transfer takes place at time τ and $H = e^{-iA\tau}$, then there is $\gamma \in \mathbf{C}$ such that $|\gamma| = 1$ and $H|u\rangle = \gamma|v\rangle$. So

$$\gamma P|v\rangle = PH|u\rangle = HP|u\rangle = H|u\rangle = \gamma|v\rangle$$

and thus v is fixed by P as well. Thus, $\mathrm{Aut}(G)_u \subseteq \mathrm{Aut}(G)_v$. The argument is same when we replace u and v, hence $\mathrm{Aut}(G)_v \subseteq \mathrm{Aut}(G)_u$ as well. □

Vertices u and v of G are *cospectral* if $\phi(G-u,t) = \phi(G-v,t)$, where $\phi(G,t) = \prod_{k=1}^{n}(t-\lambda_k)$ is the characteristic polynomial of G. Alternatively, u and v are cospectral if they have the same angles [32].

Lemma 4.2. [40] *If G admits perfect state transfer from u to v, then u and v are cospectral.*

Proof. By Cramer's rule,

$$((tI-A)^{-1})_{u,u} = \frac{\phi(G-u,t)}{\phi(G,t)}$$

and so using the spectral decomposition we find that

$$\frac{\phi(G-u,t)}{\phi(G,t)} = \sum_{k=1}^{n} \frac{\langle \mu_k|u\rangle^2}{t-\lambda_k}.$$

Let $\theta_1, \ldots, \theta_r$ be all distinct values among $\lambda_1, \ldots, \lambda_n$, and let $\mu_{j_i}, \mu_{j_i+1}, \ldots, \mu_{j_{i+1}-1}$ be the eigenvectors corresponding to θ_i, $1 \leqslant i \leqslant r$. The orthogonal projection onto the eigenspace corresponding to θ_i is given by

$$E_i = \sum_{k=j_i}^{j_{i+1}-1} |\mu_k\rangle\langle\mu_k|.$$

Assume we have perfect state transfer from u to v at time τ and set $H = e^{-iA\tau}$. Then there is $\gamma \in \mathbf{C}$ such that $|\gamma| = 1$ and $H|u\rangle = \gamma|v\rangle$. Since H is a polynomial in A, it commutes with each projection E_i and therefore

$$\gamma E_i|v\rangle = E_i H|u\rangle = HE_i|u\rangle.$$

As H is unitary, this implies that $E_i|v\rangle$ and $E_i|u\rangle$ have the same length, i.e.,

$$\sum_{k=j_i}^{j_{i+1}-1} \langle \mu_k|v\rangle^2 = \sum_{k=j_i}^{j_{i+1}-1} \langle \mu_k|u\rangle^2.$$

From this we conclude that $G-u$ and $G-v$ have the same characteristic polynomial. Thus u and v are cospectral. □

5. Eigenvalue ratio condition and periodic graphs

We say that G is *periodic relative to the vertex* u if there is a time t such that

$$|\langle u|e^{-iAt}|u\rangle| = 1.$$

We say that G is *periodic* if there is a time t such that e^{-iAt} is diagonal, i.e., if G is periodic relative to each of its vertices at the same time.

Theorem 5.1. [27, 39] *If G has perfect state transfer from u to v at time t_0, then G is periodic relative to u and v at time $2t_0$.*

Proof. With G initialized in the state $|u\rangle$, after time t_0 we have the state

$$e^{-iAt_0}|u\rangle = e^{i\phi}|v\rangle.$$

Since A is a symmetric matrix, it also holds that

$$e^{-iAt_0}|v\rangle = e^{i\phi}|u\rangle.$$

Thus, after another period of time t_0 we have the state

$$e^{-iA2t_0}|u\rangle = e^{-iAt_0}e^{i\phi}|v\rangle = e^{i2\phi}|u\rangle,$$

and the graph is periodic with period $2t_0$. □

The above proof also shows that if there is perfect state transfer between u and v at time t_0, then perfect state transfer also occurs for all times t of the form

$$t = (2k+1)t_0, \qquad \text{where } k \in \mathbf{Z}.$$

Theorem 5.2. [27, 39] *Let G has eigenvalues λ_j with corresponding eigenvectors $|x_j\rangle$, $j = 1, \ldots, n$. If G is periodic relative to the vertex u, then for each quadruple λ_k, λ_l, λ_r, λ_s of eigenvalues of G, such that $\langle x_k|u\rangle$, $\langle x_l|u\rangle$, $\langle x_r|u\rangle$, $\langle x_s|u\rangle \neq 0$ and $\lambda_r \neq \lambda_s$,*

$$\frac{\lambda_k - \lambda_l}{\lambda_r - \lambda_s} \in \mathbf{Q}. \tag{5.1}$$

The condition (5.1) is called the *eigenvalue ratio condition*.

Proof. Let $|u\rangle = \sum_j a_j|x_j\rangle$ and examine the state of a periodic graph with period $2t_0$:

$$e^{-iA_G 2t_0}|u\rangle = \sum_j a_j e^{-i\lambda_j 2t_0}|x_j\rangle = e^{i2\phi}\sum_j a_j|x_j\rangle = e^{i2\phi}|u\rangle.$$

Since the eigenvectors $|x_j\rangle$ are linearly independent, we have that for each j with $a_j = \langle x_j|u\rangle \neq 0$

$$2\lambda_j t_0 + 2\phi = 2m_j\pi \quad \text{for some } m_j \in \mathbf{Z}.$$

Thus,

$$\frac{\lambda_k - \lambda_l}{\lambda_r - \lambda_s} = \frac{m_k - m_l}{m_r - m_s} \in \mathbf{Q}.$$

□

Note that the condition $\langle x_k|u\rangle$, $\langle x_l|u\rangle$, $\langle x_r|u\rangle$, $\langle x_s|u\rangle \neq 0$ in the above theorem does not appear in [27].

Periodicity of a graph at each of its vertices may be characterized by its spectrum alone.

Lemma 5.1. [39] *Let the eigenvalues of G be $\lambda_1, \ldots, \lambda_n$. Then G is periodic if and only if the ratio of any two non-zero eigenvalues is rational.*

Theorem 5.3. [39] *A graph G is periodic if and only if either:*

(a) *The eigenvalues of G are integers, or*
(b) *The eigenvalues of G are rational multiples of $\sqrt{\Delta}$, for some square-free integer Δ. In this case, G is bipartite.*

The graphs whose eigenvalues are all integers are called *integral graphs*. They have been a sort of a mathematical curiosity for a number of years: cubic integral graphs have been, for example, characterized 25 years ago in [21], and independently in [78]. A number of other results on integral graphs with bounded maximum degree and on integral trees are surveyed in [7, 89]. For application of integral graphs in multiprocessor systems, see the chapter "Multiprocessor interconnection networks" in this book.

The graphs whose eigenvalues are all rational multiples of $\sqrt{\Delta}$ have not been explicitly studied before. They are, perhaps, most easily found among semiregular graphs.

We have shown that perfect state transfer exists in paths with two and three vertices. We will now show, following [27], that there is no perfect state transfer in path P_n for $n \geqslant 4$. Suppose contrary, that there exists perfect state transfer between u and v in P_n for some $n \geqslant 4$. We will show that there is a set of eigenvalues λ_k, λ_l, λ_r, λ_s of P_n that violates the eigenvalue ratio condition.

The eigenvalues of P_n are given by $\lambda_i = 2\cos\frac{\pi i}{n+1}$ for $i = 1, \ldots, n$, and the eigenvectors are given by [28]

$$x_i = \sqrt{\frac{2}{n+1}} \sum_{j=1}^{n} \sin\frac{\pi ij}{n+1} |j\rangle.$$

Choosing $k = 2$, $l - 1$, $r = 1$ and s, we see that the eigenvalue ratio condition requires that

$$\frac{\cos\frac{2\pi}{n+1}}{\cos\frac{\pi}{n+1}} \in \mathbf{Q}. \tag{5.2}$$

Further, $\langle x_1|u\rangle$, $\langle x_n|u\rangle \neq 0$ for all u, and $\langle x_2|u\rangle$, $\langle x_{n-1}|u\rangle \neq 0$ unless n is odd and u is the center of P_n (however, in such case, v has to satisfy $\langle x_2|v\rangle$, $\langle x_{n-1}|v\rangle \neq 0$). Assume that

$$\frac{\cos\frac{2\pi}{n+1}}{\cos\frac{\pi}{n+1}} = \frac{p}{q}, \quad \text{for } p, q \in \mathbf{Z}.$$

Using the trigonometric identity

$$\cos 2\theta = 2\cos^2\theta - 1$$

we can write

$$\Big(\cos\frac{\pi}{n+1}\Big)^2 - \frac{p}{2q}\cos\frac{\pi}{n+1} - \frac{1}{2} = 0$$

which is a monic polynomial in $\cos\frac{\pi}{n+1}$ with rational coefficients. Thus, $\cos\frac{\pi}{n+1}$ has to be an algebraic integer with degree $\leqslant 2$.

On the other hand, Lehmer proved (see, for example, [70]) that if $n > 1$ and $\gcd(k, n+1) = 1$, then $\cos\frac{\pi k}{n+1}$ is an algebraic integer of degree $\phi(2(n+1))/2$, where ϕ is the Euler phi function. For $n \geqslant 3$ it can be shown [74] that

$$\phi(n) \geqslant \frac{n}{e^{\gamma}\log\log n + 3/\log\log n}$$

holds, with $\gamma \approx 0.5772$ Euler's constant. Using this bound, and inspecting values not covered by it, we can see that $\phi(2(n+1))/2 \geqslant 3$ for $n \geqslant 6$. Thus, $\cos\frac{\pi}{n+1}$ is an algebraic number of degree $\geqslant 3$, and so $\cos\frac{2\pi}{n+1}/\cos\frac{\pi}{n+1}$ has to be irrational, violating the eigenvalue ratio condition (5.2). Hence, perfect state transfer is impossible in paths with $n \geqslant 6$. The cases $n = 4$ and $n = 5$ are easily proved by direct evaluation.

6. Some regular graphs with perfect state transfer

Integral graphs represent a class of graphs that naturally satisfies eigenvalue ratio condition. There are only thirteen connected cubic integral graphs [21, 78], so the next theorem follows easily:

Theorem 6.1. [79] *The 3-dimensional cube is the only periodic, connected cubic graph with perfect state transfer between two different vertices.*

4-regular integral graphs are not fully characterized, except those that do not have ± 3 as an eigenvalue [82]. However, all 4-regular integral graphs with up to 24 vertices are known [83]. Among them, there is a triplet of cospectral graphs on 16 vertices with perfect state transfer, one of which is a 4-dimensional cube (Fig. 2).

Regular graphs with perfect state transfer are not necessarily periodic. An example of such graph was found by Matthew Russell [75], who showed that the complement of the union of four cycles C_3, C_4, C_4 and C_5 has perfect state transfer at time $\pi/2$ between antipodal vertices in both C_4s, but it is not periodic at time π relative to vertices belonging to C_3 and C_5. At time 2π it is periodic relative to vertices belonging to C_3, but still not periodic relative to vertices in C_5.

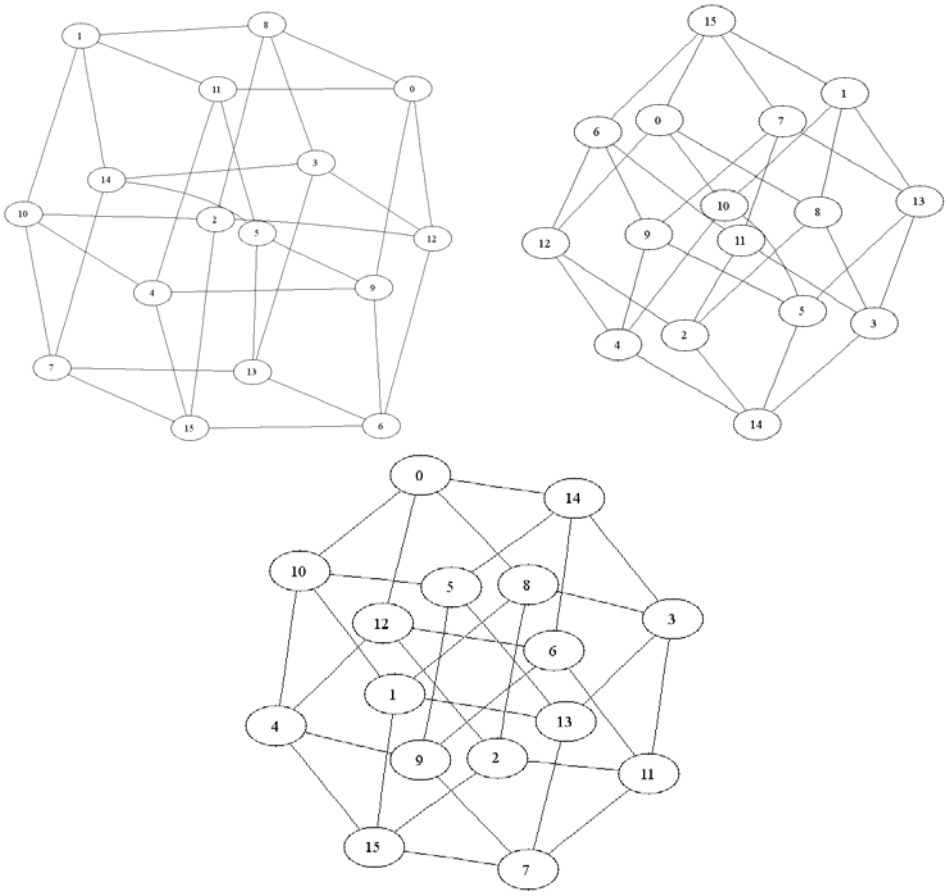

FIGURE 2. 4-regular integral graphs on 16 vertices with perfect state transfer.

