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Preface

This book is on graph energy. Graph energy is an invariant that is calculated from the eigenvalues of the adjacency matrix of the graph, see Definition 2.1 in Chap. 2. In the mathematical literature, this quantity was formally put forward in 1978, but its chemical roots go back to the 1940s. In spite of this, 20 years ago, only a few mathematicians would know what graph energy is, and only few of those would consider it as a topic worth of their interest.

Then, sometime around the turn of the century, a dramatic change occurred, and graph energy started to attract the attention of a remarkably large number of mathematicians, all over the globe. Since 2001, authors from Australia, Austria, Brazil, Canada, Chile, China, Croatia, France, Germany, India, Iran, Ireland, Italy, Japan, Mexico, Netherlands, Pakistan, Portugal, Rumania, Russia, Serbia, South Africa, South Korea, Spain, Sweden, Thailand, Turkey, UK, USA, and Venezuela participated in research of graph energy. The following diagram shows the expansion of the field, reflected by the number of published papers (Fig. 1).

By now, the theory of graph energy achieved a level of maturity that both permits and requires the writing of a monograph summarizing the main (certainly not all!) results in this field. The present book is an attempt to accomplish this task.

The readers of the book are expected to be familiar with details of linear algebra and graph theory at an undergraduate level. Yet, all relevant notions from graph theory are properly defined (mainly in not only Sects. 1.4 and 1.5, but also elsewhere where needed). Less well-known concepts of linear algebra are also briefly described.

The anticipated readers of the book are mathematicians and students of mathematics, whose fields of interest are *graph theory*, *spectral graph theory*, *combinatorics*, and/or *linear algebra*. Nowadays, every textbook on spectral graph theory mentions graph energy (see Sect. 2.2). Therefore, topics related to graph energy may be a part of any graduate course dealing with the spectra of graphs. Consequently, the present book will be found suitable for such courses. The exposition of the details of the proofs of all main results will enable students to understand and eventually master not only the methods of the theory of graph energy, but also of a good part of graph theory and combinatorics.

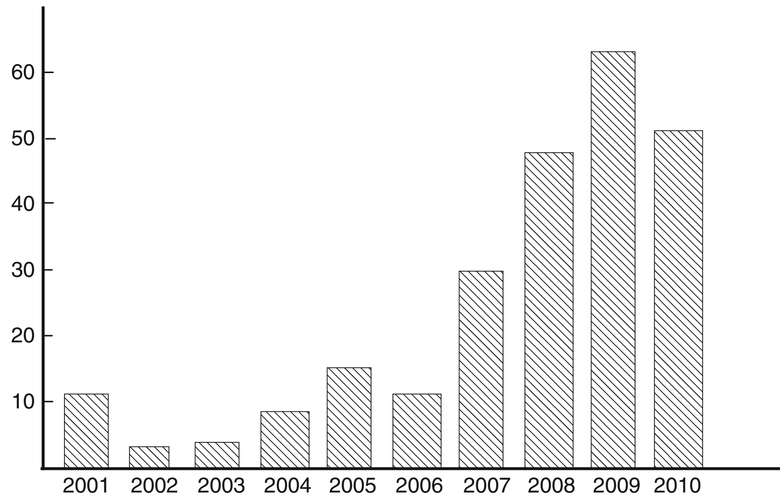

Fig. 1 Number of published mathematical papers on graph energy, of which the authors of the book are aware. At the time of the completion of the book, papers dated by year 2010 were still appearing. By May 2011, the count for 2011 was already 31, with an additional few dozen articles in press

Another major group of expected readers of our book will be scholars involved in research in what nowadays is referred to as *chemical graph theory*. Indeed, in this area, graph energy is a topic of great current interest.

Theoretical chemist may also be interested in some aspects of the book. They will find it amusing and exciting that a chemical concept (total π-electron energy), conceived in the 1940s within chemical studies based on quantum theory, has evolved to an object of mathematical interest per se. Graph energy is one of the rare cases of chemistry-motivated and chemistry-initiated directions of research in mathematics.

Mathematicians (both "pure" and "applied") whose interests lie far from spectral graph theory may be surprised by the fact that graph energy is a special kind of matrix norm (Sect. 1.2). They will then recognize that the concept of graph energy (under different names, of course) is encountered in a number of seemingly unrelated areas of their own expertise, namely *analysis*, *matrix theory*, *probability theory*, and even *statistics*. These readers should pay special attention to Chap. 11, in which a variety of other graph energies are described.

Combinatorial designs and strongly regular graphs play a significant role in problems related to graphs with maximal energy. In the present book, the theory of these combinatorial objects is not outlined in due detail, and thus readers interested in such details should consult other specialized monographs. In contrast to this, experts for combinatorial designs and strongly regular graphs may find it most pleasing and stimulating to learn that their theory found a new and important field of application.

Information on how the theory of graph energy is outlined in this book and partitioned in its eleven chapters is found in Sect. 1.3. Open problems in the theory of graph energy are abound. The readers of this book will find them stated at appropriate places of the text.

Many of the results outlined in the book are given with complete proofs. These proofs are sometimes lengthy, split into cases and subcases, based on earlier established lemmas. Yet, in our opinion, this is a valuable feature of our book. The readers will learn not only *what* the known results on graph energy are, but also *how* these have been obtained.

Although extensive and rapidly growing, it was still possible to collect a practically complete bibliography on graph energy. We believe that this bibliography gives our book an additional value.

The material presented in this book was used in the course "*Chemical Graph Theory*," held three times at the Nankai University, in 2009, 2010, and 2011. The authors wish to thank the graduate students Wenxue Du, Bofeng Huo, Jing Li, Lei Li, Shasha Li, Wei Li, Yiyang Li, Hongping Ma, Yuefang Sun, Xiangmei Yao, and Wenli Zhou for help in the preparation of the text of this book, and for pointing out and correcting numerous errors in it.

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Contents

Chapter 1
Introduction

1.1 Introduction to Graph Energy

Let G be a finite and undirected simple graph, with vertex set $V(G)$ and edge set $E(G)$. The number of vertices of G is n, and its vertices are labeled by $v_1, v_2, \ldots, v_n$. The adjacency matrix $\mathbf{A}(G)$ of the graph G is a square matrix of order n, whose (i, j)-entry is equal to 1 if the vertices v_i and v_j are adjacent and is equal to zero otherwise. The characteristic polynomial of the adjacency matrix, i.e., $\det(x\,\mathbf{I}_n - \mathbf{A}(G))$, where $\mathbf{I}_n$ is the unit matrix of order n, is said to be the *characteristic polynomial of the graph* G and will be denoted by $\phi(G, x)$. The eigenvalues of a graph G are defined as the eigenvalues of its adjacency matrix $\mathbf{A}(G)$, and so they are just the roots of the equation $\phi(G, x) = 0$. Since $\mathbf{A}(G)$ is symmetric, its eigenvalues are all real. Denote them by $\lambda_1, \lambda_2, \ldots, \lambda_n$, and as a whole, they are called the *spectrum* of G and denoted by $\mathrm{Spec}(G)$.

Spectral properties of graphs, including properties of the characteristic polynomial, have been extensively studied; for details, we refer to [81, 89].

One of the remarkable chemical applications of spectral graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of π-electrons in conjugated hydrocarbons (see [85, 133, 216, 238]). Whereas details are given in Chap. 2, here, we only mention that within the Hückel molecular orbital (HMO) approximation, the energy levels of the π-electrons in molecules of conjugated hydrocarbons are related to the eigenvalues of a pertinently constructed graph, the so-called molecular graph, as

$$\mathscr{E}_i = \alpha + \beta\,\lambda_i$$

where α and β are parameters of the HMO model; for our considerations, it suffices to say that α and β are constants. Within the HMO approximation, the total energy

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of the π-electrons, denoted by $\mathscr{E}_\pi$, is then obtained by summing the individual electron energies:

$$\mathscr{E}_\pi = \sum_{i=1}^{n} g_i\, \mathscr{E}_i$$

where g_i is the count of π-electrons with energy $\mathscr{E}_i$, the so-called occupation number. This yields

$$\mathscr{E}_\pi = n\,\alpha + \beta \sum_{i=1}^{n} g_i\, \lambda_i$$

because in conjugated hydrocarbons, the total number of π-electrons is equal to the number of vertices of the associated molecular graph.

For reasons whose physical origin is explained in textbooks of quantum chemistry (see, e.g., [76, 101, 503]), $g_i \in \{0, 1, 2\}$. Moreover, for the majority (but not all!) of conjugated hydrocarbons, $g_i = 2$ if $\lambda_i > 0$ and $g_i = 0$ if $\lambda_i < 0$, implying

$$\mathscr{E}_\pi = n\,\alpha + 2\beta \sum_{+} \lambda_i$$

where $\sum_{+}$ indicates the summation over the positive eigenvalues of the molecular graph. Since the sum of all graph eigenvalues is equal to zero, we arrive at

$$\mathscr{E}_\pi = n\,\alpha + \beta \sum_{i=1}^{n} |\lambda_i| \,. \qquad (1.1)$$

Because n, α, and β are constants, the only nontrivial term on the right-hand side of Eq. (1.1) is the sum of the absolute values of the eigenvalues of the molecular graph. This fact was, in an implicit manner, known already in the 1940s [73]. Yet, only in the 1970s, one of the authors of this book recognized [149] that the quantity

$$\mathscr{E} = \mathscr{E}(G) := \sum_{i=1}^{n} |\lambda_i| \qquad (1.2)$$

could be viewed as a graph-spectrum-based invariant, with interesting and worth-to-study mathematical properties. Contrary to the right-hand side of Eq. (1.1), the right-hand side of Eq. (1.2) is, by definition, applicable to any graph. In the general case, $\mathscr{E}$ should not have any "chemical" interpretation: It is just an abstract (hopefully, mathematically interesting) graph invariant. Only in some rather restricted cases, and within a relatively rough approximation, is $\mathscr{E}$ related to a physically meaningful quantity "total π-electron energy," cf. Eq. (1.1). Nevertheless, the name *graph energy* was proposed [149] for the invariant occurring on the right-hand side of Eq. (1.2), a name that nowadays seems to be accepted and used by the entire mathematical and mathematico–chemical community.

More on the chemical background of graph energy is found in Chap. 2.

The right-hand side of Eq. (1.2) is related to several other concepts of analysis, linear algebra, and graph spectral theory. These details are outlined in the following section.

1.2 Other Mathematical Connections

The singular values $s_1, s_2, \ldots, s_n$ of a real symmetric matrix $\mathbf{M}$ of order n coincide with the absolute values of the eigenvalues of $\mathbf{M}$. If the singular values are labeled in a nonincreasing order, then the *Ky Fan k-norm* of $\mathbf{M}$ is $\sum_{j=1}^{k} s_j$. For $k = n$, the Ky Fan k-norm is sometimes referred to as the *Ky Fan trace norm* or *nuclear norm*. Evidently, the graph energy is just the Ky Fan n-norm of the adjacency matrix.

Recall that this latter norm is widely studied in matrix theory and functional analysis. We refer the readers to [31] (p. 35) or to [364, 385, 386].

The *p-norm*, also called *Schatten p-norm*, defined as $\left(\sum_{j=1}^{n} |\lambda_j|^p\right)^{1/p}$, which is originally defined by singular values $\left(\sum_{j=1}^{n} s_j^p\right)^{1/p}$, is another norm that is frequently used in analysis, where p is a real number and $p \geq 1$. Its special cases are the Ky Fan trace norm ($p = 1$) and the Frobenius norm ($p = 2$). Again, the graph energy is the p-norm of the adjacency matrix for $p = 1$.

Remark 1.1. Among n-vertex trees, the star S_n and the path P_n have, respectively, minimum and maximum energy. It is interesting that this fact remains valid for any p-norm of the adjacency matrix, $p \in (0, 2)$, but is inverted for $p > 2$ (S. Wagner, 2011, private communication).

Remark 1.2. Let G' and G'' be two graphs with equal number n of vertices, and let their eigenvalues be $\lambda_1' \geq \lambda_2' \geq \cdots \geq \lambda_n'$ and $\lambda_1'' \geq \lambda_2'' \geq \cdots \geq \lambda_n''$, respectively. The *spectral difference* between G' and G'' is defined as [300] $\sum_{j=1}^{n} |\lambda_j' - \lambda_j''|$. Thus, the energy of a graph G can be viewed as the spectral difference between G and the empty graph $\overline{K_n}$.

1.3 Outline of the Book

This book has 11 chapters, followed by a detailed (hopefully not far from complete) bibliography on graph energy.

In Chap. 1, the basic notation and terminology are specified, and the main definitions given.

In Chap. 2, we explicate the chemical origin of the graph–energy concept and briefly survey the almost countless papers dealing with chemical applications of total π-electron energy.