One can also find examples of nonintegral periodic graphs with perfect state transfer. Besides already known P_3, such graph is the bipartite complement of the union of $2k$ copies of P_3, $k \geqslant 1$, which has perfect state transfer between end vertices of the same copy of P_3 at time $\pi/\sqrt{2}$. It has even number of vertices and distinct eigenvalues $\pm(2k-1)\sqrt{2}, \pm\sqrt{2}$ and 0, thus answering a problem (a) from Section 10 in the first version of Godsil' paper [39].

7. Cartesian product of graphs

Perfect state transfer is impossible in paths of length larger than two. Clearly it is desirable to find a graph that allows perfect state transfer over larger distances, and with that goal in mind, we examine the d-fold Cartesian product of the path P_3, which we denote by $P_3^{\otimes d}$.

The Cartesian product of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is a graph $G_1 + G_2$ whose vertex set is set $V_1 \times V_2$ and two of its vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if one of the following holds: (i) $u_1 = v_1$ and $\{u_2, v_2\} \in E_2$, or (ii) $u_2 = v_2$ and $\{u_1, v_1\} \in E_1$. Let A_{G_1} and A_{G_2} be the adjacency matrices of G_1 and G_2, and let $\{\lambda_i(G_1)\colon 1 \leqslant i \leqslant |V_1|\}$ and $\{\lambda_j(G_2)\colon 1 \leqslant j \leqslant |V_2|\}$ denote the sets of eigenvalues of G_1 and G_2, respectively. The adjacency matrix of $G_1 + G_2$ is given by

$$A_{G_1+G_2} = A_{G_1} \otimes I_{G_2} + I_{G_1} \otimes A_{G_2},$$

where $\otimes$ denotes the Kronecker product of matrices. The eigenvalues of $G_1 + G_2$ are then precisely the numbers $\lambda_i(G_1) + \lambda_j(G_2)$. For the Hamiltonian of $G_1 + G_2$ we have

$$\begin{aligned} e^{-iA_{G_1+G_2}t} &= e^{-i(A_{G_1}\otimes I_{G_2} + I_{G_1}\otimes A_{G_2})t} \\ &= e^{-i(A_{G_1}\otimes I_{G_2})t} e^{-i(I_{G_1}\otimes A_{G_2})t} \\ &= (e^{-iA_{G_1}t} \otimes I_{G_2})(I_{G_1} \otimes e^{-iA_{G_2}t}) \\ &= e^{-iA_{G_1}t} \otimes e^{-iA_{G_2}t}. \end{aligned}$$

Cartesian product of graphs is thus well related to perfect state transfer.

Theorem 7.1. [5] *For $j = 1, \ldots, m$, the graph G_j has perfect state transfer from a_j to b_j at time t^* if and only if $\mathcal{G} = G_1 + \cdots + G_m$ has perfect state transfer from $(a_1, \ldots, a_m)$ to $(b_1, \ldots, b_m)$ at time t^*.*

Proof. We prove the claim for $m = 2$. From above,

$$\langle b_1, b_2|e^{-iA_{G_1+G_2}t}|a_1, a_2\rangle = \langle b_1|e^{-iA_{G_1}t}|a_1\rangle\langle b_2|e^{-iA_{G_2}t}|a_2\rangle.$$

This shows that G_1+G_2 has perfect state transfer from (a_1, a_2) to (b_1, b_2) at time t^* if and only if G_1 has perfect state transfer from a_1 to b_1 at time t^* and G_2 has perfect state transfer from a_2 to b_2 at time t^*. The general claim now follows by induction. □

Let $A = (1, 1, \ldots, 1)$ and $B = (3, 3, \ldots, 3)$ denote the antipodal points of $P_3^{\otimes d}$. If we select time $t^* = \pi/\sqrt{2}$, we get perfect state transfer from 1 to 3 in each copy of P_3. Thus, we achieve perfect state transfer between A and B in $P_3^{\otimes d}$ at time t^* (as well as between any vertex and its mirror, such as $(1, 1, 1, 2, 3) \mapsto (3, 3, 3, 2, 1)$). The communication distance provided by $P_3^{\otimes d}$ is equal to $2d = 2\log_3 n$, where $n = 3^d$ is the number of vertices of $P_3^{\otimes d}$.

Perfect state transfer can also be achieved between the antipodal vertices of the hypercube Q_d in time $t^* = \pi/2$ for arbitrary d. This is because $Q_d = P_2^{\otimes d}$ and perfect transfer occurs across P_2 in this time. In this case, the communication distance is somewhat smaller and equal to $\log_2 n$.

The Cartesian product is a special case of non-complete extended p-sum (NEPS) of graphs. Let $\mathcal{B} \subseteq \{0, 1\}^n \setminus \{(0, \ldots, 0\}$ such that there exists $\beta \in \mathcal{B}$ with $\beta_i = 1$ for each $i = 1, \ldots, n$. The NEPS$(G_1, \ldots, G_n; \mathcal{B})$ is the graph with the vertex set $V(G_1) \times \cdots \times V(G_n)$, in which two vertices $(u_1, \ldots, u_n)$ and $(v_1, \ldots, v_n)$ are

adjacent if there exists $\beta \in \mathcal{B}$ such that for each $i = 1, \ldots, n$, $u_i = v_i$ if $\beta_i = 0$ and $\{u_i, v_i\} \in E(G_i)$ if $\beta_i = 1$.

The simplest case, NEPS of P_2s, has been studied in [13] under the name of *cubelike graphs*.

8. Cubelike graphs

Let $\mathbf{Z}_2^n$ be the additive abelian group $(\mathbf{Z}_2)^{\times n}$. Each element of $\mathbf{Z}_2^n$ is represented as a binary vector of length n. Let Ω be an arbitrary subset of $\mathbf{Z}_2^n \setminus \{0\}$. If w and v are two binary vectors of the same length, then $w \oplus v$ denotes the vector obtained by elementwise addition modulo 2. The Cayley graph $X(\mathbf{Z}_2^n, \Omega)$, having the binary vectors of length n as its vertices, with two vertices w and v adjacent if and only if $w \oplus v \in \Omega$, is called *cubelike graph* [13]. Note that the cubelike graph $X(\mathbf{Z}_2^n, \Omega)$ is actually the same as $\mathrm{NEPS}(P_2, \ldots, P_2; \Omega)$.

The above definition of a cubelike graph embraces every possible set $\Omega \neq \{0\}$. When Ω is the standard generating set of $\mathbf{Z}_2^n$, the graph $X(\mathbf{Z}_2^n, \Omega)$ is isomorphic to the hypercube Q_n.

Theorem 8.1. [13] *Let $X(\mathbf{Z}_2^n, \Omega)$ be a cubelike graph and let $a, b \in \mathbf{Z}_2^n$. For $t = \pi$, perfect state transfer exists between a and b if and only if $a = b$. For $t = \pi/2$, perfect state transfer exists between a and b if and only if $a \oplus b = u$ and $u = \bigoplus_{w \in \Omega} w \neq 0$.*

As a simple consequence, there are various ways to *route* information between any two nodes of a network whose vertices correspond to the elements of $\mathbf{Z}_2^n$. Let $\Omega = \{w_1, \ldots, w_r\}$ be a generating set of $\mathbf{Z}_2^n$. Let $\bigoplus_{w_i \in \Omega} w_i = w \neq 0$. Let us define $C = \{w, w_1, \ldots, w_r\}$ and $C_i = C \setminus \{w_i\}$. Since the sum of the elements of C_i is nonzero, the Cayley graph $X(\mathbf{Z}_2^n, C_i)$ has perfect state transfer between a and b such that $a \oplus b = w_i$ at time $\pi/2$. The simplest case arises when we choose r and take the vectors $w_1, \ldots, w_r$ to be the standard basis of $\mathbf{Z}_2^n$. Then $X(\mathbf{Z}_2^n, C_i)$ is the *folded d-cube* and by using a suitable sequence of the graphs $X(\mathbf{Z}_2^n, C_i)$, we can arrange perfect state transfer from the zero vector to any desired element of $\mathbf{Z}_2^n$.

For example, consider the case $\Omega = \{w_1, w_2, w_3\}$ with $w_1 = (100)$, $w_2 = (010)$ and $w_3 = (001)$. Then $w = (111)$. The graph $X(\mathbf{Z}_2^3, C)$ is illustrated in Fig. 3-left. Since $w_1 = w_2 \oplus w_3 \oplus w$, there is perfect state transfer between 000 and $w_1 = 100$ at time $\pi/2$, given that $000 \oplus 100 = 100$ (see Fig. 3-right). Also, there is perfect state transfer for the pairs $\{010, 110\}$, $\{001, 101\}$ and $\{011, 111\}$. Note that $X(\mathbf{Z}_2^3, C_1)$ is isomorphic to the 3-dimensional hypercube.

A special case has been left open in the above theorem: when $\bigoplus_{w \in \Omega_f} w = 0$. Although it was suggested in [13] that cubelike graphs with this property do not allow perfect state transfer, examples of such graphs on 32 vertices were recently found in [29]. Let M be the matrix with the elements of Ω as its columns. Its row space is a binary code, with $\mathrm{supp}(x)$ and $\mathrm{wt}(x)$ denoting the support and the Hamming weight of x (i.e., the set of positions and the number of 1s in binary string x).

Theorem 8.2. [29] *Let $X(\mathbf{Z}_2^n, \Omega)$ be a cubelike graph with matrix M and suppose u is its vertex distinct from 0. Then the following are equivalent:*

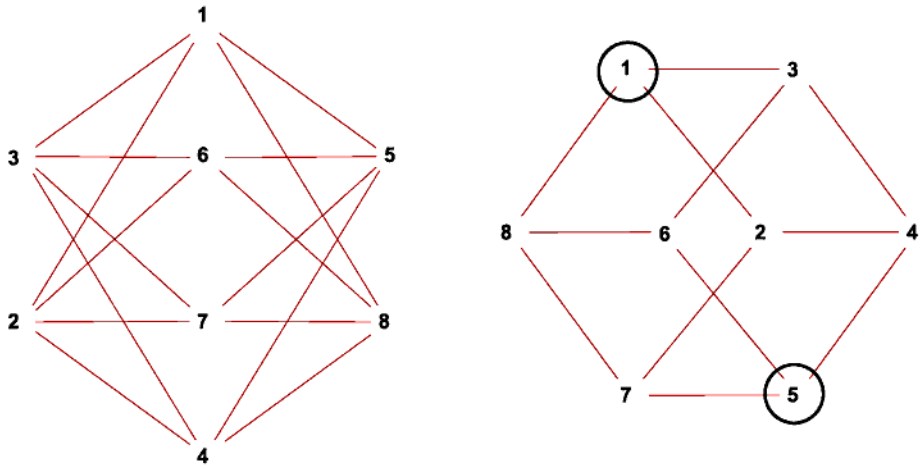

FIGURE 3. Left: The graph $X(\mathbf{Z}_2^3, C)$, where $C = \{100, 010, 001, 111\}$. This graph is isomorphic to the complete bipartite graph $K_{4,4}$. Right: The graph $X(\mathbf{Z}_2^3, C_1)$, where $C_1 = \{010, 001, 111\}$. This graph is isomorphic to the hypercube of dimension 3.

(a) *There is perfect state transfer from* 0 *to* u *at time* $\pi/2\Delta$.
(b) *All words in* Ω *have weight divisible by* Δ *and* $\Delta^{-1}\mathrm{wt}(a^T M)$ *and* $a^T u$ *have the same parity for all vectors* $a \in \mathbf{Z}_2^n$.
(c) Δ *divides* $|\mathrm{supp}(u) \cap \mathrm{supp}(v)|$ *for any two code words* u *and* v.

9. Integral circulant graphs

Circulant graphs are an important class of interconnection networks used in parallel and distributed computing [48]. They are another class of graphs extensively studied for the existence of perfect state transfer. For $n \in \mathbf{N}$ and $S \subseteq \{1, \ldots, n-1\}$, the *circulant graph* $G(n, S)$ is the graph with n vertices, labelled with integers modulo n, such that each vertex i is adjacent to $|S|$ other vertices $i + s \pmod n$ for each $s \in S$. The set S is called the *symbol* of $G(n, S)$. As we consider undirected graphs, we assume that $s \in S \Leftrightarrow n - s \in S$, so that the vertex i is adjacent to both $i \pm s \pmod n$ for each $s \in S$. The adjacency matrix A of the circulant graph $G(n, S)$ is diagonalizable by the Fourier matrix F whose columns $|F_k\rangle$ are defined as $\langle j|F_k\rangle = \omega_n^{jk}/\sqrt{n}$, where $\omega_n = e^{2\pi i/n}$ [5]. In fact, we have $FAF^\dagger = \sqrt{n}\mathrm{diag}(FA_0)$, for any circulant matrix A, where A_0 is the first column of A. This shows that the eigenvalues of A are given by

$$\lambda_j = \sum_{k=0}^{n-1} a_{n-k}\omega_n^{jk}.$$

So [81] has characterized the integral circulant graphs. Let

$$G_n(d) = \{k\colon \gcd(n,k) = d,\ 1 \leqslant k < n\}$$

be a set of all integers less than n having the same greatest common divisor d with n. In particular, $|G_n(d)| = \phi(n/d)$, where

$$\phi(m) = |\{s\colon \gcd(m,s) = 1,\ 1 \leqslant s < m\}$$

denotes the Euler phi-function. Let D_n be a set of positive divisors d of n, with $d \leqslant n/2$.