The Coulson integral formula for $\mathcal{E}$ is not only the very first great result of the theory of graph energy (obtained as early as 1940) but also plays a crucial role in much of the contemporary research, especially in finding graphs extremal w. r. t. $\mathcal{E}$. This topic is outlined in Chap. 3.

In Chap. 4, some fundamental methods, useful for solving problems on graph energy, are summarized.

In Chap. 5, numerous upper and lower bounds for graph energy are given, and in many cases, the graphs achieving these bounds are characterized.

In Chap. 6, we discuss the energy of random graphs.

Chapter 7 outlines some selected (of the very many existing) results on graphs extremal with regard to energy.

Chapter 8 is concerned with hyperenergetic ($\mathcal{E} > 2n - 2$) and pairs of equienergetic graphs ($\mathcal{E}(G_1) = \mathcal{E}(G_2)$).

In Chap. 9, hypoenergetic ($\mathcal{E} < n$) and strongly hypoenergetic ($\mathcal{E} < n - 1$) graphs are investigated.

Those results on graph energy that did not fit into any of the first 9 chapters, but which deserve to be mentioned in this book, are collected in Chap. 10.

In Chap. 11, we briefly describe some other energy-like quantities that recently have emerged in the mathematical and mathematico–chemical literature.

Open problems and conjectures are stated in the appropriate sections.

1.4 Basic Notation and Terminology

1.4.1 Graph Theory

As before, we use $G = (V(G), E(G))$ to denote a finite and undirected simple graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex u of G, we write $u \in G$ instead of $u \in V$. The *order* of G is the number of vertices in G, denoted by $|G|$, and thus $|G| = |V(G)|$. A graph of order n is also called an *n-vertex graph*. The *size* of G is the number of edges in G. Similarly, $G(n, m)$ denotes an arbitrary graph of order n and size m, which is also called an *(n, m)-graph*. The graph of order n and size $\binom{n}{2}$ is the *complete graph* and is denoted by K_n. A graph G is *connected* if there exists a path between every pair of vertices. Otherwise, G is *disconnected*, and we denote by $\omega(G)$ the number of its connected components. A *tree* T is a connected acyclic graph, and so a tree of order n has size $m = n - 1$. A graph G of order n and size m is called *unicyclic*, *bicyclic*, and *tricyclic* if G is simple and connected with $m = n$, $m = n + 1$, and $m = n + 2$, respectively. The *cyclomatic number* of a connected graph with order n and size m is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is said to be *k-cyclic*. A *bipartite graph* is composed of two independent sets of vertices (bipartition), with p and q vertices respectively, and some edges joining pairs of vertices u and v such that u and v are not in the same partition. If a bipartite graph contains such edges for all pairs, then it is a *complete* *bipartite graph*, denoted by $K_{p,q}$. The graph $K_{1,n-1}$ is also called the *star* of order n, denoted by S_n. The *complement* $\overline{G}$ of a graph $G = (V, E)$ is the graph with the same vertex set V, such that two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G. The *empty graph* of order n is the graph $\overline{K_n}$.

For any vertex $v \in G$, denote by $N(v)$ the *neighborhood* of v and by $d(v)$ the *degree* of v. The *minimum degree* of G is denoted by $\delta(G)$, while the *maximum degree* is denoted by $\Delta(G)$. A vertex of degree 0 is said to be an *isolated vertex*. A vertex of degree 1 is called a *leaf vertex* (or simply, a *leaf*); sometimes, it is also called a *pendent vertex*. The edge incident with a leaf is called a *pendent edge*.

Denote by $\pi(G) = [d_1, d_2, \ldots, d_n]$ the degree sequence of the graph G, where d_i stands for the degree of the i-th vertex and $d_1 \geq d_2 \geq \cdots \geq d_n$. For convenience, we sometimes write $\pi(G) = [d_1^{\alpha_1}, d_2^{\alpha_2}, \ldots, d_s^{\alpha_s}]$, where $d_1 > d_2 > \cdots > d_s$ and $d_i^{\alpha_i}$ indicate that the number of vertices with degree d_i is α_i.

As usual, we use P_n and C_n to denote the *path* and the *cycle* of order n, respectively. The *length* of a path (cycle) is the number of edges in the path (cycle). The *distance* $d(u, v)$ between two vertices u and v of a graph G is the length of a shortest path between u and v in G. If G has no path between vertices u and v, then $d(u, v)$ is not defined. The *diameter* $d(G)$ of G is the maximum distance between any pair of vertices of G, i.e., $d(G) = \max_{u,v \in V(G)} d(u, v)$. The *eccentricity* of a vertex u, written as $\epsilon(u)$, is $\max_{v \in V} d(u, v)$. Note that the diameter equals the maximum of the vertex eccentricities. The *radius* of a graph G is $r(G) = \min_{u \in V} \varepsilon(u)$. The *center* of a graph is the set of vertices of the graph whose eccentricities equal to the radius of the graph. The center of a tree is a single vertex, called the *center vertex*, or the two ends of an edge, called the *center edge*.

Let $P = v_0 v_1 \ldots v_k$ $(k \geq 1)$ be a path of a tree T. If $d_T(v_0) \geq 3$, $d_T(v_k) \geq 3$, and $d_T(v_i) = 2$, $(0 < i < k)$, then we say that P is an *internal path* of T. If $d_T(v_0) \geq 3$, $d_T(v_k) = 1$, and $d_T(v_i) = 2$, $(0 < i < k)$, we call P a *pendent path* of T with root v_0. In particular, when $k = 1$, we call P a *pendent edge*.

For a given graph $G = (V, E)$, a subset M of E is called a *matching* of G if no two edges in M are incident in G. The two ends of an edge in M are said to be *matched* under M. If every vertex of G is matched under M, then M is a *perfect matching*. M is a *maximum matching* if G has no matching M' with $|M'| > |M|$. Clearly, every perfect matching is maximum.

For a given graph G, a vertex coloring of G is said to be *proper* if any two adjacent vertices are assigned different colors. The *chromatic number* $\chi(G)$ of G is the minimum number of colors that are needed to color G properly.

A tree is called a *double star* $S_{p,q}$ if it is obtained by joining the centers of two stars S_p and S_q by an edge. So, for a double star $S_{p,q}$ with n vertices, we have $p + q = n$.

A *comet* or a *broom* is a tree composed of a star and an appended path. For any numbers n and $2 \leq k \leq n - 1$, we denote by $P_{n,k}$ the comet of order n with k pendent vertices, i.e., a tree formed by a path P_{n-k} of which one end vertex coincides with a pendent vertex of a star S_{k+1} of order $k + 1$.

We use $G - u$ or $G - uv$ to denote the graph obtained from G by deleting the vertex $u \in G$ or the edge $uv \in E$, respectively. Similarly, $G + uv$ is a graph obtained from G by adding an edge $uv \notin E$, where $u, v \in G$. Suppose that $V' \subset V$. We denote by $G - V'$ the graph obtained from G by deleting the vertices in V' together with their incident edges. An edge e of G is said to be *contracted* if it is deleted and its ends are identified; the resulting graph is denoted by G/e.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. The *union* $G_1 \cup G_2$ of G_1 and G_2 is the graph $G = (V, E)$ for which $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$. A union of (at least two) trees is a (disconnected) acyclic graph referred to as a *forest*. The *Cartesian product* of G_1 and G_2, denoted by $G_1 \times G_2$, is the graph with vertex set $V_1 \times V_2$ specified by putting (u_1, u_2) adjacent to (u'_1, u'_2) if and only if $u_1 = u'_1$ and $u_2u'_2 \in E_2$, or $u_2 = u'_2$ and $u_1u'_1 \in E_1$.

A graph G is *regular* if there exists a constant r, such that $d(v) = r$ holds for every $v \in G$, in which case G is said to be r*-regular*. Further, a graph G is (a, b)-*semiregular* if $\{d(v), d(w)\} = \{a, b\}$ holds for all edges $vw \in E(G)$. A semiregular graph that is not regular will henceforth be called *strictly semiregular*. Clearly, a connected strictly semiregular graph must be bipartite. Let a and b be integers such that $1 \leq a < b$. A graph is said to be (a, b)*-biregular* if the degrees of its vertices assume exactly two different values: a and b. Similarly, let x, a, and b be integers, $1 \leq x < a < b$. A graph is said to be (x, a, b)*-triregular* if the degrees of its vertices assume exactly three different values: x, a, and b.

A k-regular graph G on n vertices which is neither empty nor complete is said to be *strongly regular* with parameters (n, k, λ, μ) if the following conditions hold: Each pair of adjacent vertices has the same number $\lambda \geq 0$ of common neighbors, and each pair of nonadjacent vertices has the same number $\mu \geq 0$ of common neighbors. If $\mu = 0$, then G is a disjoint union of complete graphs, whereas if $\mu \neq 0$ and G is noncomplete, then the eigenvalues of G are k and the roots r, s of the quadratic equation

$$x^2 + (\mu - \lambda)x + (\mu - k) = 0 \,. \tag{1.3}$$

The eigenvalue k has multiplicity 1, whereas the multiplicities m_r of r and m_s of s can be calculated by solving the simultaneous equations:

$$m_r + m_s = n - 1, \qquad k + m_r\, r + m_s\, s = 0 \,.$$

For more details see [125].

For more notation and terminology, we refer the readers to the standard textbooks by Bondy and Murty [39, 40] and Bollobás [37].

1.4.2 Hadamard Matrix and Latin Square Graph

A square $(+1, -1)$-matrix $\mathbf{H}$ of order n is called a *Hadamard matrix* whenever $\mathbf{HH}^T = n\, I_n$. Note that the order of the Hadamard matrix n must be 1, 2, or a multiple of 4. For example,

$$\mathbf{H}_+ = \begin{bmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{H}_- = \begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{bmatrix}$$

are two Hadamard matrices of order 4. A Hadamard matrix is said to be *graphical* if it is symmetric with constant diagonal. For more details, see [77].

A *Latin square* consists of n sets of the numbers 1 to n arranged in such a way that no orthogonal row or column contains the same number twice. Ball and Coxeter define a *lattice graph* as the graph obtained by taking the n^2 ordered pairs of the first n positive integers as vertices and drawing an edge between all pairs having exactly one number in common. The more usual definition of a lattice graph $L_{m,n}$ (confusingly called the $m \times n$ grid by Brouwer et al.) is the line graph of the complete bipartite graph $K_{m,n}$. The lattice graph is also isomorphic to the *Latin square graph*. The vertices of such a graph are defined as the n^2 elements of a Latin square of order n, with two vertices being adjacent if they lie in the same row or column or contain the same symbol. It turns out that all Latin squares of order n produce the same lattice graph. For more results, see [48].

For further details, the readers are referred to [33, 81, 125]. Specific terminology and notions are defined at the places where they are used.

1.5 Characteristic Polynomial of a Graph

Let G be a graph of order n and $\mathbf{A}(G)$ its adjacency matrix. As before, let the characteristic polynomial $\phi(G,x)$, or $\phi(G)$ for short, of G be

$$\phi(G,x) = \det(x\,\mathbf{I}_n - \mathbf{A}(G)) = \sum_{k=0}^{n} a_k\, x^{n-k} \ .$$

For the coefficients of the characteristic polynomial of a graph, we have the famous Sachs theorem [81].

Theorem 1.1 (Sachs theorem). *Let G be a graph with characteristic polynomial $\phi(G) = \sum_{k=0}^{n} a_k\, x^{n-k}$. Then for $k \geq 1$,*

$$a_k = \sum_{S \in L_k} (-1)^{\omega(S)}\, 2^{c(S)}$$

where L_k denotes the set of Sachs subgraphs of G with k vertices, that is, the subgraphs in which every component is either a K_2 or a cycle; $\omega(S)$ is the number of connected components of S, and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$.

In the following, we list some basic properties of the characteristic polynomial $\phi(G)$, which can be found in any appropriate books, e.g. in [81, 89]. These will be used in the forthcoming chapters of this book.

Theorem 1.2. *If $G_1, G_2, \ldots, G_t$ are the connected components of a graph G, then*

$$\phi(G) = \prod_{i=1}^{t} \phi(G_i).$$

Theorem 1.3. *Let uv be an edge of G. Then*

$$\phi(G) = \phi(G - uv) - \phi(G - u - v) - 2 \sum_{C \in \mathscr{C}(uv)} \phi(G - C)$$

where $\mathscr{C}(uv)$ is the set of cycles containing uv. In particular, if uv is a pendent edge with pendent vertex v, then $\phi(G) = x\,\phi(G - v) - \phi(G - u - v)$.