Theorem 9.1. [81] *A circulant graph $G(n,S)$ is integral if and only if*

$$S = \bigcup_{d\in D} G_n(d)$$

for some set of divisors $D \subseteq D_n$.

Actually, integral circulants were characterized long before by Bridges and Mena in 1979 [16], they also extended their result to Cayley graphs of abelian groups in 1982 [17].

For a set of divisors $D = \{d_1,\dots,d_k\} \subseteq D_n$, we shortly denote by $\mathrm{ICG}_n(D)$ an integral circulant graph $G\big(n, \bigcup_{i=1}^{k} G_n(d_i)\big)$. $\mathrm{ICG}_n(D)$ is connected if and only $\gcd(n,d_1,\dots,d_k) = 1$ [81].

It was shown in [10] that perfect state transfer is possible in $\mathrm{ICG}_n(D)$ for even n only, in which case perfect state transfer exists between antipodal vertices a and $a + n/2$, for each a.

The integral circulants with $D = \{1\}$ are also called the *unitary Cayley graphs.*

Theorem 9.2. [10] *The only unitary Cayley graphs* $\mathrm{ICG}_n(\{1\})$ *with perfect state transfer are P_2 and $C_4 \cong P_2^{\otimes 2}$.*

The cocktail-party graph, which is a complete graph K_n minus a perfect matching, has perfect state transfer between antipodal vertices at distance two [86]. It is another example of an integral circulant graph with $S = \{1,\dots,n-1\} \setminus \{n/2\}$.

Among other integral circulant graphs (non-unitary and non-cocktail-party), the smallest graphs with perfect state transfer are $\mathrm{ICG}_8(\{1,2\})$ and $\mathrm{ICG}_8(\{1,4\})$, shown in Fig. 4. They represent two infinite families of integral circulants with perfect state transfer.

Theorem 9.3. [8] *For n divisible by 8, the integral circulant graphs* $\mathrm{ICG}_n(\{1,n/2\})$ *and* $\mathrm{ICG}_n(\{1,n/4\})$ *have perfect state transfer between antipodal vertices.*

Further examples of integral circulants with perfect state transfer have been found in [5], using the concept of circulant join. For a n-vertex graph G and a $n \times n$ $(0,1)$-matrix C, the *circulant join* $G \bigtriangledown_C G$ is a graph with adjacency matrix

$$A_{G\bigtriangledown_C G} = \begin{bmatrix} A_G & C \\ C & A_G \end{bmatrix}.$$

This operation generalizes the usual join $G \bigtriangledown G = G \bigtriangledown_J G$ and $K_2 + G = G \bigtriangledown_I G$. If u is a vertex of G, then we denote by (u,s), $s \in \{0,1\}$, the vertex u in the s-th copy of G in $G \bigtriangledown_C G$.

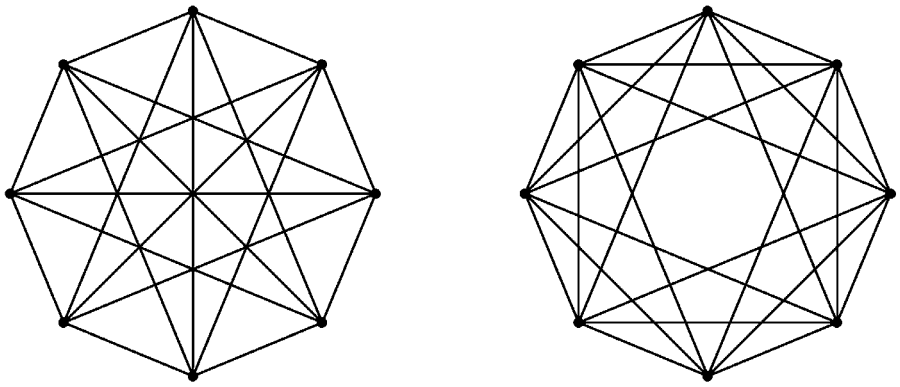

FIGURE 4. The integral circulant graphs $\mathrm{ICG}_8(\{1,2\})$ and $\mathrm{ICG}_8(\{1,4\})$.

Theorem 9.4. [5] *Let C be a $n \times n$ circulant matrix. If G is a n-vertex circulant graph with perfect state transfer from a to b at time t^*, then the circulant join $G \bigtriangledown_C G$ has perfect state transfer from vertex $(a,0)$ to vertex (b,s), $s \in \{0,1\}$, at time t^* provided that*

$$\left[\cos\left(t^*\sqrt{B}\right)\right]^{1-s}\left[\sin\left(t^*\sqrt{B}\right)B^{-1/2}C^T\right]^s = \pm I$$

where $B = C^TC$ and B^{-1} exists whenever $s = 1$. Also, $G \bigtriangledown_C G$ is a circulant graph if C is a palindrome circulant matrix, where $c_j = c_{n-1-j}$, for $j = 0, 1, \ldots, n-1$.

Corollary 9.1. [5] *If G is a n-vertex circulant graph that has perfect state transfer from a to b at time t^*, then so does the circulant graph $G \bigtriangledown G$ provided $nt^* \in 2\pi\mathbf{Z}$.*

Theorem 9.5. [5] *Let $n = 2^u m$, where $u \geqslant 3$ and $m \geqslant 3$ is an odd number. Suppose that $G = \mathrm{ICG}_n(D)$, for $D = \{1, n/4\}$ or $D = \{1, n/2\}$. For any subset $Q \subset D_m \cup \{m\}$, there is an $(0,1)$-circulant matrix $C \notin \{I_n, J_n, O_n\}$ so that*

$$G \bigtriangledown_C G = \mathrm{ICG}_{2n}(2D \cup Q)$$

has perfect state transfer from 0 to $n/2$ in G at time $t^* = \pi/2$.

Corollary 9.2. [5] *For $n = 2^u$, for $u \geqslant 3$, the integral circulants $\mathrm{ICG}_{2n}(\{1,2,n/2\})$ and $\mathrm{ICG}_{2n}(\{1,2,n\})$ have perfect state transfer from 0 to n at time $t^* = \pi/2$.*

Still, the integral circulants with perfect state transfer exhibit very small communication distance, as their diameter is of order $O(\ln\ln n)$ [84], inferior to the communication distance $2\log_3 n$ found in a P_3-cube [27].

Besides few examples of perfect state transfer above, one can actually find more results in the literature on the nonexistence of perfect state transfer in integral circulants:

Theorem 9.6. *An integral circulant graph $\mathrm{ICG}_n(D)$ does not have perfect state transfer if any of the following conditions hold:*

(i) *n is odd* [76];
(ii) *n/d is odd for every $d \in D$* [10];
(iii) *n is an even square-free integer* [8];
(iv) *$n = 2p^2$ for a prime number p* [9].
(v) *n is not square-free, $D \neq \{1, n/2\}$, there exists an* isolated divisor $d_0 \in D$ *such that* $\gcd(d_0, d) = 1$ *for every $d \in D \setminus \{d_0\}$ and n/d_0 is square-free* [9];
(vi) *$n \in 4\mathbf{N} + 2$ and n/d is not square-free for each divisor $d \in D$* [9];

10. Other graph compositions

Angeles-Canul et al. [5] and Ge et al. [37] have considered a number of graph compositions which yield graphs with perfect state transfer under suitable conditions. Here we review the results on perfect state transfer in direct product, generalized lexicographic product and join of graphs.

The *direct product* $G \times H$ is a graph defined on $V(G) \times V(H)$ where (g_1, h_1) is adjacent to (g_2, h_2) if $(g_1, g_2) \in E(G)$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G \times H$ is $A_G \otimes A_H$.

Theorem 10.1. [37] *Let G be a graph with perfect state transfer at time t_G so that*

$$t_G \operatorname{Spec}(G) \subset \mathbf{Z}\pi.$$

Then $G \times H$ has perfect state transfer if H is a circulant graph with odd eigenvalues.

Note that Q_{2n} has eigenvalues $\lambda_k = 2n - 2k$, for $k = 0, 1, \ldots, 2n$ and perfect state transfer time $t = \pi/2$. Also, $P_3^{\otimes n}$ has eigenvalues from $\lambda_k \in \mathbf{Z}\sqrt{2}$ and perfect state transfer time $t = \pi/\sqrt{2}$. In both cases, we have $t\lambda_k \in \mathbf{Z}\pi$ for all k. Thus, $Q_{2n} \times H$ and $P_3^{\otimes n} \times H$ have perfect state transfer for any circulant H with odd eigenvalues. For example, we may let $H = K_m$ be the complete graph of order m, for an even integer m.

The *generalized lexicographic product* $G_C[H]$ of graphs G and H, under the square $(0,1)$-matrix C indexed by vertices of H, is a graph on $V_G \times V_H$ where (g_1, h_1) is adjacent to (g_2, h_2) if and only if either $(g_1, g_2) \in E_G$ and $C(h_1, h_2) = 1$, or, $g_1 = g_2$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G_C[H]$ is $A_{G_C[H]} = A_G \otimes A_C + I_G \otimes A_H$. The standard lexicographic product $G[H]$ is obtained by setting $C = J_H$.

Theorem 10.2. [37] *Let G and H be perfect state transfer graphs with a common time t, with H being a circulant graph. Suppose that*

$$t|V_H| \operatorname{Spec}(G) \subset 2\pi\mathbf{Z}.$$

Then the lexicographic product $G_{J_H - I_H}[H]$ has perfect state transfer at time t.

Theorem 10.3. [37] *Let G be an arbitrary graph and let H be a regular graph with perfect state transfer at time t_H from h_1 to h_2, for $h_1, h_2 \in V_H$. Then $G[H]$ has perfect state transfer from (g, h_1) to (g, h_2) for any $g \in V_G$, if*

$$t_H|V_H| \operatorname{Spec}(G) \subset 2\pi\mathbf{Z}.$$

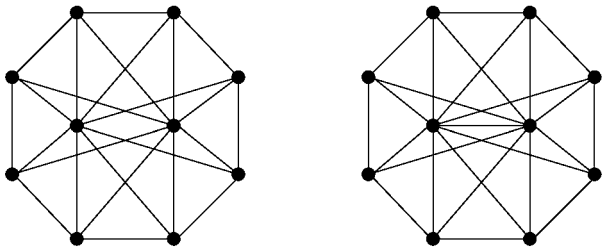

FIGURE 5. Double cones $\overline{K_2} \bigtriangledown C_8$ and $K_2 \bigtriangledown C_8$.

Corollary 10.1. [37] *Suppose H is a k_H-regular graph with perfect state transfer at time $t_H = \frac{\pi}{2}k_H$ and G is an integral graph. Then $G[H]$ has perfect state transfer provided $k_H|V_H| \operatorname{Spec}(G) \subset 4\mathbf{Z}$.*

The n-cube Q_n is a n-regular graph on 2^n vertices which has perfect state transfer at time $n\frac{\pi}{2}$. Thus, for any integral graph G, the composition graph $G[Q_n]$ has perfect state transfer if $n \geqslant 2$.

The *join* $G \bigtriangledown H$ is a graph defined on $V(G) \cup V(H)$ obtained by taking disjoint copies of G and H and by connecting all vertices of G to all vertices of H. The adjacency matrix of $G \bigtriangledown H$ is $\left[\begin{smallmatrix} A_G & J \\ J & A_H \end{smallmatrix}\right]$. The *cone* of a graph G is defined as $K_1 \bigtriangledown G$. The *double cone* of G is $\overline{K_2} \bigtriangledown G$, whereas the *connected double cone* is $K_2 \bigtriangledown G$.

Bose et al. [15] observed that, although K_n does not exhibit perfect state transfer, perfect state transfer is created between any two of its vertices by removing an edge between them. Note that this graph is the double cone $\overline{K_2} \bigtriangledown K_{n-2}$.

The existence of perfect state transfer in a join of two arbitrary regular graphs may be reduced to the existence of perfect state transfer in one of the graphs along with certain structure-independent constraints on the sizes and degrees of the graphs.

Theorem 10.4. [5] *Let G be a m-vertex k_G-regular graph and let H be an n-vertex k_H-regular graph. Let a and b be two vertices in G. Then*

$$\langle b|e^{-iA_{G\bigtriangledown H}t}|a\rangle = \langle b|e^{-iA_G t}|a\rangle + \frac{e^{-ik_G t}}{m}\Big\{e^{it\delta/2}\Big[\cos\Big(\frac{\Delta t}{2}\Big) - i\Big(\frac{\delta}{\Delta}\Big)\sin\Big(\frac{\Delta t}{2}\Big)\Big] - 1\Big\}$$

where $\delta = k_G - k_H$ and $\Delta = \sqrt{\delta^2 + 4mn}$.

This theorem may be applied to the double cones $\overline{K_2} \bigtriangledown G$ and $K_2 \bigtriangledown G$. For a prime p, let $S_p(n)$ denote the largest non-negative integer j so that $p^j|n$.

Corollary 10.2. [5] *For any k-regular graph G on n vertices, $\overline{K_2} \bigtriangledown G$ has perfect state transfer between the two non-adjacent vertices of $\overline{K_2}$ if $\Delta = \sqrt{k^2 + 8n}$ is an integer and $k, \Delta \equiv 0 \pmod 4$ with $S_2(k) \neq S_2(\Delta)$.*

This corollary may be used to answer a question of Godsil [39, Section 10, question (b)]: for $l \geqslant 2$, the double-cone graphs $\overline{K_2} \bigtriangledown (C_{2(2l-1)} + C_{2l+1})$ are nonperiodic and have perfect state transfer. They have mixture of integral and irrational eigenvalues, so they violate the eigenvalue ratio condition, and hence cannot be periodic.

Corollary 10.3. [5] *For any k-regular graph G on n vertices, $K_2 \bigtriangledown G$ has perfect state transfer between the two adjacent vertices of K_2 if $\Delta = \sqrt{(k-1)^2 + 8n}$ is an integer and $k - 1, \Delta \equiv 0 \pmod 8$.*

11. Perfect routing of quantum states

The transfer of quantum states was introduced as a protocol to simplify interaction between distant qubits in a quantum architecture that has locality restrictions, as in solid state systems [71]. The perfect transfer protocols are designed to transfer a quantum state which is input on a given site, onto a specific, corresponding output site. Although it is desirable to assume no interaction with the system, and just let its (fixed) Hamiltonian generate the state transfer, this assumption does not use a vital element of the state transfer protocol—it is implicitly assumed that one is able to introduce the quantum state onto the input node, and remove it from the output node, quickly in comparison to the Hamiltonian dynamics. This additional level of control enables several new features, as recently observed in [72].

We start by considering a one-dimensional system of $3N + 1$ qubits, as depicted in Fig. 6(a), in order to illustrate the basic idea of the construction. The fixed XY Hamiltonian takes the form

$$H = \frac{1}{2} \sum_{\{i,j\} \in E} J_{i,j} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$

where E is the set of edges of the graph depicted in Fig. 6(a) and $J_{i,j} = 1$ unless $\{i, j\} = \{3k, 3k+1\}$ for some k, in which case $J_{i,j} = -1$. Same as in Section 3, the Hamiltonian is spin preserving,

$$\left[H, \sum_{i=1}^{3N+1} \sigma_i^z \right] = 0,$$

and we assume that all spins are initialised in the $|0\rangle$ state. By introducing the state to be transferred on a particular spin, the system is placed in a superposition of 0 and 1 excitations. The 0 excitation subspace is a single state, which is invariant under the Hamiltonian evolution, and we concentrate on the single excitation subspace. The basis states in this subspace are denoted by $|n\rangle = |0\rangle^{\otimes n-1} |1\rangle |0\rangle^{\otimes 3N+1-n}$.

The crucial observation is that, for example, $(|2\rangle + |3\rangle)/2$ is a 0 eigenstate for $(\sigma_2^x \sigma_4^x + \sigma_2^y \sigma_4^y) - (\sigma_3^x \sigma_4^x + \sigma_3^y \sigma_4^y)$, and similarly, $(|2\rangle - |3\rangle)/2$ is a 0 eigenstate for $(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + (\sigma_1^x \sigma_3^x + \sigma_1^y \sigma_3^y)$. This means that one can rewrite the basis states as $|\lambda_{3n+1}\rangle = |3n+1\rangle$, $|\lambda_{3n+2}\rangle = (|3n+2\rangle + |3n+3\rangle)/2$, and $|\lambda_{3n+3}\rangle = (|3n+2\rangle - |3n+3\rangle)/2$, leaving the Hamiltonian with a direct sum structure as depicted in Fig. 6(b). Each subsystem is now a uniformly coupled path of length 2 or 3, which achieves perfect transfer in time $\pi/\sqrt{2}$ or $\pi/2$, respectively.

Thus, starting with a state $|\lambda_{3n}\rangle$, after a time $\pi/2$, we obtain $|\lambda_{3n+2}\rangle$ from Hamiltonian dynamics. Now, observe that a fast application of the local rotations (but globally applied) $U = \prod_{i=1}^{N} \sigma_{3n}^z$ converts between states $|\lambda_{3n+2}\rangle$ and $|\lambda_{3n+3}\rangle$, i.e., it transfers the state from one subsystem to the next. Hence, starting from

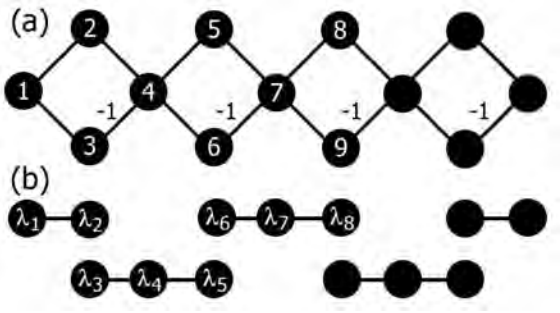

FIGURE 6. (a) A quasi-one-dimensional routing structure. The circles represent qubits, and the lines indicate a coupling between pairs of qubits of strength $+1$, unless -1 is indicated. (b) Under a basis transformation, a simple direct sum structure is apparent. In this case, all coupling strengths are equal to $\sqrt{2}$.

$|\lambda_{3n+2}\rangle$, we apply U every $\pi/2$ and after $|m-n|\pi/2$, we get the state $|\lambda_{3m+2}\rangle$. This achieves the long range transfer, and a few further details given in [71] are needed to show how to convert from the input state, either $|3n+1\rangle$ or $|3n+2\rangle$ to $|\lambda_{3n+2}\rangle$ and back to the output state, with the help of the local magnetic fields.

Thus, we can perfectly propagate a quantum state along the length of the system, between any two vertices in a time proportional to the distance between them. Since the subsystems in Fig. 6(b) are independent, we can actually have multiple excitations in the system provided they are each separated by at least one subsystem. Thus, multiple states can be transferred at once, enabling a transfer rate which is in excess of that achievable in perfect state transfer schemes. These results are easily generalized to two and more dimensions, yielding networks which can perfectly route quantum states from arbitrary vertices in a time linear in the distance to be covered.

Perfect routing of quantum states has also been studied in [30], where it is shown that multiple vertices can faithfully send entanglement through the oscillator hypercube network *at the same time*.

12. Conclusion

Due to the bound in the total length of this article, we have surveyed here the perfect state transfer in uniformly coupled spin networks (simple graphs) only. When one allows non-uniform couplings in the network, such as in the previous section on routing of quantum states, then it is possible, for example, to engineer the couplings such that an arbitrarily long path enables the perfect state transfer between its ends, leading to the notion of quantum wires [27].

Another aspect of perfect state transfer that we did not consider here is its physical implementation. There is a large body of physics literature on this topic, and most of it is listed in references below, so that the interested researcher may find it as a useful start point. The technique of perfect routing of quantum states [30,

71, 72] appears to be especially promising in bringing the quantum state transfer closer to its physical realization.

The problem of the maximum communication distance is very much untouched. The largest known communication distance of $2\log_3 n$ was achieved already for one of the very first perfect state transfer networks, the Cartesian product $P_3^{\otimes d}$ of three-vertex paths [28]. The integral circulants, due to their extremely small diameter $O(\log\log n)$, are unable to provide larger communication distances. The situation is similar with other constructions, which in some cases cannot perform better than to achieve perfect state transfer between vertices at a small constant distance (2 or 3). Thus, it is a main open problem to see whether a larger communication distance, for example, of order $O(\sqrt{n})$, may be achieved.

Among graph compositions, most elegant connection to the perfect state transfer is exhibited by the Cartesian product of graphs, which is a particular case of NEPS. Bernasconi et al. [13] have, with a single unresolved case, managed to characterize perfect state transfer in cubelike graphs, which itself is NEPS of P_2s. Thus, the next interesting question is to find out whether similar conditions will enable perfect state transfer in NEPS of P_3s.

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Ivan Gutman

HYPERENERGETIC AND 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 "hyperenergetic" if $E > 2n - 2$, and to be "hypoenergetic" if $E(G) < n$. In this chapter we outline the main hitherto obtained results related to hyperenergetic and hypoenergetic graph.

Mathematics Subject Classification (2010): 05C50; 05C90; 92E10

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

Contents

1. Energy of a graph

Definition 1. Let G be a graph on n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues [7, 11]. Then the *energy* of G is

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

Although in the chemical literature the sum of absolute values of the eigenvalues of some graphs was (in a more-or-less implicit manner) considered already since the 1940s (see e.g., [5, 20, 41, 55, 59]), it was the present author who in the 1970s used Eq. (1) as a *definition*, noticing that practically all results that until then were obtained for the total π-electron energy (cf. the next section), pertain to the quantity occurring on the right–hand side of (1).

Definition 1 was advocated by the present author on several lectures and seminars held in the 1970s. In written form it was first stated in the paper [21]. Since this paper is extremely difficult to acquire, it is not quite surprising that the graph-energy concept was for a long time not recognized by other scholars. The same definition was later given in the book [37], and elsewhere [22].

Nowadays, this is history. Its details have been outlined on several occasions [10, 28, 29].

What from the present–day's point of view is important is the following.

First, Eq. (1) does not require (and, in fact: does not permit) a chemical interpretation. Consequently, the graph G needs not satisfy any of the several chemistry-based conditions, such as that it must be connected, that its maximum vertex degree must not exceed 3, etc. [37]. The graph energy is defined for all graphs and mathematicians may study it without being restricted by any chemistry-caused limitation.

Second, somewhere around the turn of the century mathematicians realized the mathematical value (and, let us say: mathematical beauty) of graph energy, 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, 2008, and 2009 this number increased to 30, 47, and 59, respectively. In the time of completion of this chapter (August 2010) the author is aware of 54 papers on graph energy published in 2010 or in press. Solely in the 21-th century several hundreds of mathematicians from Australia, Austria, Brazil, Canada, Chile, China, Croatia, Germany, India, Iran, Ireland, Italy, Mexico, Netherlands, Pakistan, Portugal, Rumania, Russia, Serbia, South Africa, South Korea, Spain, Sweden, Turkey, UK, USA, and Venezuela participated or are participating in research on graph energy.

Details of the (mathematical) theory of graph energy can be found in the reviews [26, 29, 35, 54] and in the references cited therein. In this chapter we are going to outline only two aspects of this theory, namely the results pertaining to the conditions $E > 2n - 2$ and $E(G) < n$. Before doing this, in the subsequent section we briefly repeat the details on E related to chemistry.

2. The chemical connection

Researches related to 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 [6, 62, 66].

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

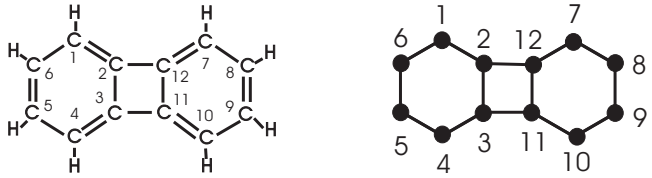
$$\hat{H}\,\Psi = \mathcal{E}\,\Psi \tag{2}$$

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. (2), which evidently is an eigenvalue–eigenvector problem of the Hamiltonian operator. In order that the solution of (2) 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. (2) 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.



H *G*

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. (3) and (4).

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 [6, 62, 66].

For instance, the HMO Hamiltonian matrix of biphenylene is:

$$\mathbf{H} = \begin{bmatrix} \alpha & \beta & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta \\ 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & 0 & 0 & 0 & \beta & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha & \beta & 0 & 0 & 0 & \beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 \\ 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta \\ 0 & \beta & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & \beta & \alpha \end{bmatrix} \tag{3}$$

which can be written also as

(4)

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

The first matrix on the right-hand side of Eq. (4) 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

$$\mathbf{H} = \alpha\, \mathbf{I}_n + \beta\, \mathbf{A}(G) \tag{5}$$

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 (5), which was first noticed only in 1956 [19]. Much later, not knowing of [19], the same observation was made by the present author (for details see [8, 30]). Anyway, the mere observation of the existence of the connection between HMO theory and spectral graph theory had little impact on theoretical chemistry. Chemists became interested in this connection only after it was shown (to them) how by means of the Sachs theorem some long-time open problems of HMO theory could easily be resolved [18, 27].

As a consequence of (5), 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 [13,17,37] and reviews [28,29]. 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

$$E = \sum_{j=1}^{n} g_j\, \lambda_j. \tag{6}$$

The right-hand side of Eq. (6) 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. (6) 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

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

which by form (but not by "physical meaning") is identical to Eq. (1).

3. Hyperenergetic graphs

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

$$E > 2n - 2.$$

In order to understand the reason for defining "hyperenergeticity" in such a seemingly awkward manner, one needs to recall the following.

In the times when computers were not commonly available, the calculation of HMO total π-energy (that is, E) was not an easy task. Therefore, much work was done on finding simple algebraic expressions that would make it possible to obtain an approximate numerical value of E knowing the simple structural details of the underlying molecular graph. A particularly successful such approximation was discovered by McClelland [55], viz.

$$E \approx a\sqrt{2mn}$$

where n and m are the number of vertices (resp., number of carbon atoms) and number of edges (resp., number of carbon–carbon bonds) of the corresponding molecular graph (resp., conjugated hydrocarbon), and where a is an empirical constant ($a \approx 0.9$). Eventually, scores of other such (n, m)-type approximate expressions for E were designed, whose details can be found in the surveys [23, 39].

Most of the (n, m)-type approximate expressions for E are monotonically increasing functions of the parameter m. This, indeed, is in good agreement with the observed E-values of molecular graphs, which because of the requirement $2m/n \leqslant 3$, necessarily have small number of edges.

By extrapolating this kind od m-dependence of E, one readily arrives at the conclusion that among n-vertex graphs, the complete graph K_n would have maximal energy. Since $E(K_n) = 2n - 2$, one would thus arrive at:

Conjecture 3.1. [21] If G is an n-vertex graph, $G \ncong K_n$, then $E(G) < 2n - 2$.