By Theorem 1.3, one easily obtains:

Corollary 1.1. *Let G be a forest and $e = uv$ be an edge of G. Then the characteristic polynomial of G satisfies $\phi(G) = \phi(G - e) - \phi(G - u - v)$.*

Corollary 1.2. *Let P_n denote the path with n vertices. Then for $i = 1, 2, \ldots, n-1$, $\phi(P_n) = \phi(P_i)\phi(P_{n-i}) - \phi(P_{i-1})\phi(P_{n-i-1})$, where $\phi(P_0) \equiv 1$.*

Theorem 1.4. *Let G be a forest and v be a vertex of G. Then the characteristic polynomial of G satisfies $\phi(G) = x\phi(G - v) - \sum_u \phi(G - u - v)$, where the summation extends over all vertices adjacent to v.*

Theorem 1.5. *For a given graph G, denote by H the graph obtained by adding a set V_i of k new isolated vertices to each vertex x_i of G and joining x_i by an edge to each of the k vertices of V_i $(i = 1, 2, \ldots, n)$. Then*

$$\phi(H, x) = x^{nk}\, \phi\left(G,\ x - \frac{k}{x}\right).$$

Denote by $m(G, k)$ the number of k-matchings of the graph G, i.e., the number of ways in which k independent edges can be selected in G. By definition, $m(G, 0) = 1$ for all graphs, and $m(G, 1)$ is equal to the number of edges of G.

Theorem 1.6. *If G is a forest on n vertices, then*

$$\phi(G, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, m(G, k)\, x^{n-2k}.$$

The right-hand side of the above expressions (which in the case of cycle-containing graphs differs from the characteristic polynomial) is referred to as the *matching polynomial* of the graph G. In the later parts of the book, it will be denoted by $m(G,x)$. Thus,

$$m(G,x) =: \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \, m(G,k) \, x^{n-2k} \, . \tag{1.4}$$

Details of the theory of matching polynomials can be found in the book [80] and in the papers [111, 112, 124, 151].

Chapter 2
The Chemical Connection

2.1 Hückel Molecular Orbital Theory

Research on what we call the *energy of a graph* can be traced back to the 1940s or even to the 1930s. In the 1930s, the German scholar Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called conjugated hydrocarbons. Details of this approach, often referred to as the "Hückel molecular orbital (HMO) theory" can be found in appropriate textbooks [76, 101].

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

$$\hat{H}\,\Psi = \mathscr{E}\,\Psi \tag{2.1}$$

where Ψ is the so-called wave function of the system considered, $\hat{H}$ the so-called Hamiltonian operator of the system considered, and $\mathscr{E}$ 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. (2.1), which evidently is an eigenvalue–eigenvector problem of the Hamiltonian operator. In order that the solution of (2.1) be feasible (yet not completely exact), one needs to express Ψ as a linear combination of a finite number of pertinently chosen basis functions. If so, then Eq. (2.1) is converted into

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

where now **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 a conjugated molecule, especially of conjugated hydrocarbons. In Fig. 2.1, depicted is 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.

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_2,

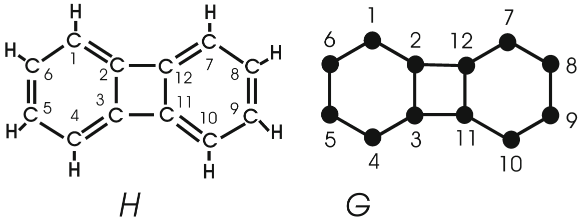

Fig. 2.1 Biphenylene H is a typical conjugated hydrocarbon. Its carbon–atom skeleton is represented by the molecular graph G. The carbon atoms in the chemical formula H and the vertices of the graph G are labeled by $1, 2, \ldots, 12$ so as to be in harmony with Eqs. (2.2) and (2.3)

In the HMO model, the wave functions of a conjugated hydrocarbon with n carbon atoms are expanded in an n-dimensional space of orthogonal basis functions, whereas the Hamiltonian matrix is a square matrix of order n, defined such 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 [76, 101, 503].

For instance, the HMO Hamiltonian matrix of biphenylene is

$$\mathbf{H} = \begin{bmatrix} \alpha & \beta & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta \\ 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta & 0 & 0 & 0 & \beta & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha & \beta & 0 & 0 & 0 & \beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta & 0 \\ 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & \alpha & \beta \\ 0 & \beta & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & \beta & \alpha \end{bmatrix} \tag{2.2}$$

which can be written also as

$$\mathbf{H} = \alpha \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1 \end{bmatrix} + \beta \begin{bmatrix} 0&1&0&0&0&1&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0&0&1 \\ 0&1&0&1&0&0&0&0&0&0&1&0 \\ 0&0&1&0&1&0&0&0&0&0&0&0 \\ 0&0&0&1&0&1&0&0&0&0&0&0 \\ 1&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0&0&1 \\ 0&0&0&0&0&0&1&0&1&0&0&0 \\ 0&0&0&0&0&0&0&1&0&1&0&0 \\ 0&0&0&0&0&0&0&0&1&0&1&0 \\ 0&0&1&0&0&0&0&0&0&1&0&1 \\ 0&1&0&0&0&0&1&0&0&0&1&0 \end{bmatrix} . \tag{2.3}$$

The first matrix on the right-hand side of Eq. (2.3) is just the unit matrix of order $n = 12$, whereas the second matrix can be understood as the adjacency matrix of a graph on $n = 12$ vertices. This graph is also depicted in Fig. 2.1 and in an obvious 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

$$\mathbf{H} = \alpha\,\mathbf{I}_n + \beta\,\mathbf{A}(G) \tag{2.4}$$

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

As a curiosity, we mention that neither Hückel himself nor the scientists who did early research in HMO theory were aware of the identity (2.4), which was first noticed only in 1956 [139].

As a consequence of Eq. (2.4), the energy levels $\mathscr{E}_j$ of the π-electrons are related to the eigenvalues λ_j of the graph G by the simple relation

$$\mathscr{E}_j = \alpha + \beta\,\lambda_j\,; \qquad j = 1, 2, \ldots, n\,.$$

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

$$\mathscr{E}_\pi = \sum_{j=1}^{n} g_j\,\mathscr{E}_j$$

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 $\mathscr{E}_\pi$ and the way in which the molecular graph G is constructed can be found in the books [133, 216] and reviews [161, 174, 238]. More information on the chemical applications of $\mathscr{E}_\pi$ is found in Sect. 2.3 and in the references quoted therein.

For what follows, it is only important that because the number of π-electrons in the conjugated hydrocarbons considered is equal to n, it must be

$$g_1 + g_2 + \cdots + g_n = n$$

which immediately implies

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

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

$$\mathscr{E} = \sum_{j=1}^{n} g_j\, \lambda_j\,. \tag{2.5}$$

The right-hand side of Eq. (2.5) is just what in the chemical literature is referred to as "total π-electron energy"; if necessary, then one says "total π-electron energy in β-units."

If the π-electron energy levels are labeled in a nondecreasing order

$$\mathscr{E}_1 \le \mathscr{E}_2 \le \cdots \le \mathscr{E}_n$$

then the requirement that the total π-electron energy should 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!) of chemically relevant cases,

$$g_j = \begin{cases} 2 & \text{whenever } \lambda_j > 0 \\ 0 & \text{whenever } \lambda_j < 0. \end{cases} \tag{2.6}$$

If so, then Eq. (2.5) becomes

$$\mathscr{E} = \mathscr{E}(G) = 2\sum_{+} \lambda_j$$

where $\sum_{+}$ indicates summation over positive eigenvalues. Because for all graphs the sum of eigenvalues is equal to zero, we rewrite the above equality as

$$\mathscr{E} = \mathscr{E}(G) = \sum_{j=1}^{n} |\lambda_j| \,. \tag{2.7}$$

2.2 Towards the Energy of a Graph

In the 1970s, one of the present authors noticed that practically all results that until then were obtained for the HMO total π-electron energy, in particular those in the papers [73,254,368,425,426], tacitly assume the validity of Eqs. (2.6) and (2.7) and, in turn, are not restricted to the molecular graphs encountered in the HMO theory but hold for all graphs. This observation motivated him to put forward [149] the following:

Definition 2.1. If G is a graph on n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the *energy* of G is

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

Note that Definition 2.1 just repeats what already has been given by Eq. (1.2).

The difference between Eq. (2.7) and Definition 2.1 is that Eq. (2.7) has a chemical interpretation, and therefore the graph G in it must satisfy several chemistry-based conditions (e.g., the maximum vertex degree of G must not exceed 3). On the other hand, the graph energy is defined for all graphs, and mathematicians may study it without being restricted by any chemistry-caused limitation.

Definition 2.1 was first time publicly stated on a conference held in 1978 in Austria [149]. Later, it was restated on several other lectures and conferences, as well as in the papers [155, 173] and books [80, 216].

Initially, the graph–energy concept did not attract any noteworthy attention of mathematicians, but sometime around the turn of the century, they did realize its value, and a vigorous and worldwide mathematical research of $\mathscr{E}$ started. The current activities on the mathematical studies of $\mathscr{E}$ 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 63, respectively. In the time of completing this book, in 2010 and 2011 (until May!), 51 and 31 papers on graph energy were published, which certainly are not the final numbers. Since

2001, almost 300 mathematical papers on $\mathcal{E}$ were produced, about two per month. Three reviews on the mathematical aspects of graph energy were published so far [173, 176, 200]; the books [27, 473] contain a special section devoted to this topic, and graph energy is mentioned in all newer monographs on graph spectral theory [49, 80, 81, 85, 86, 89].

2.3 Back to Total π-Electron Energy

It is not the purpose of this book to provide a detailed survey of the chemical applications of total π-electron energy. With regard to its physical basis, one should consult the articles [75, 393, 430] and the references quoted therein. For details on its chemical applications, see [71, 244] and the book [216].

In the early days, when computers were not widely available, the calculation of the HMO total π-electron energy was a serious problem. In order to overcome the difficulty, a great variety of approaches have been offered for the approximate numerical calculation of $\mathcal{E}$. Later, when the computer-aided calculation of $\mathcal{E}$ became an easy and routine task, the point of view became that the approximate formulas for $\mathcal{E}$ reveal the way in which various structural details (of the underlying molecule or of the underlying molecular graph) influence $\mathcal{E}$.

In 1971, McClelland [368] discovered the upper bound $\mathcal{E} \le \sqrt{2mn}$, but in the same paper, he showed that for molecular graphs, $\mathcal{E} \approx a\sqrt{2mn}$ is a surprisingly good approximation, where $a \approx 0.9$ is an empirical constant. This work was then followed by a remarkably extensive study of so-called (n, m)-type bounds (e.g., [62, 70, 146, 154, 188, 214, 228, 240, 305–307, 464]), approximate expressions (e.g., [153, 159–161, 163, 166, 169, 172, 187, 198, 204, 210, 224–226, 233, 239, 241, 465, 466, 468, 469, 471]), and statistics-based inferences [118, 128, 220, 229, 246]. Many other bounds (e.g., [127, 143, 150, 234, 235, 372]) and approximate expressions (e.g., [36, 56, 63–65, 147, 148, 164, 201, 205, 227, 365, 431, 443, 447, 470, 472]) for $\mathcal{E}$, mainly applicable only to some special types of molecular graphs and not mentioned in the later parts of this book, have been reported. These results are similar to the, also numerous, research aimed at relating (or correlating) $\mathcal{E}$ with some structural detail or algebraic invariant of the molecular graph, other than the number of vertices and edges. Some of these are the number of perfect matchings (in chemistry, number of Kekulé structures) [66–69, 132, 156, 157, 171, 189, 202, 203, 206, 213, 217, 230, 255], spectral moments [162, 179, 237, 297, 298, 378], number of zero eigenvalues (nullity) [181, 182, 232], coefficients of the characteristic polynomial [130, 131, 186, 194, 236], branching of molecular skeleton [155, 222], and others [74, 129, 144, 190, 208, 211, 245]. Especially much was studied in the dependence of total π-electron energy on the cycles present in the molecular graph since this problem is directly related to the, for chemistry very important, concepts of resonance energy [6, 209] and cyclic conjugation [175, 215, 231]. Hundreds of papers were published on these themes; for details, see the references quoted.

The most studied molecular graphs are those representing benzenoid hydrocarbons (for details see [183]). This is easily seen from the titles of the above-quoted papers. Also, the energies of some other types of molecular graphs were studied, e.g., [98, 152, 155, 165, 222].

As already mentioned, the "chemical" energy, given by Eq. (2.5), in some cases differs from the "mathematical" energy, given by Eq. (2.7) and Definition 2.1. These differences were pointed out by Fowler [117], resulting in a few mathematical studies on this so-called *Hückel energy* [123, 272, 303, 304].

Chapter 3
The Coulson Integral Formula

In the theory of graph energy, the so-called *Coulson integral formula* (3.1) plays an outstanding role. This formula was obtained by Charles Coulson as early as 1940 [73] and reads:

$$\mathscr{E}(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{\mathrm{i}x\, \phi'(G, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} \right] \mathrm{d}x = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - x \frac{\mathrm{d}}{\mathrm{d}x} \ln \phi(G, \mathrm{i}x) \right] \mathrm{d}x \quad (3.1)$$

where G is a graph, $\phi(G, x)$ is the characteristic polynomial of G, $\phi'(G, x) = (\mathrm{d}/\mathrm{d}x)\phi(G, x)$ its first derivative, and $\mathrm{i} = \sqrt{-1}$.