This conjecture was stated by the present author in his first paper on graph energy [21]. Soon thereafter, by means of counterexamples, Conjecture 3.1 was shown to be false [9].

At this point it is worth mentioning that in the 1990s a Chinese mathematician (whose name will be omitted) offered a proof of Conjecture 3.1. He had luck that the present author refereed his paper. The error committed in the proof was trivial: a simple quadratic equation was incorrectly solved. This minor mistake implied then the expected conclusion that $E(G) < 2n - 2$. Of course, the paper was never published.

The true work on hyperenergetic graphs started in the late 1990s, independently by a group of Indian mathematicians [64] and the present author [25, 36].

Theorem 3.2. [64] (a) *For $n \geqslant 5$ the line graph of the complete graph K_n is hyperenergetic.*
(b) *For $n \geqslant 4$ the line graph of the complete bipartite graph $K_{n,n}$ is hyperenergetic.*
(c) *For $n \geqslant 6$ the line graph of the n-vertex cocktail party graph is hyperenergetic.*

By Theorem 3.2, for the first time, infinitely many hyperenergetic graphs could be systematically constructed. Hou and the present author later extended this result as follows:

Theorem 3.3. [44] *All graphs with more than* $2n - 1$ *edges are hyperenergetic.*

In [36] graphs obtained by deleting a few edges from K_n were studied. It was shown that by deleting one, two, or three edges from K_n, the respective energy is smaller than $E(K_n)$. However, if four edges, forming a quadrangle, are deleted, then the energy exceeds $E(K_n)$. The works [25, 36] implied:

Theorem 3.4. [25] *Hyperenergetic graphs on* n*-vertices exist for all* $n \geqslant 8$*. There are no hyperenergetic graphs on less than 8 vertices.*

Eventually, hyperenergeticity was verified for a variety of other classes of graphs: Paley [46], circulant [61], Kneser [2], etc. [3]. For some other graphs, especially those for which the maximal vertex degree is 3 or less, it was shown that they cannot be hyperenergetic [32, 63].

The mortal blow to the research of hyperenergetic graphs was givew by Nikiforv, who showed:

Theorem 3.5. [56] *For almost all graphs*

$$E(G) = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2}.$$

Theorem 3.5 immediately implies that almost all graphs are hyperenergetic, making any further search for them pointless.

In view of Nikiforov's negative result, it is interesting that in a recent work [60], Shen at al. proved:

Theorem 3.6. [60] *For any* $c < \infty$*, there exists only a finite number of hyperenergetic graphs with cyclomatic number* c*. In particular, there are no hyperenergetic graphs with* $c \leqslant 8$*.*

4. Hypoenergetic graphs

Definition 3. 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 was 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 [14] 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 [37]. The authors of [14] 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 4.1. *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 4.2. *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 [4] that for all graphs, $E \geqslant 2\sqrt{m}$. Theorem 4.2 follows from $2\sqrt{m} \geqslant n$. □

Theorem 4.3. [40] *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 $n = 2ab$.

A straightforward consequence of Theorem 3.5 is:

Theorem 4.4. *Almost all graphs are non-hypoenergetic.*

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

Theorem 4.5. [31] *All hexagonal systems are non-hypoenergetic.*

Denote by $\Delta = \Delta(G)$ the maximum vertex degree of the graph G.

Theorem 4.6. [34,38] *Among trees with $\Delta \leqslant 3$, there are exactly four hypoenergetic species, G_1, G_2, G_3, and G_4, depicted in Fig. 2.*

Theorem 4.7. [34,38] *Among trees with $\Delta = 4$, there are infinitely many hypoenergetic species. The same holds also if $\Delta > 4$.*

In connection with Theorems 4.6 and 4.7 it is of importance to determine the trees with maximum vertex degree Δ, having minimum energy. This problem was recently completely solved by Heuberger and Wagner [42,43]. For an earlier attempt to treat the same problem, see [15]. Although in [15] the structure of the minimal-energy trees has not be determined, it was established that (in the general case) these differ from Volkmann trees [16, 48].

Theorem 4.8. [57] *Among connected quadrangle-free graphs with $\Delta \leqslant 3$, G_1, G_2, G_3, and G_4, and only these are hypoenergetic.*

Theorem 4.9. [49] *Among connected graphs with $\Delta \leqslant 3$, G_1, G_2, G_3, G_4, and G_5, and only these are hypoenergetic.*

Theorem 4.10. [50] *Among connected graphs with $\Delta \leqslant 3$, G_6, G_7, G_8, and G_9, and only these have energies equal to the number of vertices.*

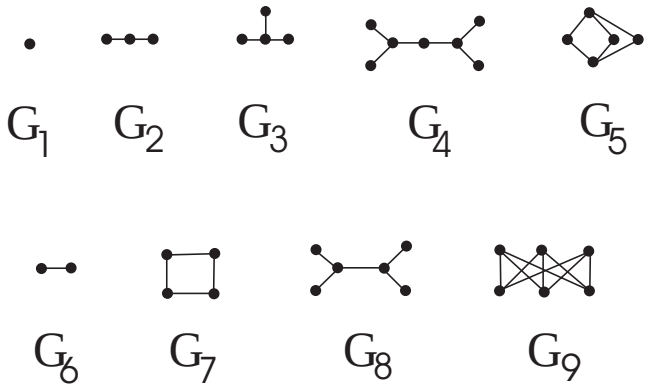


FIGURE 2. Graphs mentioned in Theorems 4.6-4.10

In connection with Theorem 4.7 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 [67] that there exist hypoenergetic connected unicyclic graphs for all $n \geqslant 7$ and hypoenergetic connected bicyclic graphs for all $n \geqslant 8$ is no surprise whatsoever.

Theorem 4.11. [67] *There are no hypoenergetic unicyclic graphs on n vertices with $n \leqslant 6$. There exist hypoenergetic unicyclic graphs on n vertices for all $n \geqslant 7$.*

Theorem 4.12. [67] *If n is even and $\Delta \in [n/2, n-1]$ or n is odd and $\Delta \in [(n+1)/2, n-1]$, then for all $n \geqslant 9$ there exist unicyclic hypoenergetic graphs of order n with maximum vertex degree Δ.*

Theorem 4.13. [67] *There are no hypoenergetic bicyclic graphs on n vertices with $n = 4$, $n = 6$, and $n = 7$. There exist hypoenergetic bicyclic graphs on n vertices for $n = 5$ and all $n \geqslant 8$.*

Theorem 4.14. [67] *If n is even and $\Delta \in [n/2+1, n-1]$ or n is odd and $\Delta \in [(n+1)/2, n-1]$, then for all $n \geqslant 9$ there exist bicyclic hypoenergetic graphs of order n with maximum vertex degree Δ.*

Results of the same kind as Theorems 4.11-4.14 have been obtained also for c-cyclic graphs with $c \geqslant 3$ [45, 51, 68]. Of these we mention here only:

Theorem 4.15. [68] *There exist hypoenergetic c-cyclic graphs for any c.*

5. Interlude: biregular and triregular graphs

A graph is said to be regular if all its vertices have equal degrees. We now generalize this simple concept to the case when the verticex degrees assume two or three different values.

Definition 4. 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.

Because biregular graphs play an important role in the subsequent part of this chapter, in Fig. 3 are depicted a few examples thereof.

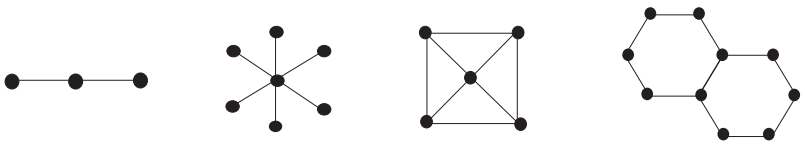


FIGURE 3. Examples of biregular graphs: a (1,2)-biregular tree (the 3-vertex path), a (1,6)-biregular tree (the 7-vertex star), a (3,4)-biregular graph, and a (2,3)-biregular graph (a hexagonal system).

Definition 5. 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.

By Theorem 4.3, the problem considered in this chapter has been completely solved for regular graphs [40]. Hexagonal systems (mentioned in Theorem 4.5) have vertex degrees equal to 2 and 3, and therefore belong to a special class of biregular graphs. From the proof of Theorem 4.5 [31], 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 [1, 33, 47, 52, 53]. In what follows we report in due detail our [1, 33] and other colleague's [65] researches on biregular graphs with cyclomatic number $c \leqslant 2$. 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. Analogous considerations for triregular graphs can be found in [32, 53] and in the survey [54]. Tricyclic biregular graphs have also been recently examined [52].

6. 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. (1), 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 [24, 69] and two times for bipartite graphs [12, 58]. Recently a generalized version thereof was obtained [70].

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 6.1. *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 6.1 will be the basis for 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).

7. On the energy of biregular graphs

In this section we use same the notation as in Definition 4. Thus the degrees of the vertices of a biregular graph are denoted by a and b, and $a < b$.

7.1. 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. The number of pendent vertices will be denoted by k.

From now on we 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, implying $n \geqslant 5$. By examining 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 see that $f'(x) > 0 \quad \forall x \in [5, +\infty)$, so f monotonically increases. Further, the 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 thus arrive at the following:

Theorem 7.1. *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 7.1 the only biregular trees that satisfy condition (14) are the paths with at least 5 vertices.

7.2. 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

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

and

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

Therefore,

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

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 that $b = 3$.

For $q = 1$ we obtain $b \leqslant 3 - 4/n$, from which we see that it must be $b < 3$. This, however, is impossible, implying that there is no unicyclic biregular graph with $q = 1$, for which the inequality (14) holds. Thus we obtain:

Theorem 7.2. *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 7.2 are shown in Fig. 4. From these examples the general structure of such graphs should be evident:

Theorem 7.3. *Let G be a connected unicyclic (a, b)-biregular graph for which* (14) *holds. Then G is obtained from a cycle C_p, by attaching to each of its vertices exactly one pendent vertex, where $p = 3$ or $p \geqslant 5$.*

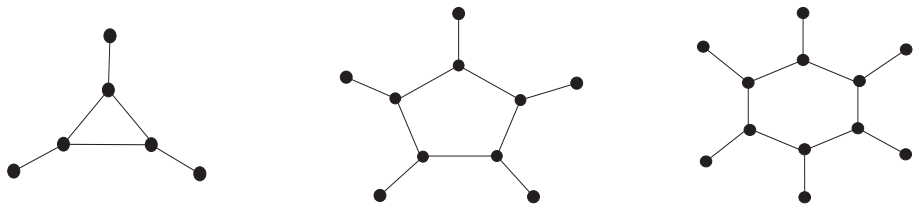


FIGURE 4. Examples of connected quadrangle-free (1,3)-biregular unicyclic graphs.

7.3. 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.

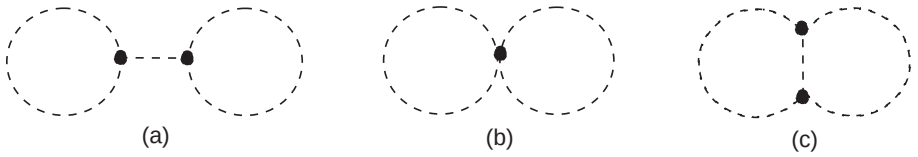


FIGURE 5. Types of bicyclic graphs.

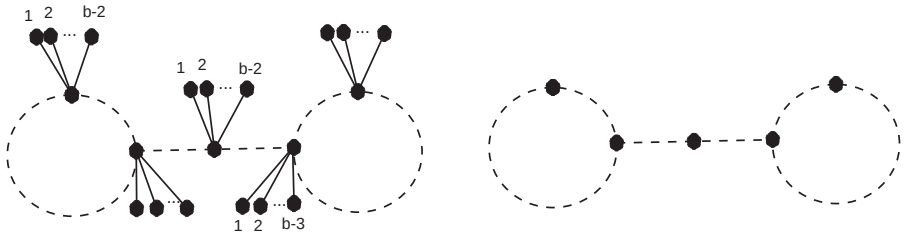


FIGURE 6. Sketches of $(1, b)$-, and $(2, 3)$-biregular bicyclic graphs with disjoint cycles. The vertices that connect cycles in a $(1, b)$-biregular graph ($b \geqslant 3$) are connected also with $b - 3$ pendent vertices, whereas all other vertices in such a graph are connected with $b - 2$ pendent 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.

7.3.1. *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

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

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 7.4. *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 7.4 are depicted in Fig. 7.

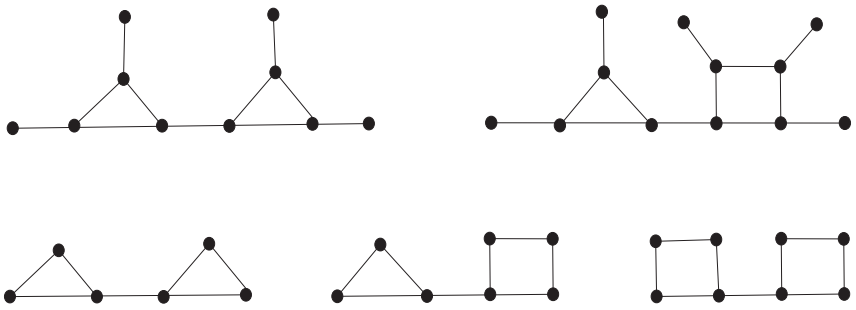


FIGURE 7. Connected bicyclic $(1, 3)$-biregular graphs with disjoint cycles, with $q = 0$ and $q = 1$, and bicyclic $(2, 3)$-biregular graphs with disjoint cycles, with $q = 0$, $q = 1$, $q = 2$. In all these examples the number of vertices is as small as possible.