Because of its importance, we introduce Coulson's formula in this early part of our book. Its numerous applications are outlined in Sect. 4.3, Chap. 7, and elsewhere.

In Eq. (3.1), as well as in what follows, $\int_{-\infty}^{+\infty} F(x)\, \mathrm{d}x$ stands for the principal value of the respective integral, i.e.,

$$\lim_{t \to +\infty} \int_{-t}^{+t} F(x)\, \mathrm{d}x .$$

The Coulson integral formula and its various modifications have important chemical applications. Namely, the Sachs theorem (Theorem 1.1) establishes the explicit dependence of the coefficients of the characteristic polynomial of a graph on the structure of this graph. The Coulson integral formula establishes the explicit dependence of the energy of a graph on the characteristic polynomial of this graph. By combining the Coulson integral formula with the Sachs theorem, we gain insight into the dependence of the energy of a graph on the structure of this graph. More on this matter can be found in [216, 238].

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_3,

3.1 A Proof of the Formula

The present derivation of the Coulson integral formula (3.1) follows that reported in [207] (see also [216, 367] and, of course, [73]). An elementary proof is reported in [436]. We assume that all λ_k, $k = 1, 2, \ldots, n$, are real numbers different from zero. We denote by $\sum_+ \lambda_k$ and $\sum_- \lambda_k$ the sum of those λ_k's that are positive and negative, respectively. Then, of course,

$$\sum_+ \lambda_k + \sum_- \lambda_k = \sum_{k=1}^{n} \lambda_k \ .$$

Let, as before, $\mathrm{i} = \sqrt{-1}$ be the imaginary unit, and let a complex number z be written in the form $z = x + \mathrm{i}y$. Then z can be presented as a point in the (x, y)-plane of a Descartes coordinate system (cf. Fig. 3.1), the so-called complex plane. The two starting points of our considerations are the following:

1. Let Γ be a simple, positively oriented contour in the complex plane and z_0 be a complex number. Then, according to the well-known Cauchy formula (see, for instance [29, 61, 72])

$$\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \frac{\mathrm{d}z}{z - z_0} = \begin{cases} 1 & \text{if } z_0 \in \mathrm{int}(\Gamma) \\ 0 & \text{if } z_0 \in \mathrm{ext}(\Gamma) \end{cases} \tag{3.2}$$

   where $z_0 \in \mathrm{int}(\Gamma)$ and $z_0 \in \mathrm{ext}(\Gamma)$ indicate that z_0 lies inside and outside the contour Γ, respectively.
2. Let $\phi(z)$ be a polynomial of degree n in the (complex) variable z, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its zeros. Then $\phi(z) = \prod_{k=1}^{n} (z - \lambda_k)$, and consequently,

$$\phi'(z) = (z - \lambda_2)(z - \lambda_3) \cdots (z - \lambda_n) + (z - \lambda_1)(z - \lambda_3) \cdots (z - \lambda_n) \\ + \cdots + (z - \lambda_1)(z - \lambda_2) \cdots (z - \lambda_{n-1})$$

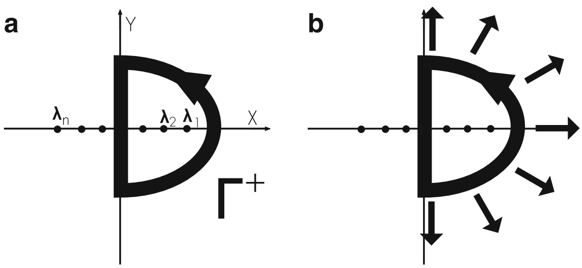

Fig. 3.1 (**a**) A simple, positively oriented contour Γ^+ in the complex plane, embracing all the positive zeros of the polynomial $\phi(z)$. The vertical part of Γ^+ lies on the y-axis. (**b**) Parts of Γ^+ are shifted to infinity so that its vertical part remains on the y-axis

from which follows

$$\frac{\phi'(z)}{\phi(z)} = \sum_{k=1}^{n} \frac{1}{z - \lambda_k} \,. \tag{3.3}$$

In our considerations, we need the relation

$$\frac{z\,\phi'(z)}{\phi(z)} - n = \sum_{k=1}^{n} \frac{\lambda_k}{z - \lambda_k} \,. \tag{3.4}$$

Actually, from Eq. (3.3), it follows

$$\frac{z\,\phi'(z)}{\phi(z)} = \sum_{k=1}^{n} \frac{z}{z-\lambda_k} = \sum_{k=1}^{n} \frac{z-\lambda_k+\lambda_k}{z-\lambda_k} = \sum_{k=1}^{n}\left(1+\frac{\lambda_k}{z-\lambda_k}\right) = n + \sum_{k=1}^{n}\frac{\lambda_k}{z-\lambda_k} \,.$$

Because, evidently, $\lambda_k/(z-\lambda_k) \to 0$ for $|z| \to \infty$ holds for all $k = 1, 2, \ldots, n$, from Eq. (3.4), we get

$$\left[\frac{z\,\phi'(z)}{\phi(z)} - n\right] \to 0, \qquad \text{for} \qquad |z| \to \infty \,. \tag{3.5}$$

Note that for the validity of the relations (3.3)–(3.5), it is not necessary that the zeros of the polynomial $\phi(z)$ be mutually distinct. As a consequence, also, the Coulson formula (3.1) holds irrespective of the multiplicity of the zeros of the underlying polynomial.

Consider now the contour Γ^+ shown in Fig. 3.1a. In view of the relations (3.2) and (3.4), we have

$$\frac{1}{2\pi \mathrm{i}} \oint\limits_{\Gamma^+} \left[\frac{z\,\phi'(z)}{\phi(z)} - n\right] \mathrm{d}z = \frac{1}{2\pi \mathrm{i}} \oint\limits_{\Gamma^+} \sum_{k=1}^{n} \frac{\lambda_k}{z-\lambda_k}\,\mathrm{d}z = \sum_{k=1}^{n} \frac{\lambda_k}{2\pi \mathrm{i}} \oint\limits_{\Gamma^+} \frac{\mathrm{d}z}{z-\lambda_k} = \sum_{+} \lambda_k \,. \tag{3.6}$$

Because the value of the integral (3.7)

$$\frac{1}{2\pi \mathrm{i}} \oint\limits_{\Gamma^+} \left[\frac{z\,\phi'(z)}{\phi(z)} - n\right] \mathrm{d}z \tag{3.7}$$

is independent of the actual form of the contour Γ^+ (provided it embraces all the positive-valued zeros of $\phi(z)$), we may inflate Γ^+ as indicated in Fig. 3.1b.

The idea behind the Coulson formula (3.1) is that in the limit case when Γ^+ becomes infinitely large, then by Eq. (3.5), we know that the only nonvanishing contribution to the integral (3.7) comes from integration along the y-axis. That is,

$$\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma^+} \left[\frac{z\,\phi'(z)}{\phi(z)} - n \right] \mathrm{d}z = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma^+ \setminus \text{ vertical part of } \Gamma^+} \left[\frac{z\,\phi'(z)}{\phi(z)} - n \right] \mathrm{d}z$$

$$+ \frac{1}{2\pi \mathrm{i}} \int_{\text{vertical part of } \Gamma^+} \left[\frac{z\,\phi'(z)}{\phi(z)} - n \right] \mathrm{d}z$$

$$= \frac{1}{2\pi \mathrm{i}} \int_{+\infty}^{-\infty} \left[\frac{\mathrm{i}y\,\phi'(\mathrm{i}y)}{\phi(\mathrm{i}y)} - n \right] d(\mathrm{i}y)$$

which when combined with Eq. (3.6) straightforwardly results in formula (3.1).

3.2 More Coulson-Type Formulas

Let G_1 and G_2 be two graphs with equal number of vertices. Then, by a direct application of (3.1), one obtains [74]

$$\mathscr{E}(G_1) - \mathscr{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \frac{\phi(G_1, \mathrm{i}x)}{\phi(G_2, \mathrm{i}x)} \, \mathrm{d}x \,. \tag{3.8}$$

Equation (3.8) is often referred to as the *Coulson–Jacobs formula*.

The integrand in Eq. (3.8) may be complex valued, although its left-hand side is necessarily real. In view of the fact that the real part of $\ln z$ is $\ln |z|$, we can rewrite Eq. (3.8) as

$$\mathscr{E}(G_1) - \mathscr{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(G_1, \mathrm{i}x)}{\phi(G_2, \mathrm{i}x)} \right| \mathrm{d}x \,. \tag{3.9}$$

If we choose $G_2 \cong \overline{K_n}$, namely if the graph G_2 is without edges, then $\mathscr{E}(G_2) = 0$, and the right-hand side of (3.8) becomes equal to the energy of the graph G_1. Bearing in mind that

$$\phi(G, x) = \sum_{k \geq 0}^{n} a_k \, x^{n-k} \qquad \text{and} \qquad \phi(\overline{K_n}, x) = x^n$$

we obtain

$$\mathscr{E}(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \sum_{k \geq 0} a_k \, (\mathrm{i}x)^{-k} \right| \mathrm{d}x \,. \tag{3.10}$$

Therefore,

$$\mathscr{E}(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{k \geq 0} (-1)^k \, a_{2k} \, x^{2k} \right)^2 + \left(\sum_{k \geq 0} (-1)^k \, a_{2k+1} \, x^{2k+1} \right)^2 \right] \mathrm{d}x. \tag{3.11}$$

For a graph G, let $b_{2k}(G) = |a_{2k}(G)|$ and $b_{2k+1}(G) = |a_{2k+1}(G)|$, respectively, for $0 \leq k \leq \lfloor n/2 \rfloor$. Clearly, $b_0(G) = 1$, $b_2(G) = |E(G)|$.

If G is a bipartite graph, then its characteristic polynomial is of the form $\sum_{k \geq 0} (-1)^k \, b_{2k} \, x^{n-2k}$, where $b_{2k} \geq 0$ for all k. Then Eq. (3.10) can be simplified as

$$\mathscr{E}(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln \left[\sum_{k \geq 0} b_{2k} \, x^{2k} \right] \mathrm{d}x = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k \geq 1} b_{2k} \, x^{2k} \right] \mathrm{d}x. \tag{3.12}$$

For applications of Eqs. (3.10) and (3.12) in the theory of graph energy (which are quite numerous), see later in this book in Sect. 4.3 and Chap. 7.

Chapter 4
Common Proof Methods

After the concept of graph energy was proposed [149], there was much research on this topic. One basic problem is to find the extremal values or the best bounds for the energy within some special classes of graphs and graphs from these classes with extremal values of energy. Finding answers to such questions is often far from elementary. In this chapter we outline some fundamental methods that are frequently used for solving problems of this kind.

4.1 Method 1: Direct Comparison

For given graphs G and H, if we want to compare the energies $\mathscr{E}(G)$ and $\mathscr{E}(H)$, one trivial way is to compute the characteristic polynomials $\phi(G)$ and $\phi(H)$ and then to compute $\mathscr{E}(G) = \sum |\lambda_i|$ and $\mathscr{E}(H) = \sum |\mu_j|$, where λ_i and μ_j are the eigenvalues of G and H, respectively. Notice that this trivial method is only effective for graphs with small order or some special graphs. In what follows we give a few examples.

It is well known that the spectrum of the complete graph K_n is $n-1$ with multiplicity 1 and -1 with multiplicity $n-1$, thus the energy of K_n is $\mathscr{E}(K_n) = n-1+(n-1)\times 1 = 2n-2$. Actually, there is a naive conjecture [149]: Among all graphs of order n, the complete graph K_n has the maximal energy. It was soon shown (first by Godsil in the early 1980s) that there exist graphs whose energy exceeds $\mathscr{E}(K_n)$, which are now called *hyperenergetic graphs*; for details, see Chap. 8.