7.3.2. *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.

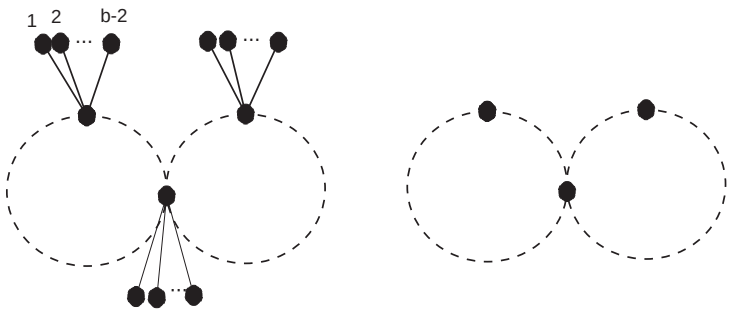


FIGURE 8. Connected bicyclic $(1, b \geqslant 4)$- and $(2, 4)$-biregular graph in which cycles have one common vertex. For the $(1, b)$-biregular graph, $b \geqslant 4$, every vertex except the one belonging to both cycles is connected with $b - 2$ pendent vertices. The vertex belonging to both cycles 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.

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 7.5. *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 7.5 are shown in Fig. 9.

7.3.3. *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

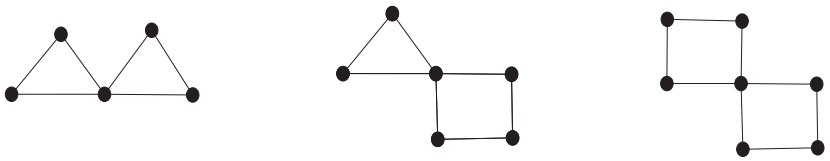


FIGURE 9. Bicyclic $(2,4)$-biregular graphs in which the cycles have one common vertex, with $q = 0, 1, 2$ quadrangles. In these examples the number of vertices is as small as possible.

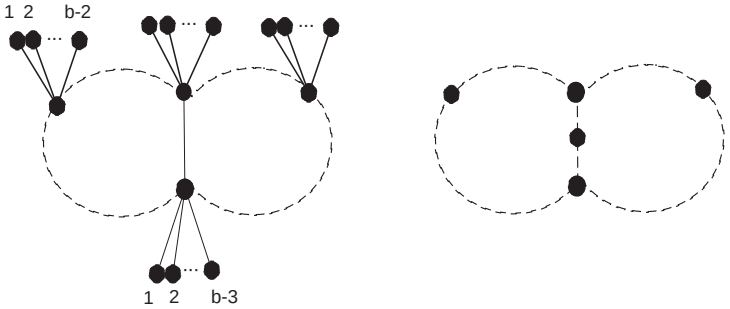


FIGURE 10. Connected bicyclic $(1, b \geqslant 3)$- and $(2,3)$-biregular graphs in which the cycles have two or more common vertices. Notice that the cycles of the graphs of the first type have only two common vertices, whereas the cycles of the graphs of the second type may have arbitrarily many common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

Fig. 11. From (22) for $b = 3$, we get the inequality $-7n^3 + 12n + 4 \geqslant 0$ that is not fulfilled for $n = 5$.

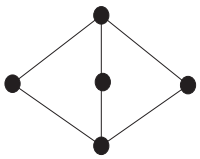


FIGURE 11. The only bicyclic biregular graph in which the number of quadrangles q is 3. For this graph inequality (14) is violated. Recall that according to Theorem 4.9 this graph is hypoenergetic.

Theorem 7.6. *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 7.6 holds are shown in Fig. 12.

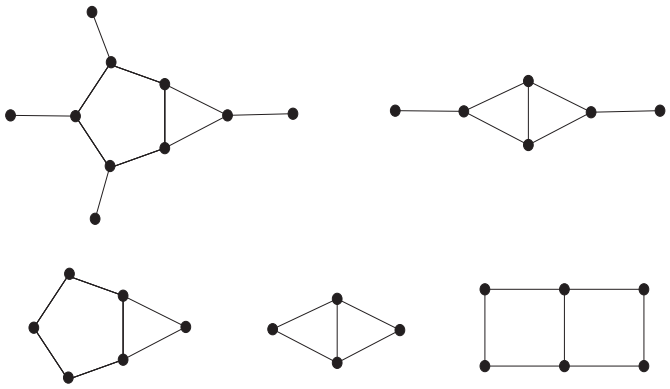


FIGURE 12. Bicyclic $(1,3)$-biregular graphs in which cycles have two common vertices and $q = 0, 1$, and bicyclic $(2,3)$-biregular graphs with $q = 0, 1, 2$.

7.3.4. *Concluding remark.* In this sections we established necessary and sufficient conditions for the validity of the inequality (14), for certain types of acyclic, unicyclic, and bicyclic graphs. In these considerations the graph energy was not mentioned at all. Therefore, at this point it seems to be purposeful to re-state Theorem 6.1:

Theorem 6.1.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 that violate inequality* (14)*.*

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NULLITY OF GRAPHS: AN UPDATED SURVEY

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 in an updated version of the an earlier survey [B. Borovićanin, I. Gutman, *Nullity of graphs*, in: D. Cvetković, I. Gutman, Eds. *Applications of Graph Spectra*, Math. Inst., Belgrade, 2009, pp. 107–122] and 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 (2010): 05C50; 05C90; 92E10

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

Contents

1. Graph nullity and its chemical applications

This chapter is an updated, extended, and modified version of the survey [3] that was a part of the booklet "*Applications of Graph Spectra*". Since the completion of [3], a number of relevant results came to the authors' attention, that now are appropriately taken care of.

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.[1]

In addition to its evident relevance in "pure" spectral graph theory, the nullity has a noteworthy application in chemistry. The recognition of this fact, first outlined in [8], was not only an important discovery per se, but happened to be the starting point of an unprecedented activity in theoretical and mathematical chemistry, resulting in thousands of published papers, and leading to a new field of research, nowadays referred to as *Chemical Graph Theory* [13, 19, 23, 40].

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 [12]. 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* [28]. Nowadays, this method is known under the name *Hückel molecular orbital* (*HMO*) *theory* [5, 12, 41].

A quarter of century was needed to recognize that the mathematics on which the HMO theory is based is graph spectral theory [20, 35]. In a nutshell: The (approximate) energies $E_1, E_2, \ldots$ that the electrons may possess are related to the

[1]The symbol η for nullity was first used by I. G. in his correspondence with Dragoš Cvetković, which eventually resulted in the paper [8]. The choice for η was fully arbitrary. Yet, nowadays this symbol is used by the majority of scholars. Another notation for nullity is n_0.

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 [19, 23]. 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 [33].

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*" [6]. 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 [7].

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 [32]:

- 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. [7, 8, 36] (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. [11] *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. [11] *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. [11] *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 $\mathrm{gir}(G)$ is given by:

Corollary 2. [11] *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. [11] *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. [11] *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. [11] *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)

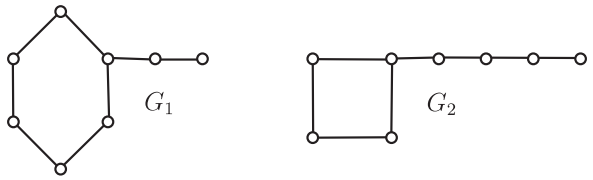

FIGURE 1

In what follows we consider mostly bipartite graphs, although some of the theorems stated below can be extended to non-bipartite graphs (see [9]).

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 [7]

$$a_i = \sum_U (-1)^{p(U)}\, 2^{c(U)} \quad (i = 1, 2, \ldots, n), \tag{2}$$

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 [8].

Theorem 1. [8] *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. [10] *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 $4s$) [22]. 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" [22], Sachs and John produced an independent paper on this "discovery" and (together with Fajtlowicz) published it [15].

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. [32] *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. [8] $\eta(G) \geqslant \max(|X|, |Y|) - \min(|X|, |Y|)$.

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 ([8], [10]) 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. [8] *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. [8] *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. [8] *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.

Theorem 5. [10] *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. [10] *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 $\eta(G)$.*

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 [9].

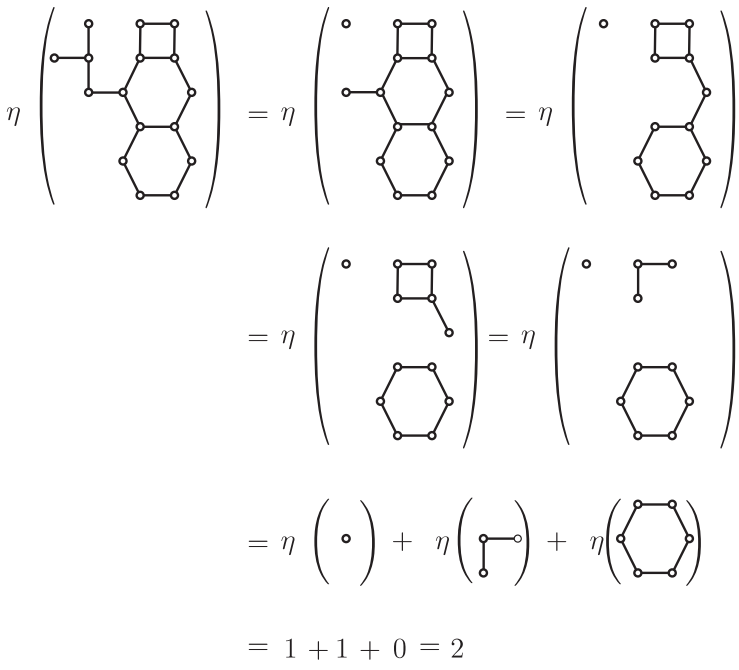

FIGURE 2

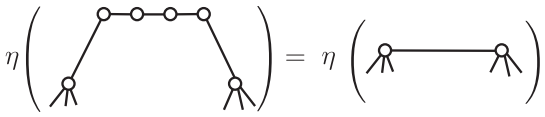

FIGURE 3

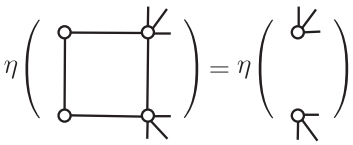

FIGURE 4

Example 2. See Fig. 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.

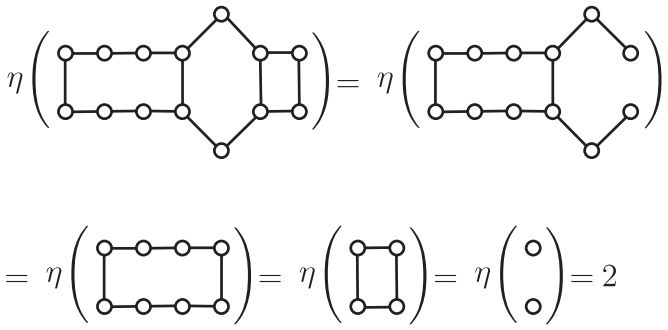

FIGURE 5

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. [11] *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 graphs satisfying $\eta = n-t$ for some fixed value t, $t > 3$ 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 [30]. Then we proceed recursively, as in [30], 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. [30] *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.*

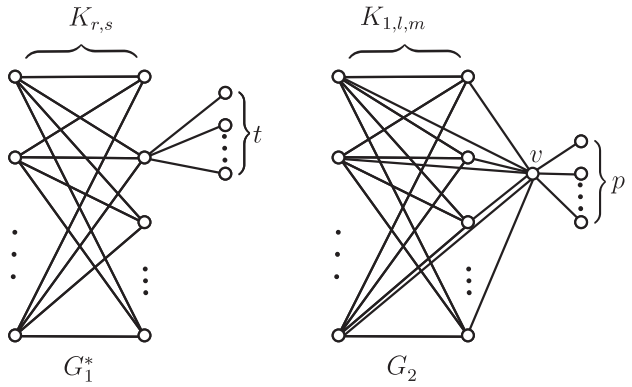

FIGURE 6

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 $l + m + p + d + 1 = n$.

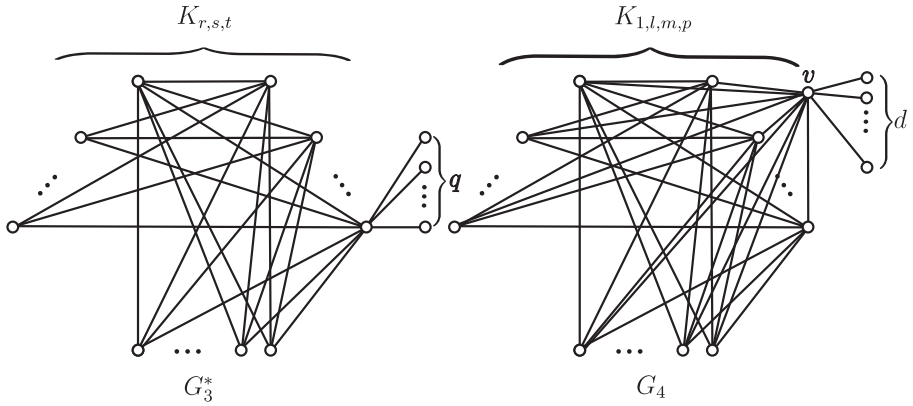

FIGURE 7

Theorem 9. [30] *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 [30]. Recently, also graphs with pendent trees were examined with regard to their nullity [18].

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. [14, 30] *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 $T \cong S_n$* [14].

(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 [30].

(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 [30].

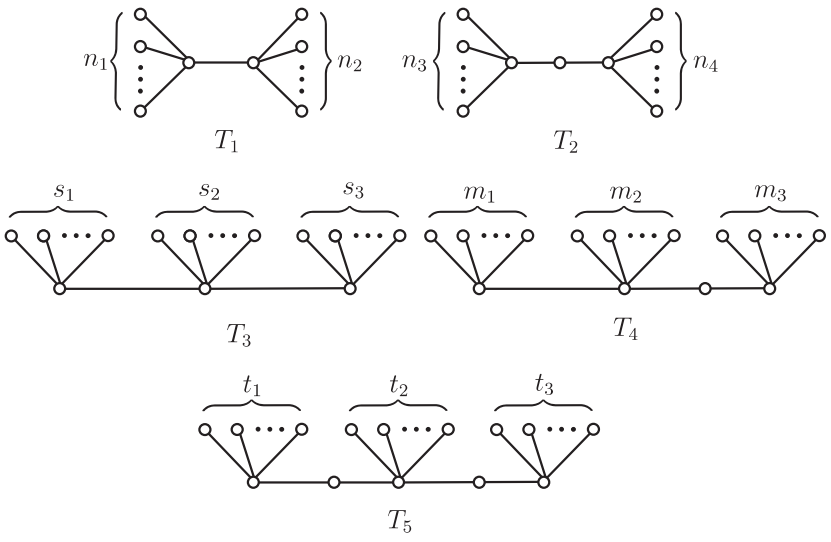

FIGURE 8

Just as in Theorem 10, we can use graphs in $\mathcal{T}_n$ (see [30]) whose nullity is $n-6$ to determine n-vertex trees whose nullity is $n-8$, and so on. This implies:

Corollary 8. [30] *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.*

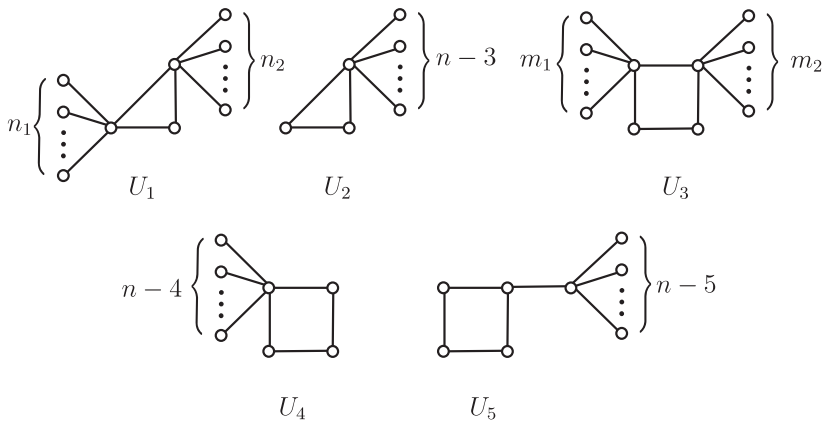

FIGURE 9

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 Tan and Liu obtained:

Theorem 11. [39] *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 was also determined in [39].

Theorem 12. [39] *The nullity set of $\mathcal{U}_n$ $(n \geqslant 5)$ is $[0, n-4]$.*

Recently, Guo, Yan, and Yeh [21] have somewhat extended the results of [39] by characterizing unicyclic graphs for which $\eta = n-5$. They also proved:

Theorem 13. [21] *Let $G \in \mathcal{U}_n$. Let m be the size of a maximum matching of G. Then $\eta(G) = n-2m-1$ or $\eta(G) = n-2m$ or $\eta(G) = n-2m+2$.*

In [21] the structure of the graphs belonging to each of the three cases in Theorem 13 was fully determined.

In [39] the characterization of unicyclic graphs for which $\eta = 0$ remained as an open problem. In [21] the following was shown:

Theorem 14. *Let $G \in \mathcal{U}_n$ and let C_ℓ be the unique cycle of G. Then $\eta(G) = 0$ holds if and only if either G has a unique perfect matching, or ℓ is odd and $G - C_\ell$ has a perfect matching, or $\ell \not\equiv 0 \pmod 4$ and G has two perfect matchings.*

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 [26, 29]. Thus, the following results are proved.

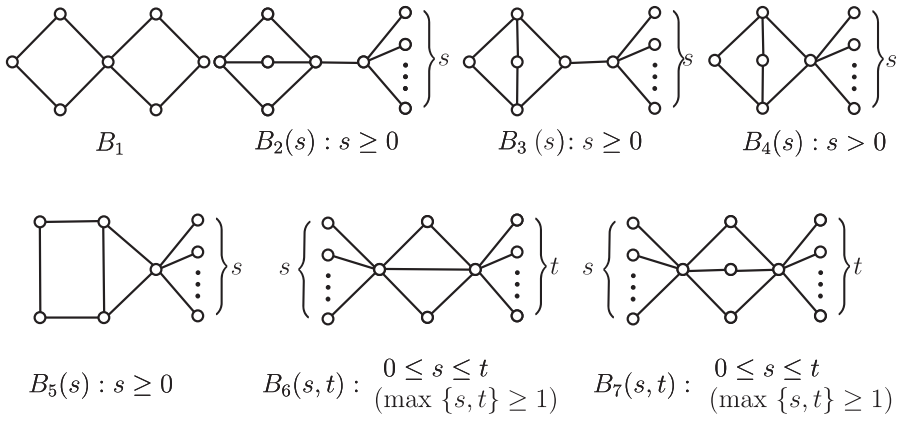

FIGURE 10

Theorem 15. [26, 29] *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 16. [26, 29] *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 [17].

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 17. [17] *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 [17] 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 [31] 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 18. [31] $\mathcal{T}(n, \Delta, \max) = \mathcal{T}_1^*(n, \Delta, \max) \cup \mathcal{T}_2^*(n, \Delta, \max)$.

A result analogous to Theorem 17 has recently been proved for bipartite graphs:

Theorem 19. [34] *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 $\eta(G) \leqslant n - 2\lceil e/\Delta \rceil$.*

For bipartite graphs Fan and Qian [16] obtained the following results. Let Bip_n be the set of all bipartite graphs on n vertices.

Theorem 20. [16] *The nullity set of* Bip_n *is* $\{n - 2k \mid k = 0, 1, 2, \ldots, \lfloor n/2 \rfloor\}$.

In order to formulate the next two theorems, we need to define the concepts of *extended path* and *extended cycle*.

Let for $n \geqslant 2$, $P_n := v_1 v_2 \cdots v_n$ be a path on vertices $v_1, v_2, \ldots, v_n$ with edges $(v_i, v_{i+1}$ for $i = 1, 2, \ldots, n-1$. Let O_p denote the p-vertex graph without edges, an empty graph. Replace each vertex v_i of P_n by an empty graph O_{p_i} for $i = 1, 2, \ldots, n$, and add edges between each vertex of O_{p_i} and each of $O_{p_{i+1}}$ for $i = 1, 2, \ldots, n-1$. The graph thus obtained is of order $N = p_1 + p_2 + \cdots + p_n$ and will be referred to as an *extended path* of length n. In an analogous manner we construct an *extended cycle* of length n, $n \geqslant 3$, by additionally joining all vertices of O_{p_1} with all vertices of O_{p_n}.

At this point we note that the nullity of an extended path of length n, $n \geqslant 2$, and of order N is equal to $N - n$ if n is even, and is equal to $N - n + 1$ if n is odd [16].

Theorem 21. [16] *Let $G \in \mathrm{Bip}_n$, $n \geqslant 4$. Then $\eta(G) = n - 4$ if and only if G is isomorphic to a graph H to which possibly some isolated vertices are added, where H is either the union of two extended paths of length 2, or an extended path of length 4, or an extended path of length 5.*

Theorem 22. [16] *Let $G \in \mathrm{Bip}_n$, $n \geqslant 6$. Then $\eta(G) = n - 6$ if and only if G is isomorphic to a graph H to which possibly some isolated vertices are added, where*

H is either the union of three extended paths of length 2, or an extended cycle of length 6, or an extended cycle of length 8, and in any of these graphs the number of all extended vertices (i.e., the p_i-values) are mutually equal.

Finally, we mention another family of graphs where the nullity problem has been solved [25]. 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).

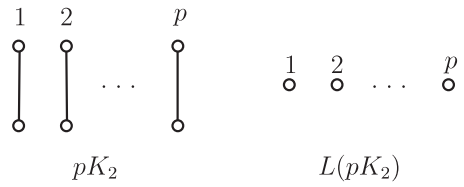

FIGURE 11

If we restrict ourselves to connected graphs then the nullity of the line graph may still be any positive integer. For instance [25], for the graph G_r depicted in Fig. 12, $\eta(L(G_r)) = r + 1$.

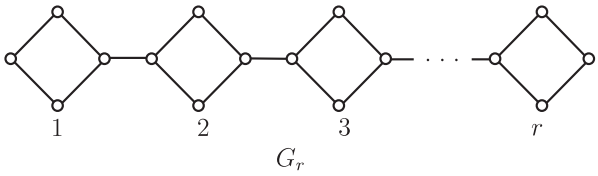

FIGURE 12

With the line graphs of trees the situation is different:

Theorem 23. [25] *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 [37, 38].

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THE ESTRADA INDEX: AN UPDATED SURVEY

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.

This chapter in an updated version of the an earlier survey by the same authors, published in the book D. Cvetković, I. Gutman (Eds.), *Applications of Graph Spectra*, Math. Inst., Belgrade, 2009, pp. 123–140.

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Contents

1. Introduction: the Estrada index and its various applications

This chapter is an updated, extended, and modified version of the survey [12] that was a part of the booklet "*Applications of Graph Spectra*". Since the completion of [12], a number of relevant results came to the authors' attention, that now are appropriately taken care of.

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 [4] 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 books [4, 5].

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 [8] to call it the *Estrada index*, a name that in the meantime has been commonly accepted.

Although invented in year 2000 [15], 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 [15–17]; 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 [21, 22]. 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 [18]. In [23] 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 [20] and later further extended in [19]. Recently, Carbó–Dorca [3] endeavored to find connections between EE and the Shannon entropy.

The proposed biochemical [15–17], physico–chemical [20,23], network–theoretical [18, 21, 22], and infomation–theoretical [3] applications of the Estrada index are nowadays widely accepted and used by other members of the scientific community; see, for example [6, 14, 30, 44, 45, 47, 51, 57]. 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 [22, 33].

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 [4] 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 [4]:

$$M_0 = n; \quad M_1 = 0; \quad M_2 = 2m; \quad M_3 = 6t$$

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 $G \cong \bar{K}_n$ [24].

4° The eigenvalues of a bipartite graph satisfy the pairing property [4]: $\lambda_{n-i+1} = -\lambda_i$, $i = 1, 2, \ldots, n$. 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. [8] *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 $\bar{K}_n$ [4].

By this the proof of Theorem 3.1 is completed. □

Recently Zhou [54] arrived at the following generalizations of Theorem 3.1:

Theorem 3.2. [54] *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. [54] *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. [54] *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. [54] *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. [31] *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. [31] *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. [31,38] *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 [38] and eventually extended to all graphs. The same result was later communicated also in [54].

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 $-r$ [4]. Bearing these facts in mind, some of the above bounds could have been simplified [8]:

Theorem 3.9. [8] *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. [8] *Let G be a bipartite regular graph of degree r and of order n. Then*

$$2\cosh(r) + \sqrt{(n-2)^2 + 2nr - 4\,r^2} \leqslant EE(G) \leqslant n - 4 + 2\cosh(r) + 2\cosh\left(\sqrt{nr/2 - r^2}\right).$$

In recent works [2, 7] several bounds for the Estrada index were obtained, of which we state here the neat:

Theorem 3.11. [7] *Let G be a connected graph with n vertices and m edges. Then,*

$$EE(G) \geqslant n + \left(\frac{2m}{n}\right)^2 + \frac{1}{12}\left(\frac{2m}{n}\right)^4.$$

4. Estrada indices of some graphs

For graphs whose spectra are known [4], 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 $EE(Q_n) = [2\cosh(1)]^n$ [24].

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 $EE(W_{n+1}) = EE(C_n) - e^2 + 2e\cosh\left(\sqrt{n-1}\right)$ [24].

The Estrada index of the cycle C_n can be approximated as $EE(C_n) \approx n\, I_0$, [36] 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, 36]

$$\begin{aligned} EE(P_n) &\approx (n+1)\, I_0 - \cosh(2) \\ EE(Z_n) &\approx (n+2)\, I_0 \\ EE(ZZ_n) &\approx (n+1)\, I_0 + 2 + \cosh(2) \end{aligned}$$

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 [26]

$$EE(P_{n,m}) \approx (m-1)n + 2(n+1)\, J_m,$$

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 [52]. Expressions and approximate expressions for EE of several other graphs can be found in [24].

In [41] 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 [41] also some more complicated approximations for EE of (n, m)-graphs were proposed.

4.1. Estrada index of line graphs.

Theorem 4.1. [1] *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 $G \cong C_n$ [24]. 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. [1] *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 [1] 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 [1] 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. [24] *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. [24] *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. [24] $EE(G \times H) = EE(G)\, EE(H)$. *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 [8] 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.