Since the characteristic polynomial of the star S_n is $\phi(S_n) = x^n - (n-1)\,x^{n-2}$, its energy is $\mathscr{E}(S_n) = 2\sqrt{n-1}$. Similarly, we can compute the energies of the cycle C_n and the path P_n as

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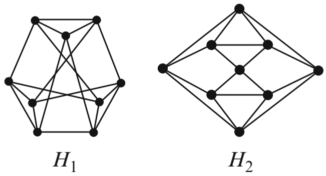

Fig. 4.1 Graphs H_1 and H_2

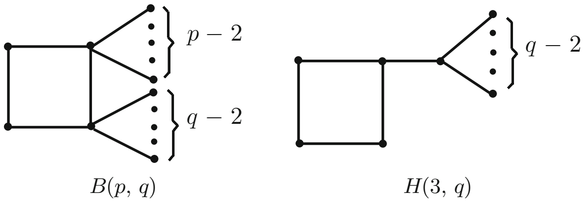

Fig. 4.2 The graphs $B(p,q)$ $(q \geq p \geq 2)$ and $H(3,q)$ $(q \geq 3)$

$$\mathscr{E}(C_n) = \begin{cases} \dfrac{4\cos\frac{\pi}{n}}{\sin\frac{\pi}{n}} & \text{if } n \equiv 0 \pmod 4 \\[2ex] \dfrac{4}{\sin\frac{\pi}{n}} & \text{if } n \equiv 2 \pmod 4 \\[2ex] \dfrac{2}{\sin\frac{\pi}{2n}} & \text{if } n \equiv 1 \pmod 2 \end{cases}$$

$$\mathscr{E}(P_n) = \begin{cases} \dfrac{2}{\sin\frac{\pi}{2(n+1)}} - 2 & \text{if } n \equiv 0 \pmod 2 \\[2ex] \dfrac{2\cos\frac{\pi}{2(n+1)}}{\sin\frac{\pi}{2(n+1)}} - 2 & \text{if } n \equiv 1 \pmod 2 \end{cases} .$$

In Sect. 4.3, we will prove that among all trees of order n, S_n attains the minimal energy, while P_n attains the maximal energy.

Example 4.1. Let H_1 and H_2 be the graphs depicted in Fig. 4.1. Then $\mathscr{E}(H_1) = \mathscr{E}(H_2)$.

Proof. It is not difficult to get that $\phi(H_1) = (x-4)(x-1)^4\,(x+2)^4$ and $\phi(H_2) = (x-4)(x-2)(x-1)^2\,(x+1)^2\,(x+2)^3$. Hence, $\mathscr{E}(H_1) = \mathscr{E}(H_2) = 16$. ∎

Let $B(p,q)$ denote the graph obtained by attaching $p-2$ and $q-2$ vertices to two adjacent vertices of a quadrangle, respectively, and $H(3,q)$ the graph formed by attaching $q-2$ vertices to a pendent vertex of $B(2,3)$. The graphs $B(p,q)$, $(q \geq p \geq 2)$ and $H(3,q)$, $(q \geq 3)$ are shown in Fig. 4.2. In [312], the relation between their energies was left undecided.

Example 4.2. $\mathscr{E}(B(3,q)) > \mathscr{E}(H(3,q))$ for $q \geq 3$.

Proof. It is easy to calculate the characteristic polynomials of $B(3,q)$ and $H(3,q)$ as follows:

$$\phi(B(3,q)) = x^{q-3}\left[x^6 - (q+3)x^4 + (3q-4)x^2 - (q-2)\right]$$

and

$$\phi(H(3,q)) = x^{q-1}\left[x^4 - (q+3)x^2 + (4q-6)\right].$$

Suppose that

$$\begin{aligned} f(x) &= x^6 - (q+3)x^4 + (3q-4)x^2 - (q-2) \\ &= \left(x - \sqrt{x_1}\right)\left(x - \sqrt{x_2}\right)\left(x - \sqrt{x_3}\right)\left(x + \sqrt{x_1}\right)\left(x + \sqrt{x_2}\right)\left(x + \sqrt{x_3}\right) \\ g(y) &= y^4 - (q+3)y^2 + (4q-6) \\ &= \left(y - \sqrt{y_1}\right)\left(y - \sqrt{y_2}\right)\left(y + \sqrt{y_1}\right)\left(y + \sqrt{y_2}\right). \end{aligned}$$

Then, from the relations between the roots and the coefficients of a polynomial, we have $x_1 + x_2 + x_3 = q + 3$, $x_1 x_2 + x_2 x_3 + x_1 x_3 = 3q - 4$, $x_1 x_2 x_3 = q - 2$, $y_1 + y_2 = q + 3$, and $y_1 y_2 = 4q - 6$.

Let $f_0(x) = x^3 - (q+3)x^2 + (3q-4)x - (q-2)$. It is easy to check that $f_0(0) < 0$, $f_0(0.6) > 0$, $f_0(q) < 0$, $f_0(q^{10}) > 0$ since $q \geq 3$. Suppose that $x_1 \leq x_2 \leq x_3$. Then, clearly, $x_3 > q$ and $\sqrt{x_1} + \sqrt{x_2} + \sqrt{x_3} > \sqrt{x_3} > \sqrt{q}$. Therefore,

$$\begin{aligned} \left(\sqrt{x_1 x_2} + \sqrt{x_2 x_3} + \sqrt{x_1 x_3}\right)^2 &= x_1 x_2 + x_2 x_3 + x_1 x_3 \\ &\quad + 2\sqrt{x_1 x_2 x_3}\left(\sqrt{x_1} + \sqrt{x_2} + \sqrt{x_3}\right) \\ &> 3q - 4 + 2\sqrt{q-2}\,\sqrt{q} > 4q - 6 \end{aligned}$$

from which

$$\begin{aligned} (\sqrt{x_1} + \sqrt{x_2} + \sqrt{x_3})^2 &= x_1 + x_2 + x_3 + 2(\sqrt{x_1 x_2} + \sqrt{x_2 x_3} + \sqrt{x_1 x_3}) \\ &> q + 3 + 2\sqrt{4q-6} \\ &= y_1 + y_2 + 2\sqrt{y_1 y_2} = (\sqrt{y_1} + \sqrt{y_2})^2. \end{aligned}$$

Finally, we get that for $q \geq 3$,

$$\mathscr{E}(B(3,q)) = 2\left(\sqrt{x_1} + \sqrt{x_2} + \sqrt{x_3}\right) > 2\left(\sqrt{y_1} + \sqrt{y_2}\right) = \mathscr{E}(H(3,q)).$$

The inequality is thus proven. ■

4.2 Method 2: Spectral Moments

The first inequality that we state here is a lower bound on graph energy (see Ineq. (4.2)), which was independently discovered several times: two times for general graphs [168,529] and two times for bipartite graphs [99,400]. A generalized version thereof was obtained in [540]. One of the proofs is outlined in the following.

The *k-th spectral moment* of a graph G with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ is $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$. Note that if G is a graph with n vertices and m edges, possessing Q quadrangles, then $M_2(G) = 2m$ and $M_4(G) = 2\sum_{i=1}^{n} d_i^2 - 2m + 8Q$.

Lemma 4.1. *Let $a_1, a_2, \dots, a_n$ be positive real numbers and define*

$$x_k = \sum_{i=1}^{n} a_i^k \qquad \text{for } k \geq 1 \; .$$

Then $t+s = 2k$ implies $x_t\, x_s \geq x_k^2$. The equality holds if and only if either $a_i = a_j$ for all $1 \leq i, j \leq n$ or $t = s$.

Proof. Compute

$$x_k^2 = \left(\sum_{i=1}^{n} a_i^k \right)^2 = \sum_{i=1}^{n} a_i^{2k} + \sum_{i \neq j} a_i^k\, a_j^k$$

$$x_t\, x_s = \left(\sum_{i=1}^{n} a_i^t \right) \left(\sum_{j=1}^{n} a_j^s \right) = \sum_{i=1}^{n} a_i^{t+s} + \sum_{i \neq j} a_i^t\, a_j^s \; .$$

For $t + s = 2k$ and $i < j$, it is sufficient to show that $a_i^t\, a_j^s + a_i^s\, a_j^t \geq 2a_i^k\, a_j^k$. Assume that $s \leq t$. Then we have to show that $a_i^{t-s} + a_j^{t-s} \geq 2a_i^{k-s}\, a_j^{k-s}$. Since $t - s = 2(k-s)$, the latter inequality is equivalent to $(a_i^{k-s} - a_j^{k-s})^2 \geq 0$. Equality holds only when $a_i^{k-s} = a_j^{k-s}$ for all $i \neq j$. ■

Theorem 4.1. *Let G be a bipartite graph with at least one edge, and let r, s, t be even positive integers, such that $4r = s + t + 2$. Then*

$$\mathscr{E}(G) \geq M_r(G)^2 \, [M_s(G) M_t(G)]^{-1/2} \; .$$

Proof. Let G be a bipartite graph with vertices $1, 2, \dots, n$ and a_{ij} be the number of edges between i and j. Then the adjacency matrix is $\mathbf{A} = \mathbf{A}(G) = (a_{ij})_{n \times n}$. Assume that $2k = s + t$ and that k is odd. Define $G^{(k)}$ as the graph with vertices $1, 2, \dots, n$ and $a_{ij}^{(k)}$ edges between i and j, where $a_{ij}^{(k)}$ is the number of walks of length k in G between i and j. We have $\mathbf{A}(G^{(k)}) = (a_{ij}^{(k)}) = \mathbf{A}^k$. Denote by $\mathscr{E}^{(k)} = \mathscr{E}(G^{(k)})$ the energy of $G^{(k)}$.

Suppose that $\lambda_1, \lambda_2, \ldots, \lambda_h$ are the nonzero eigenvalues of G. Then we apply Lemma 4.1 for the positive numbers $a_i = |\lambda_i|$, $1 \le i \le h$, and $x_s = \sum_{i=1}^{h} a_i^s$, $s \ge 1$. Then $(\mathscr{E}^{(k)})^2 = x_k^2 \le x_t\, x_s = M_t\, M_s$, and so $\mathscr{E}^{(k)} \le \sqrt{M_t\, M_s}$. On the other hand, $M_r^2 = x_r^2 \le x_1\, x_k = \mathscr{E}(G) \cdot \mathscr{E}^{(k)}$, so we get the conclusion. ■

The above result is presented in [99]. Applying Theorem 4.1 for $t = 2$, $s = 4$, and $r = 2$, we obtain $\mathscr{E}(G) \ge M_2 \sqrt{M_2/M_4}$. Furthermore, Rada and Tineo [400] proved the following result:

Theorem 4.2. *Let G be a bipartite graph with $2N$ vertices. Suppose that $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_N \ge \lambda_{N+1} \ge \cdots \ge \lambda_{2N}$ are the eigenvalues of G and $q = \sum_{i=1}^{N} \lambda_i^4$. Then*

$$\mathscr{E}(G) \ge M_2 \sqrt{\frac{M_2}{M_4}} \ge 2m \sqrt{\frac{m}{q}}. \tag{4.1}$$

(i) Equality in (4.1) is attained if and only if $G = N\, K_2$ or G is the direct sum of isolated vertices and complete bipartite graphs $K_{r_1,s_1}, \ldots, K_{r_j,s_j}$, such that $r_1\, s_1 = \cdots = r_j\, s_j$.

(ii) If G is a bipartite graph with $2N + 1$ vertices, then Ineq. (4.1) remains true. Moreover, the equality holds if and only if G is the direct sum of isolated vertices and complete bipartite graphs $K_{r_1,s_1}, \ldots, K_{r_j,s_j}$ such that $r_1\, s_1 = \cdots = r_j\, s_j$. ■

Since $M_4(G) = 2\sum_{i=1}^{n} d_i^2 - 2m + 8Q$ by Theorem 4.2, it is easy to obtain the following result for bipartite graphs. Furthermore, it can be extended to general graphs.

Theorem 4.3. *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. Then*

$$\mathscr{E}(G) \ge M_2 \sqrt{\frac{M_2}{M_4}} = \sqrt{\frac{(2m)^3}{2\sum\limits_{i=1}^{n} d_i^2 - 2m + 8Q}}\,. \tag{4.2}$$

Proof. Our starting point is the Cauchy–Schwarz inequality

$$\sum_{i=1}^{n} x_i\, y_i \le \sqrt{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2}$$

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

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

By another application of the Cauchy–Schwarz inequality,

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

which when substituted back into the previous inequality yields

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

The relation (4.2) follows. ■

A graph G is called *hypoenergetic* if the energy of G is less than the number of vertices of G. By Ineq. (4.2), we have the following lemma, which is a basic result for determining nonhypoenergetic graphs; for details, see Chap. 9.

Lemma 4.2. *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*

$$2m \sqrt{\frac{2m}{2\sum_{i=1}^{n} d_i^2 - 2m + 8Q}} \geq n \tag{4.3}$$

is obeyed, then G is nonhypoenergetic. ■

For a bipartite graph, the odd spectral moments are necessarily equal to zero. In order to overcome this limitation, we define the moment-like quantities

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

In order to prove Theorem 4.4 [540], we need the following lemma:

Lemma 4.3. *Let $a_1, a_2, \ldots, a_h$ be positive real numbers, $h > 1$, and let r, s, t be nonnegative real numbers, such that $4r = s + t + 2$. Then*

$$\left[\sum_{i=1}^{h} (a_i)^r\right]^4 \leq \left(\sum_{i=1}^{h} a_i\right)^2 \sum_{i=1}^{h} (a_i)^s \sum_{i=1}^{h} (a_i)^t .$$

If $(s,t) \neq (1,1)$, then equality holds if and only if $a_1 = a_2 = \cdots = a_h$.

Proof. By the Cauchy–Schwarz inequality,

$$\left[\sum_{i=1}^{h}(a_i)^r\right]^4 = \left[\sum_{i=1}^{h}(a_i)^{(s+t)/4}(a_i)^{1/2}\right]^4 \leq \left[\sum_{i=1}^{h}(a_i)^{(s+t)/2}\sum_{i=1}^{h}a_i\right]^2$$

$$= \left[\sum_{i=1}^{h}(a_i)^{s/2}(a_i)^{t/2}\right]^2\left(\sum_{i=1}^{h}a_i\right)^2 \leq \sum_{i=1}^{h}(a_i)^s\sum_{i=1}^{h}(a_i)^t\left(\sum_{i=1}^{h}a_i\right)^2.$$

This proves the lemma, and equality holds if and only if both a_i^{s+t-2} and a_i^{s-t} are constants for all $i = 1, 2, \ldots, h$. Thus if $(s, t) \neq (1, 1)$, then the equality holds if and only if $a_1 = \cdots = a_h$. ■

The following result looks similar to Theorem 4.1. However, its proof is different, especially in the analysis of the equality case, and so we prefer to give its details.

Theorem 4.4. *Let G be a graph of order n with at least one edge, and let r, s, t be nonnegative real numbers, such that $4r = s + t + 2$. Then*

$$\mathscr{E}(G) \geq M_r^*(G)^2\,[M_s^*(G)M_t^*(G)]^{-1/2} \tag{4.4}$$

with equality if and only if the components of the graph G are isolated vertices and/or complete bipartite graphs $K_{p_1,q_1}, \ldots, K_{p_k,q_k}$ for some $k \geq 1$, such that $p_1\,q_1 = \cdots = p_k\,q_k$.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G, and suppose that $\lambda_{j1} \geq \lambda_{j2} \geq \cdots \geq \lambda_{jh}$ are the nonzero eigenvalues of G. Since G has at least one edge, we have $\lambda_{j1} = \lambda_1 > 0$ and $\lambda_{jh} = \lambda_n < 0$. Using Lemma 4.3 for the positive numbers $a_i = |\lambda_{ji}|$, $i = 1, 2, \ldots, h$, and noting that in this case $\sum_{i=1}^{h}(a_i)^k = M_k^*(G)$ and, in particular, $\sum_{i=1}^{h} a_i = \mathscr{E}(G)$, we have $M_r^*(G)^4 \leq \mathscr{E}(G)^2 M_s^*(G)M_t^*(G)$, from which (4.4) follows.

If G is a graph specified in the theorem with $p_i\,q_i = c$ as a constant for $i = 1, \ldots, k$, it is easy to check that its nonzero eigenvalues are $\sqrt{c}$ (k times) and $-\sqrt{c}$ (k times), and so the equality in (4.4) holds.

If $s = t = 1$, then in a trivial manner, (4.4) becomes an equality. If $(s, t) \neq (1, 1)$, then equality in (4.4) holds if and only if $|\lambda_{j1}| = |\lambda_{j2}| = \cdots = |\lambda_{jh}|$, and it must be $\sum_{i=1}^{h} \lambda_{ji} = 0$. Therefore, the spectrum of G must be symmetric with respect to the origin, and thus G is a bipartite graph. Note also that G has either two (λ_{j1} and $-\lambda_{j1}$) or three (λ_{j1}, $-\lambda_{j1}$, and 0) distinct eigenvalues. Then G is the disjoint union of complete bipartite graphs $K_{p_1,q_1}, \ldots, K_{p_k,q_k}$ for some $k \geq 1$, such that $p_1\,q_1 = \cdots = p_k\,q_k$, and possibly isolated vertices. ■

Denote by $n_0(G)$ the nullity (i.e., the multiplicity of zero in the spectrum) of G. By setting $s = 0$ and $t = 2$ in Theorem 4.4 (which implies $r = 1$), we obtain the following theorem, which was first reported in [142].

Theorem 4.5. *If the nullity of G is n_0, then $\mathscr{E}(G) \leq \sqrt{2m(n-n_0)}$.* ■

The inequality in Theorem 4.5 is the second result outlined here, which is widely used in finding hypoenergetic graphs; for details, see Chap. 9.

4.3 Method 3: Quasi-Order

Based on Eq. (3.12) in Sect. 3.2, we can define a quasi-order for bipartite graphs, which is of great value for comparing their energies.

For two bipartite graphs G_1 and G_2, we define the quasi-order $\preceq$ and write $G_1 \preceq G_2$ or $G_2 \succeq G_1$ if $b_{2k}(G_1) \leq b_{2k}(G_2)$ for all k [248, 249, 515, 516, 525]. If, moreover, at least one of the inequalities $b_{2k}(G_1) \leq b_{2k}(G_2)$ is strict, then we write $G_1 \prec G_2$ or $G_2 \succ G_1$. Thus, we have

$$\begin{aligned} G_1 \preceq G_2 &\Rightarrow \mathscr{E}(G_1) \leq \mathscr{E}(G_2) \\ G_1 \prec G_2 &\Rightarrow \mathscr{E}(G_1) < \mathscr{E}(G_2)\ . \end{aligned} \tag{4.5}$$

As before, let $m(G,k)$ denote the number of matchings of size k of G, i.e., the number of selections of k independent edges in G. For convenience, let $m(G,0) = 1$ and $m(G,k) = 0$ for all $k < 0$. If G is an acyclic graph, then by the Sachs theorem, $b_{2k}(G) = m(G,k)$ for all $0 \leq k \leq \lfloor n/2 \rfloor$. If G is a tree (or, more generally, a forest), then, as already stated in Theorem 1.6,

$$\phi(G,x) = \sum_{k \geq 0} (-1)^k \, m(G,k) \, x^{n-2k}\ . \tag{4.6}$$

In this case,

$$\mathscr{E}(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k \geq 1} m(G,k) \, x^{2k} \right] \mathrm{d}x\ . \tag{4.7}$$

Practically all results on graphs that are extremal with regard to energy were obtained by establishing the existence of the relation $\preceq$ between the elements of some class of graphs. Details on this matter are found in Chap. 7. In the following, we give some examples to explain this method, which are some basic results on trees [145] and are frequently used. First, we give a useful lemma [81]:

Lemma 4.4. *Let $e = uv$ be an edge of a tree T with n vertices. Then the number $m(T,k)$ of k-matchings of T obeys:*

$$m(T,k) = m(T-uv,k) + m(T-u-v,k-1) \quad \textit{for} \quad k = 1,2,\ldots,\lfloor n/2 \rfloor$$

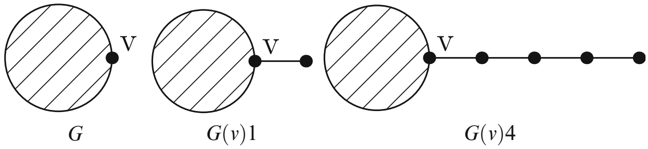

Fig. 4.3 Graphs G, $G(v)1$, and $G(v)4$

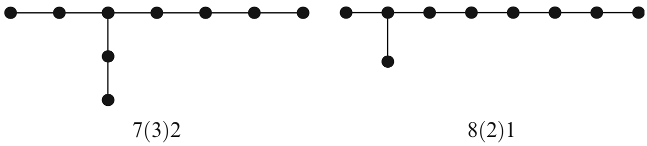

Fig. 4.4 The graphs 7(3)2 and 8(2)1

where $m(T, 0) = 1$. *Moreover, if* u *is a pendent vertex, then*

$$m(T, k) = m(T - u, k) + m(T - u - v, k - 1).$$ ■

By the above lemma, the following result is obvious:

Lemma 4.5. *Let* T *be an acyclic graph with* n *vertices* ($n > 1$) *and* T' *a spanning subgraph (resp. a proper spanning subgraph) of* T. *Then* $T \succeq T'$ *(resp.* $T \succ T'$*).* ■

Let $\mathscr{T}_n$ be the set of all trees with n vertices. Let the vertices $1, 2, \ldots, n$ of the path P_n be labeled so that vertices 1 and n are leaves and vertices j and $j + 1$ are adjacent ($j = 1, 2, \ldots, n - 1$).

Further, let G be an arbitrary graph and $v \in G$. Then we denote by $G(v)m$ the graph obtained by joining one leaf of P_m to the vertex v of G (see Fig. 4.3). In particular, $P_n(v)m$ is obtained by joining one leaf of P_m to the v-th vertex of P_n. For convenience, we denote $P_n(v)m$ in an abbreviated manner as $n(v)m$. As an example, in Fig. 4.4 we present 7(3)2 and 8(2)1.

For any $T \in \mathscr{T}_n$, by Eq. (4.6), $\phi(T, x)$ can be written in the form

$$\phi(T, x) = x^n - b_2\, x^{n-2} + b_4\, x^{n-4} - \cdots + (-1)^k\, b_{2k}\, x^{n-2k} + \cdots \tag{4.8}$$

By Lemma 4.4, for any edge $e = uv$,

$$b_{2j}(T) = b_{2j}(T - uv) + b_{2j-2}(T - u - v)\,. \tag{4.9}$$

Note that if v is a leaf of T, then

$$b_{2j}(T) = b_{2j}(T - v) + b_{2j-2}(T - u - v)\,. \tag{4.10}$$

In particular, if $T = T_0(v)m$, then $b_{2j}(T) = b_{2j}(T_0(v)m - 1) + b_{2j-2}(T_0(v)m - 2)$.

Theorem 4.6 [145]. *For any $T \in \mathscr{T}_n$,*

$$\mathscr{E}(S_n) \le \mathscr{E}(T) \le \mathscr{E}(P_n)\ . \tag{4.11}$$

Proof. The characteristic polynomial of the star is $\phi(S_n, x) = x^n - (n-1)x^{n-2}$. But all other trees $T \in \mathscr{T}_n$ have also $b_2 = n-1$, but $b_4 > 0$. Hence, $\mathscr{E}(T) \ge \mathscr{E}(S_n)$.

We now prove that $\mathscr{E}(T) \le \mathscr{E}(P_n)$. It is easy to check the above statement for small values of n, say $n = 2, 3, 4$. Now, suppose that $P_n \succ T$ holds for $n = 2, 3, \dots, m-1$, where $T \in \mathscr{T}_n$. Let T_0 be the tree such that $T_0 \succ T$ for all $T \in \mathscr{T}_m$. We show that $T_0 \cong P_m$.

Let v be a leaf of T_0 adjacent to the vertex w. Then by Eq. (4.10),

$$b_{2j}(T_0) = b_{2j}(T_0 - v) + b_{2j-2}(T_0 - v - w)\ .$$

Now, $b_{2j}(T_0)$ will be maximal if both $b_{2j}(T_0 - v)$ and $b_{2j-2}(T_0 - v - w)$ are maximal. According to our assumption and Lemma 4.5, this implies $T_0 - v \cong P_{m-1}$ and $T_0 - v - w \cong P_{m-2}$. This, however, is possible only if $T_0 \cong P_m$. ∎

Thus, we have found that among all trees, the path has maximal energy and the star has minimal energy. Note that Lovász and Pelikán [360] proved the intriguing result that for all trees T with n vertices,

$$\lambda_1(S_n) \ge \lambda_1(T) \ge \lambda_1(P_n)\ . \tag{4.12}$$

The analogy between Ineqs. (4.11) and (4.12) is evident. However, the readers' attention is drawn to the fact that a naive extension of Ineq. (4.12) would lead to a conclusion which is just the contrary of Theorem 4.6, namely, $\mathscr{E}(S_n) \ge \mathscr{E}(T) \ge \mathscr{E}(P_n)$. Therefore, Theorem 4.6 seems to be a nontrivial result with regard to Ineq. (4.12).

Recall that $S(n-2,2)$ and $S(n-3,3)$ denote two double stars of order n, and $P_{n,n-3}$ denote a comet of order n. It is not difficult to find additional trees with minimal energies.