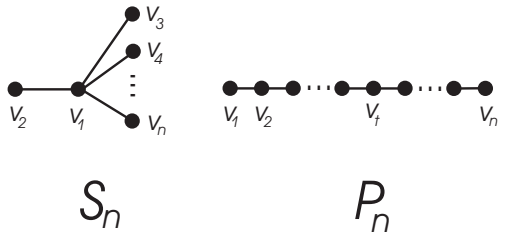

FIGURE 1. The star S_n and the path P_n, and the labelling of their vertices.

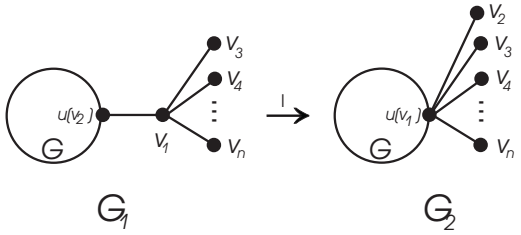

FIGURE 2. Transformation I.

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. [10] *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. [10] *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. [10] *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. [10] *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.

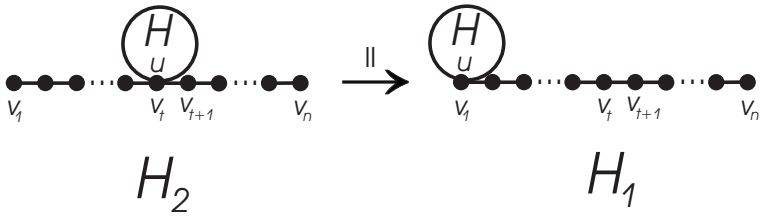

FIGURE 3. Transformation II.

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. [10] *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 [53] have determined also the trees with the second and the third greatest Estrada index. In fact, they proved:

Theorem 5.6. [53] *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.

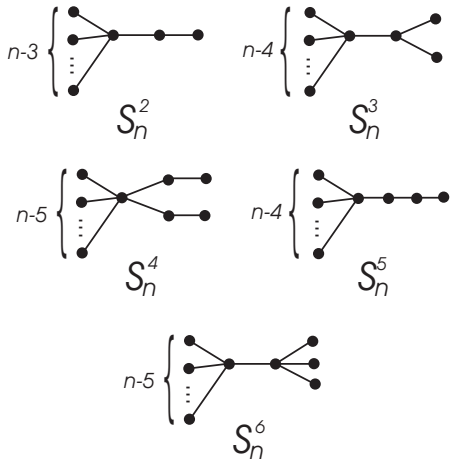

FIGURE 4. The graphs S_n^i, $i = 2, 3, 4, 5, 6$, having the second, third, fourth, fifth, and sixth greatest Estrada indices among n-vertex trees [11, 53].

Recently it was demonstrated [11] that $EE(S_n^3) > EE(S_n^4) > EE(S_n^5)$, from which follows:

Theorem 5.7. [11] *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.*

Theorem 5.5 can be extended also in another way. Denote by $B_{n,\Delta}$ the tree obtained by attaching $\Delta - 1$ pendent vertices to a pendent vertex of the path $P_{n-\Delta+1}$. This tree is usually referred to as a "*broom*" (cf. [9]).

Theorem 5.8. [42] *Among all trees on n vertices and maximum vertex degree Δ, the broom $B_{n,\Delta}$ has minimum Estrada index.*

Theorem 5.9. [42] *Observing that $B_{n,n-1} \equiv S_n$ and $B_{n,2} \equiv P_n$, we have*

$$EE(B_{n,n-1}) > EE(B_{n,n-2}) > \cdots > EE(B_{n,3}) > EE(B_{n,2}).$$

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 5.10. [10] *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 5.10 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.

Independently of the work of one of the present author [10, 11], Das and Lee also examined the Conjectures A and B [7]. For any connected (n, m)-graph G, they were able to show that $EE(G) > EE(P_n)$ provided $m \geqslant 1.8\,n + 4$, and that $EE(G) \geqslant E(P_n)$ provided $m \geqslant n^2/6$. In addition, they also proved that among trees, the star has maximum Estrada index.

6. Estrada indices of molecular graphs

In view of the chemical origin of the Estrada index, it is natural than molecular graphs [37], especially acyclic and benzenoid, were among the first whose structure–dependence was systematically examined.

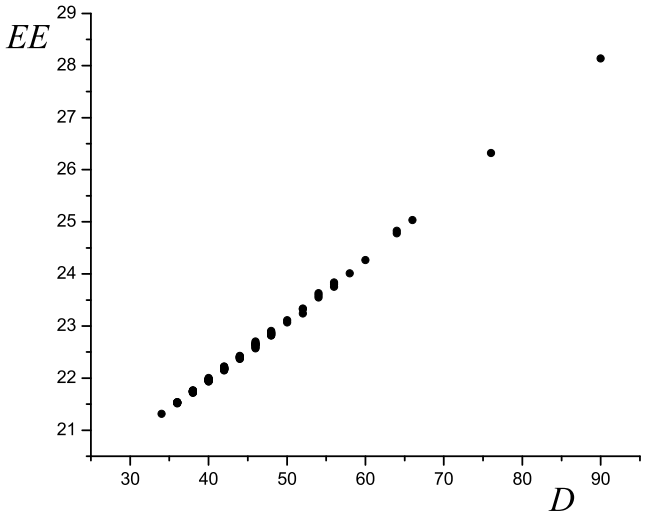

FIGURE 5. Correlation between the Estrada indices and the parameter D (= sum of squares of vertex degrees) for the 106 trees on 10 vertices.

A chemical tree is a tree in which no vertex has degree greater than four [37]. Among the n-vertex chemical trees, P_n has minimum Estrada index. For the 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 [34]. This fact motivated investigations of the relation between EE

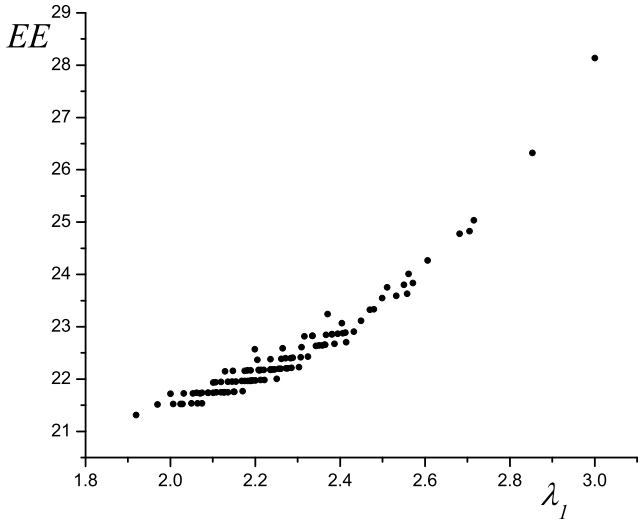

FIGURE 6. Correlation between the Estrada index (EE) and the greatest graph eigenvalue λ_1 for the 106 trees on 10 vertices.

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:

$$EE \approx 1.735\, n - 0.13 + 0.11\, D.$$

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, 40]; 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 [34, 39, 41]. For benzenoid systems, (m, n)-type approximations are capable of reproducing over 99.8% of EE-value [39, 41]. 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 [32].) Within sets of benzenoid isomers, EE is an increasing linear function of b, see Figure 7.

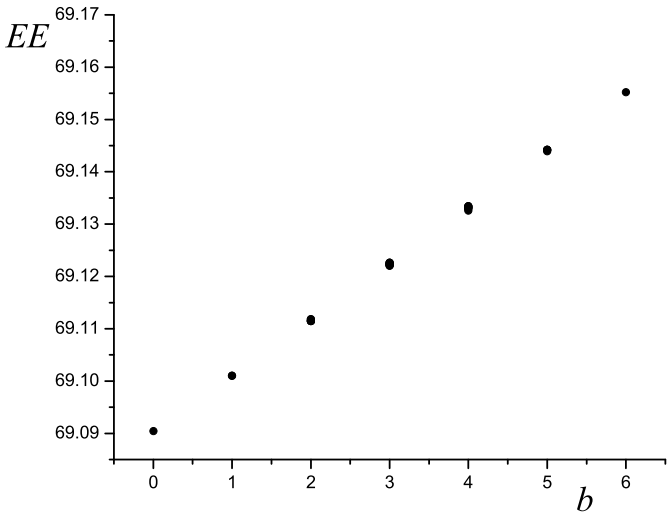

FIGURE 7. Correlation between the Estrada indices (EE) of the 36 catacondensed benzenoid systems with 6 hexagons and the number b of their bay regions.

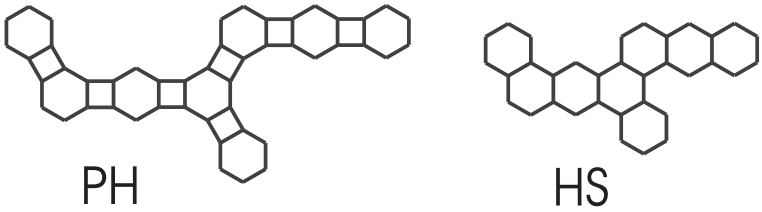

FIGURE 8. A phenylene (PH) and its hexagonal squeeze (HS).

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 [25]. 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,

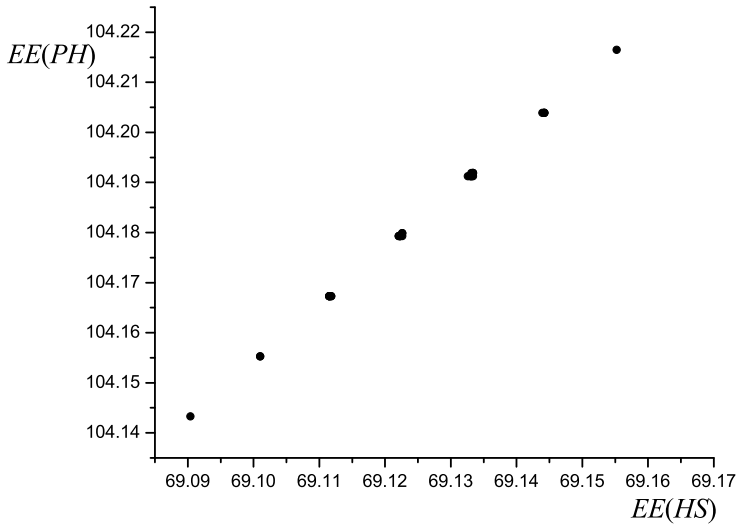

FIGURE 9. Correlation between the Estrada indices of phenylenes, $EE(PH)$, and the Estrada indices of the corresponding hexagonal squeezes, $EE(HS)$. The data points shown in this figure pertain to phenylenes with 6 hexagons; there are 37 species of this kind.

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.

7. Laplacian Estrada indices

The Estrada index is defined in terms of the ordinary graph spectrum, that is the spectrum of the adjacency matrix. Another well developed part of algebraic graph theory is the spectral theory of the Laplacian matrix [27, 28, 48–50]. The Laplacian matrix of an (n, m)-graph G is defined as $\mathbf{L}(G) = \mathbf{\Delta}(G) - \mathbf{A}(G)$, where $\mathbf{A}$ is the adjacency matrix and $\mathbf{\Delta}$ the diagonal matrix whose diagonal elements are the vertex degrees. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of $\mathbf{L}(G)$.

In view of Eq. (1), the Laplacian analogue of the Estrada index could in a natural manner be defined as

$$LEE = LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

Such a definition was, indeed, put forward in [24].

Motivated by the fact that for any (n, m)-graph, $\mu_i \geqslant 0$, $i = 1, 2, \ldots, n$, and $\sum_{i=1}^{n} \mu_i = 2m$, Li, Shiu and Chang [46] proposed a slightly different definition:

$$LEE_{LSC} = LEE_{LSC}(G) = \sum_{i=1}^{n} e^{(\mu_i - 2m/n)}.$$

Evidently,

$$LEE_{LSC}(G) = e^{-2m/n}\, EE(G)$$

and therefore it is no surprise that the lower and upper bounds for LEE obtained in [56] and those for LEE_{LSC} obtained in [46] were found to be equivalent. More bounds for LEE were reported in [2, 55].

Generally speaking, the Laplacian Estrada index has properties closely analogous to those of the ordinary Estrada index. Thus, we have:

Theorem 7.1. [43] *If T_n is a n-vertex tree different from S_n and P_n, then*

$$LEE(P_n) < LEE(T_n) < LEE(S_n).$$

This result is fully analogous to Theorem 5.5.

In [43] also the n-vertex tree with second-maximal Laplacian Estrada index was characterized. Denote by $S_n(a, b)$ the tree formed by adding an edge between the centers of the stars S_a and S_b, in which case $n = a + b$. This tree is called a "*double star*".

Theorem 7.2. [43] *For $n \geqslant 4$, the unique n-vertex tree with second-maximal Laplacian Estrada index is $S_n(2, n-2)$.*

One of the present authors together with Jie Zhang could promptly improve Theorem 7.2:

Theorem 7.3. [13] *For $n \geqslant 6$, the n-vertex tree with third-maximal Laplacian Estrada index is $S_n(3, n-3)$.*

Among results that relate the Laplacian Estrada index with the ordinary Estrada index we point out the trivial:

Theorem 7.4. *If G is a regular graph of degree r, then $LEE(G) = e^r\, EE(G)$.*

and the less straightforward:

Theorem 7.5. [56] *If G is a bipartite (n, m)-graph, then $LEE(G) = n - m + e^2\, EE(L(G))$, where $L(G)$ is the line graph of G.*

Concluding this section we mention that also the distance Estrada index was recently considered [29], in which instead of eigenvalues of the adjacency matrix one used the eigenvalues of the distance matrix.

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