Theorem 4.7. *If $T \in \mathscr{T}_n$, but $T \ncong S_n, S(n-2,2), S(n-3,3), P_{n,n-3}$, then $S_n \prec S(n-2,2) \prec S(n-3,3) \prec P_{n,n-3} \prec T$, and therefore $\mathscr{E}(S_n) < \mathscr{E}(S(n-2,2)) < \mathscr{E}(S(n-3,3)) < \mathscr{E}(P_{n,n-3}) < \mathscr{E}(T)$.*

Proof. The proof is analogous to that of Theorem 4.6 and is based on the characteristic polynomials:

$$\phi(S(n-2,2), x) = x^n - (n-1)x^{n-2} + (n-3)x^{n-4}$$
$$\phi(S(n-3,3), x) = x^n - (n-1)x^{n-2} + (2n-8)x^{n-4}$$
$$\phi(P_{n,n-3}, x) = x^n - (n-1)x^{n-2} + (2n-7)x^{n-4}.$$

∎

Theorem 4.8. *For $i = 1, 2, \dots, n$,*

$$P_1 \cup P_{n-1} \prec P_i \cup P_{n-i} \prec P_2 \cup P_{n-2} \prec P_n\ . \tag{4.13}$$

Proof. The inequalities in Ineq. (4.13) can be easily verified for $n = 6, 7$. Suppose that these hold for all $n = 6, 7, \ldots, m-1$. We now prove that Ineq. (4.13) holds for $n = m$. Because of Eq. (4.9), for arbitrary i, $b_{2j}(P_m) = b_{2j}(P_i \cup P_{m-i}) + b_{2j-2}(P_{i-1} \cup P_{m-i-1})$. Since obviously $b_{2j}(P_m)$ is independent of i, it follows that $b_{2j}(P_i \cup P_{m-i})$ is minimal if $b_{2j-2}(P_{i-1} \cup P_{m-i-1})$ is maximal. According to Theorem 4.6, this occurs when $i - 1 = 0$. Hence, $P_1 \cup P_{m-1} \preceq P_i \cup P_{m-i}$. Further, for $i \neq 0$ and $i \neq m$, $b_{2j}(P_i \cup P_{m-i})$ is maximal if $b_{2j-2}(P_{i-1} \cup P_{m-i-1})$ is minimal. According to our assumption, this occurs when $i - 1 = 1$. Hence, $P_2 \cup P_{m-2} \succeq P_i \cup P_{m-i}$. ■

By a similar way of reasoning, one can prove the following lemma: [216].

Lemma 4.6. *Let* $n = 4k$, $4k+1$, $4k+2$, *or* $4k+3$. *Then*

$$P_n \succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1}$$
$$\succ P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}. \qquad ■$$

Theorem 4.9. *Let* t *be an integer and* $k = \lfloor n/2 \rfloor$. *Then,*

$$n-1(2)1 \prec n-1(4)1 \prec \cdots \prec n-1(k)1 \prec n-1(k-1)1 \prec n-1(k-3)1$$
$$\prec \cdots \prec n-1(3)1 \prec n-1(1)1 \equiv P_n \qquad \textit{if } n = 4t \qquad (4.14)$$
$$n-1(2)1 \prec n-1(4)1 \prec \cdots \prec n-1(k-1)1 \prec n-1(k)1 \prec n-1(k-2)1$$
$$\prec \cdots \prec n-1(3)1 \prec n-1(1)1 \equiv P_n \qquad \textit{if } n = 4t+2 \qquad (4.15)$$
$$n-1(2)1 \prec n-1(4)1 \prec \cdots \prec n-1(k)1 \prec n-1(k+1)1 \prec n-1(k-1)1$$
$$\prec \cdots \prec n-1(3)1 \prec n-1(1)1 \equiv P_n \qquad \textit{if } n = 4t+1 \qquad (4.16)$$
$$n-1(2)1 \prec n-1(4)1 \prec \cdots \prec n-1(k+1)1 \prec n-1(k)1 \prec n-1(k-2)1$$
$$\prec \cdots \prec n-1(3)1 \prec n-1(1)1 \equiv P_n \qquad \textit{if } n = 4t+3\,. \qquad (4.17)$$

Proof. Application of Eq. (4.10) gives $b_{2j}(n-1(i)1) = b_{2j}(P_{n-1}) + b_{2j-2}(P_{i-1} \cup P_{n-i-1})$. Since $b_{2j}(P_{n-1})$ is independent of i, $b_{2j}(n-1(i)1)$ will be minimal if $b_{2j-2}(P_{i-1} \cup P_{n-i-1})$ is minimal, that is, if $i - 1 = 1$. Therefore, $n-1(2)1 \preceq n-1(i)1$. Similarly, $b_{2j}(n-1(i)1)$ is maximal if $b_{2j-2}(P_{i-1} \cup P_{n-i-1})$ is maximal, that is, if $i-1 = 2$. Therefore, if $i \neq 1$, $n-1(3)1 \succeq n-1(i)1$.

All other statements can be proven analogously. ■

The following simple argument enables one to find numerous new inequalities between the energies of trees:

Theorem 4.10. *Let* G *and* H *be trees with* n *vertices,* $u \in G$ *and* $v \in H$. *If* $G \succ H$ *and* $G(u)1 \succ H(v)1$, *then for arbitrary* i, $G(u)i \succ H(v)i$.

Proof. We proceed by total induction, using the facts that

$$b_{2j}(G(u)i) = b_{2j}(G(u)i-1) + b_{2j-2}(G(u)i-2)$$
$$b_{2j}(H(v)i) = b_{2j}(H(v)i-1) + b_{2j-2}(H(v)i-2)\ .$$

Then from $b_{2j}(G(u)i-1) \geq b_{2j}(H(v)i-1)$ and $b_{2j-2}(G(u)i-2) \geq b_{2j-2}(H(v)i-2)$, it immediately follows that $b_{2j}(G(u)i) \geq b_{2j}(H(v)i)$. ■

As a consequence of this theorem, we may set $n-i(v)i$ instead of $n-1(v)1$ in Ineqs. (4.14)–(4.17). We are now able to determine the tree with the second-maximal energy. First, we prove an auxiliary result:

Theorem 4.11. $n-1(i)1 \prec n-2(3)2$ *for all* $i \neq 1, n-1$ *and* $n \neq 6$.

Proof. Because of Theorem 4.9, it is sufficient to show that $n-1(3)1 \prec n-2(3)2$. This, however, follows immediately from $b_{2j}(n-2(3)2) = b_{2j}(n-2(3)1) + b_{2j-2}(P_{n-2})$ and $b_{2j}(n-1(3)1) = b_{2j}(n-2(3)1) + b_{2j-2}(n-3(3)1)$ and the fact that by Theorem 4.6, $b_{2j-2}(P_{n-2}) \geq b_{2j-2}(n-3(3)1)$. ■

Theorem 4.12. [145] *If* $T \in \mathscr{T}_n$ *and* $T \ncong P_n, n-2(3)2$*, then*

$$n-2(3)2 \succ T. \tag{4.18}$$

Proof. For small values of n $(n = 6, 7)$, Ineq. (4.18) is checked by considering the characteristic polynomials of all trees. Suppose that Ineq. (4.18) holds for all $n = 6, 7, \ldots, m-1$, and let T_0 be a tree which fulfills the relation $T_0 \succ T$ for all $T \in \mathscr{T}_m$, $T \ncong P_m$. We prove that $T_0 \cong m-2(3)2$.

Let v be a leaf of T_0 adjacent to the vertex w. Then $b_{2j}(T_0) = b_{2j}(T_0-v) + b_{2j-2}(T_0-v-w)$. Since $b_{2j}(m-2(3)2) = b_{2j}(m-3(3)2) + b_{2j-2}(m-4(3)2)$, the inequality $b_{2j}(T_0) \geq b_{2j}(m-2(3)2)$ will be fulfilled if either $T_0 \cong m-2(3)2$ or $T_0-v \cong P_{m-1}$ or $T_0-v-w \cong P_{m-2}$. If $T_0-v \cong P_{m-1}$, it must be $T_0 \cong m-1(i)1$. According to Theorem 4.11, this implies $T_0 \prec m-2(3)2$, which is impossible. If $T_0-v-w \cong P_{m-2}$, it must be $T_0 \cong m-2(i)2$. From Theorem 4.10, $m-2(3)2 \succ m-2(i)2$, and therefore $T_0 \cong m-2(3)2$. ■

Note that Theorem 4.12 was proved already in 1977 [145]. The very same result (proven in an almost identical manner) was rediscovered by Ou [391] in 2010.

Remark 4.1. The quasi-order $\preceq$ is defined for bipartite graphs, but it can be efficiently used mainly in the case of trees. Some of its applications for bipartite graphs other than trees are given in Chap. 7.

4.4 Method 4: Coulson Integral Formula

The quasi-order method is commonly used to compare the energies of two trees or bipartite graphs. However, for general graphs, it is hard to define such a partial ordering, since in this case, the Coulson integral formula cannot be used to

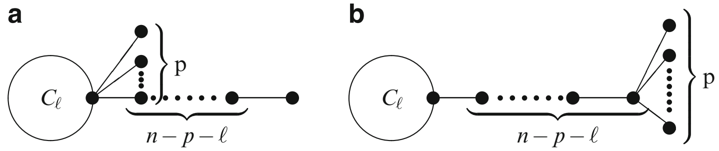

Fig. 4.5 (**a**) The graph $S_n^{\ell,p}$; (**b**) the graph $R_n^{\ell,p}$

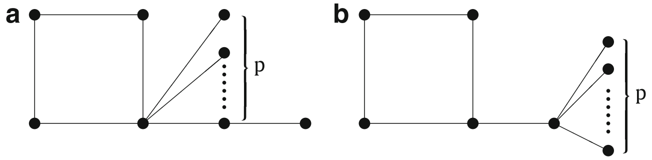

Fig. 4.6 (**a**) The graph $S_{p+5}^{4,p}$, (**b**) the graph $R_{p+5}^{4,p}$

determine whether $G_1 \preceq G_2$ implies $\mathscr{E}(G_1) \leq \mathscr{E}(G_2)$. If, for two trees or bipartite graphs, the quantities $m(T,k)$ or $|a_k(G)|$ cannot be compared uniformly, then the common comparing method is invalid, and this happens quite often. For example, in the paper [270], the unicyclic bipartite graph with maximal energy could not be determined. In the same sense, in [327, 434], one could not determine the tree with the fourth-maximal energy; in [340], the bicyclic graph with maximal energy; in [339], the tree with two maximum degree vertices that has maximal energy; in [517], the conjugated trees with the third- and fourth-minimal energies; and in [324], the conjugated trees with the third- through sixth-minimal energies.

For a long time, much effort has been made to attack these quasi-order-incomparable problems. Efficient approaches to solving these problems were found only quite recently. By means of the Coulson integral formula, combined by methods of real analysis, algebra, and combinatorics, almost all of these problems could be solved [16–18, 277–283, 316]. In what follows, we outline in detail one result of this kind [277].

Denote by $\mathscr{G}(n,p)$ the set of unicyclic graphs with n vertices and p pendent vertices. Let S_n^ℓ $(n \geq \ell+1)$ be the graph obtained by identifying the center of the star $S_{n-\ell+1}$ with any vertex of a cycle C_ℓ. Let P_n^ℓ $(n \geq \ell+1)$ be the graph obtained by attaching one pendent vertex of the path $P_{n-\ell+1}$ to any vertex of the cycle C_ℓ. Denote by $S_n^{\ell,p}$ $(n \geq \ell+p+1)$ the graph obtained by attaching one pendent vertex of the path $P_{n-\ell-p+1}$ to one pendent vertex of $S_{\ell+p}^\ell$. By $R_n^{\ell,p}$ $(n \geq \ell+p+1)$, we denote the graph obtained by attaching p pendent edges to the pendent vertex of P_{n-p}^ℓ. Hua and Wang [275] attempted to characterize graphs that have minimal energy among all graphs in $\mathscr{G}(n,p)$. They almost completely solved this problem except for the case $n = p+5$ for which the problem is reduced to finding the minimal energy species among two graphs: $S_{p+5}^{4,p}$ and $R_{p+5}^{4,p}$. In this section, we present a solution to this problem for the case $n = p+5$, i.e., we show that the graph with minimal energy is $R_{p+5}^{4,p}$ (Figs. 4.5 and 4.6).

For the minimal-energy unicyclic graphs with prescribed pendent vertices, Hua and Wang [275] obtained the following result:

Theorem 4.13. *Let* $1 \leq p \leq n-3$.

(a) *For* $p = n-3$, $S_n^{3,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$. *For* $p = n-4$, $S_n^{4,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$.
(b) *For* $p = 1$, $S_n^{4,p}$ $(= R_n^{4,p})$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$.
(c) *For* $p = n-5$ *and* $1 \leq n \leq 869$, $R_n^{4,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$, *while for* $p = n-5$ *and* $n \geq 870$, *either* $R_n^{4,p}$ *or* $S_n^{4,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$.
(d) *For* $2 \leq p \leq n-6$, $S_n^{4,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$. ■

It is obvious that both graphs have diameter 4. Their characteristic polynomials can be expressed as follows:

Lemma 4.7.

$$\phi(S_{p+5}^{4,p}, x) = x^{p-1}\,[x^6 - (p+5)x^4 + 3(p+1)x^2 - 2(p-1)]$$

$$\phi(R_{p+5}^{4,p}, x) = x^{p+1}\,[x^4 - (p+5)x^2 + (4p+2)]. \quad ■$$

Before comparing of the energies of the two graphs, we recall two useful inequalities:

Lemma 4.8. *For any real number* $X > -1$, *we have*

$$\frac{X}{1+X} \leq \ln(1+X) \leq X\ . \tag{4.19}$$

■

Lemma 4.9. *Let* A *be a positive real number and* B *and* C *be nonnegative. Then,* $X = \frac{B-C}{A+C} > -1$.

Proof. From the above conditions follows $X = \frac{B}{A+C} - \frac{C}{A+C} \geq -\frac{C}{A+C} \geq -1$. ■

We now state the main result.

Theorem 4.14. *For* $p = n-5$, $R_n^{4,p}$ *has the minimal energy among all graphs in* $\mathscr{G}(n,p)$.

Proof. Clearly, the common comparing method is inapplicable for $R_{p+5}^{4,p}$ and $S_{p+5}^{4,p}$. That is, the fact that the energy of the former graph is less than the energy of the latter cannot be determined completely by just comparing the corresponding coefficients of their characteristic polynomials. We use the Coulson integral formula to compare the energies of the two graphs. By Ineq. (3.8) and Lemma 4.7,

$$\mathscr{E}(R_{p+5}^{4,p}) - \mathscr{E}(S_{p+5}^{4,p}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \frac{x^6 + (p+5)x^4 + (4p+2)x^2}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)} \, \mathrm{d}x. \tag{4.20}$$

We denote by $f(x, p)$ the integrand in Eq. (4.20). By writing $A = x^6 + (p+5)x^4$, $B = (4p+2)x^2$, and $C = (3p+3)x^2 + (2p-2)$, we can express $f(x, p)$ as

$$f(x, p) = \ln \frac{A+B}{A+C} = \ln \left(1 + \frac{B-C}{A+C}\right),$$

i.e.,

$$f(x, p) = \ln \left(1 + \frac{(p-1)x^2 - (2p-2)}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)}\right).$$

Obviously, for $p \geq 1, x \neq 0$, we have $A > 0$, $B \geq 0$, and $C \geq 0$. Let $X = \frac{B-C}{A+C}$. Then from Lemmas 4.8 and 4.9, we get that for all $x \in \mathbb{R}$, $x \neq 0$ and any integer $p \geq 1$,

$$f(x, p) \leq \frac{(p-1)x^2 - (2p-2)}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)}$$

and

$$f(x, p) \geq \frac{(p-1)x^2 - (2p-2)}{x^6 + (p+5)x^4 + (4p+2)x^2}.$$

It follows that

$$f(x, p) \leq \frac{(p-1)x^2 - (2p-2)}{x^6 + (p+5)x^4 + (4p+2)x^2} \leq 0 \qquad \text{if } 0 < |x| \leq \sqrt{2} \tag{4.21}$$

and

$$f(x, p) \geq \frac{(p-1)x^2 - (2p-2)}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)} > 0 \qquad \text{if } |x| > \sqrt{2}. \tag{4.22}$$

Notice that the function sequence $\{f(x, p)\}$ is convergent if $x \neq 0$, and

$$\lim_{p \to +\infty} f(x, p) = \ln \frac{x^4 + 4x^2}{x^4 + 3x^2 + 2}.$$

Denote by $\varphi(x) = \ln \frac{x^4+4x^2}{x^4+3x^2+2}$ the limit of $\{f(x, p)\}$. For $x \neq 0$, we have

$$\varphi(x) - f(x,p) = \ln \frac{x^4 + 4x^2}{x^4 + 3x^2 + 2} - \ln \frac{x^6 + (p+5)x^4 + (4p+2)x^2}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)}$$

$$= \ln \frac{x^8 + (p+9)x^6 + (7p+23)x^4 + (14p+10)x^2 + (8p-8)}{x^8 + (p+8)x^6 + (7p+19)x^4 + (14p+16)x^2 + (8p+4)}.$$

By writing $A = x^8 + (p+8)x^6 + (7p+19)x^4 + (14p+10)x^2 + (8p-8)$, $B = x^6 + 4x^4$, and $C = 6x^2 + 12$, we can express the above $\varphi(x) - f(x,p)$ as

$$\varphi(x) - f(x,p) = \ln \frac{A+B}{A+C} = \ln \left(1 + \frac{B-C}{A+C}\right),$$

i.e.,

$$\varphi(x) - f(x,p) = \ln \left[1 + \frac{(x^2-2)(x^4+6x^2+6)}{x^8 + (p+8)x^6 + (7p+19)x^4 + (14p+16)x^2 + (8p+4)}\right].$$

For $x \neq 0$, it is easy to see that $A > 0$, $B \geq 0$, and $C \geq 0$. From Lemmas 4.8 and 4.9, for any $x \neq 0$, $x \in \mathbb{R}$ and any positive integer p, we have

$$\varphi(x) - f(x,p) \leq \frac{(x^2-2)(x^4+6x^2+6)}{x^8 + (p+8)x^6 + (7p+19)x^4 + (14p+16)x^2 + (8p+4)}$$

and

$$\varphi(x) - f(x,p) \geq \frac{(x^2-2)(x^4+6x^2+6)}{x^8 + (p+9)x^6 + (7p+23)x^4 + (14p+10)x^2 + (8p-8)}.$$

It follows that

$$\varphi(x) < f(x,p) \qquad \text{if } 0 < |x| < \sqrt{2}v \tag{4.23}$$

and

$$\varphi(x) > f(x,p) \qquad \text{if } |x| > \sqrt{2}. \tag{4.24}$$

Similarly, by direct calculations for $x \neq 0$, we have

$$f(x,p+1) - f(x,p) = \ln \frac{x^6 + (p+6)x^4 + (4p+6)x^2}{x^6 + (p+6)x^4 + (3p+6)x^2 + 2p}$$

$$- \ln \frac{x^6 + (p+5)x^4 + (4p+2)x^2}{x^6 + (p+5)x^4 + (3p+3)x^2 + (2p-2)}$$

$$= \ln \left[1 + \frac{(x^2-2)(x^4+6x^2+6)}{g(p,x)}\right]$$

where $g(p, x) = x^{10} + (2p + 11)x^8 + (p^2 + 18p + 38)x^6 + (7p^2 + 49p + 42)x^4 + (14p^2 + 40p + 12)x^2 + (8p^2 + 4p)$. We also have

$$f(x, p+1) - f(x, p) \leq \frac{(x^2 - 2)(x^4 + 6x^2 + 6)}{g(p, x)}$$

and

$$f(x, p+1) - f(x, p) \geq \frac{(x^2 - 2)(x^4 + 6x^2 + 6)}{g(p, x) + (x^2 - 2)(x^4 + 6x^2 + 6)}\,.$$

It follows that

$$f(x, p+1) < f(x, p) \qquad \text{if } 0 < |x| < \sqrt{2} \tag{4.25}$$

and

$$f(x, p+1) > f(x, p) \qquad \text{if } |x| > \sqrt{2}\,. \tag{4.26}$$

Combining Ineq. (4.21) with Ineq. (4.26), we have

$$\varphi(x) < f(x, p+1) < f(x, p) \leq 0 \qquad \text{if } 0 < |x| \leq \sqrt{2} \tag{4.27}$$

$$\varphi(x) > f(x, p+1) > f(x, p) > 0 \qquad \text{if } |x| > \sqrt{2}\,. \tag{4.28}$$

Based on Ineqs. (4.27) and (4.28), for $p > 2$, we immediately get

$$\int_0^{+\infty} f(x, p)\,\mathrm{d}x = \int_0^{\sqrt{2}} f(x, p)\,\mathrm{d}x + \int_{\sqrt{2}}^{+\infty} f(x, p)\,\mathrm{d}x < \int_0^{\sqrt{2}} f(x, 2)\,\mathrm{d}x + \int_{\sqrt{2}}^{+\infty} \varphi(x)\,\mathrm{d}x.$$

By means of computer-aided calculation and Lemma 4.8, it is easy to verify that for any $x \neq 0$

$$f(x, 2) = \ln \frac{x^6 + 7x^4 + 10x^2}{x^6 + 7x^4 + 9x^2 + 2} = \ln \left[1 + \frac{x^2 - 2}{x^6 + 7x^4 + 9x^2 + 2}\right]$$

$$< \frac{x^2 - 2}{x^6 + 7x^4 + 9x^2 + 2} < \frac{x^2 - 2}{x^6 + \frac{211}{30}x^4 + \frac{694}{75}x^2 + \frac{117}{50}}.$$

Furthermore,

$$\int_0^{\sqrt{2}} f(x, 2)\,\mathrm{d}x < \int_0^{\sqrt{2}} \frac{x^2 - 2}{x^6 + \frac{211}{30}x^4 + \frac{694}{75}x^2 + \frac{117}{50}}\,\mathrm{d}x$$

$$= \int_0^{\sqrt{2}} \frac{x^2 - 2}{(x^2 + \frac{27}{5})(x^2 + \frac{13}{10})(x^2 + \frac{1}{3})}\,\mathrm{d}x \doteq -0.408541$$

as well as

$$\int_{\sqrt{2}}^{+\infty} \varphi(x)\,\mathrm{d}x = \int_{\sqrt{2}}^{+\infty} \ln \frac{x^4 + 4x^2}{x^4 + 3x^2 + 2}\,\mathrm{d}x$$

$$= -\frac{\sqrt{2}}{2}\pi + 2\arctan(\sqrt{2}) - 4\arctan\left(\frac{\sqrt{2}}{2}\right) + \pi \doteq 0.368866\,.$$

Therefore, the difference between the energies of $R^{4,p}_{p+5}$ and $S^{4,p}_{p+5}$ must be less than a certain negative number since

$$\mathscr{E}(R^{4,p}_{p+5}) - \mathscr{E}(S^{4,p}_{p+5}) = \frac{2}{\pi}\int_0^{+\infty} f(x,p)\,\mathrm{d}x\,.$$

Combining with part (c) of Theorem 4.13, we conclude that $R^{4,p}_{p+5}$ has the minimal energy among all graphs in $\mathscr{G}(n, p)$. ■

The above-described method is often effective for comparing the energies of two graphs that have small diameters. For more examples of this type, we refer to [277, 278, 283]. For the case of large diameters, we also developed an effective method for comparing the energies, see [279–282, 316]. Two examples of this kind are presented in Sects. 7.1.3 and 7.2.3.

4.5 Method 5: Graph Operations

For a given class of graphs, one main problem is to determine the extremal values of graph energy and to characterize the graphs achieving these values. In order to do this, a number of graph operations have been considered. Here, we outline only two of these. For more details, see Chap. 7.

Operation I. As shown in Fig. 4.7, $T_1, T_2 \ncong P_1$ are two subtrees of T with vertices v and u as roots, respectively, and P_s $(s \geq 3)$ is the pendent path of T with s vertices and root u. If T' is obtained from T by replacing P_s with a pendent edge and replacing the edge uv with the path P_s, we say that T' is obtained from T by *Operation I*.

Operation II. As shown in Fig. 4.8, let $N_T(u) = \{u_1, u_2, \ldots, u_s, w\}$ $(s \geq 2)$ and $N_T(v) = \{v_1, v_2, \ldots, v_t, w'\}$ $(t \geq 2)$, where $u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t$ are pendent vertices of T, $d_T(w) \geq 2$ and $d_T(w') \geq 2$. Note that if $d(u_1, v_1) = 3$, then w=v. If $T' = T - \{uu_2, \ldots, uu_s\} + \{vu_2, \ldots, vu_s\}$ or $T' = T - \{vv_2, \ldots, vv_t\} + \{uv_2, \ldots, uv_t\}$, we say that T' is obtained from T by *Operation II*.

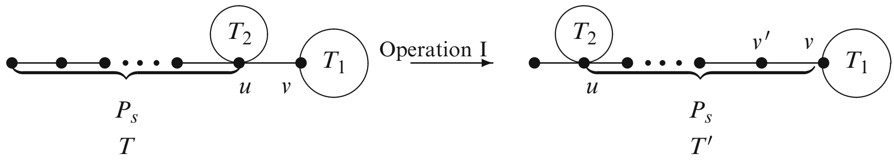

Fig. 4.7 Trees T and T' in Operation I

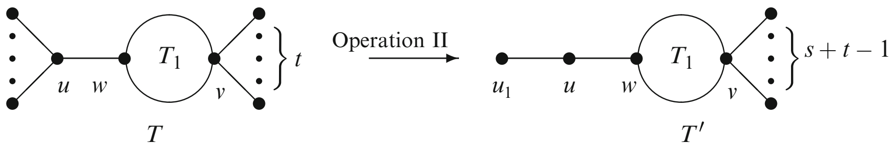

Fig. 4.8 Trees T and T' in Operation II

Note that Operations I and II do not change the number of pendent paths and hence the number of pendent vertices and that Operation II reduces the number of vertices of degree at least 3 by one.

We now show that both Operation I and Operation II strictly decrease the energy of a tree. At first, we need some useful lemmas that are easily obtained by direct calculation:

Lemma 4.10. *If T' is obtained from T by Operation I, as shown in Fig. 4.7, then*

$$\sum_{k=0}^{\lfloor n/2 \rfloor} m(T',k) < \sum_{k=0}^{\lfloor n/2 \rfloor} m(T,k). \qquad \blacksquare$$

Lemma 4.11. *Let*

$$f(x) = \sum_{k=0}^{\lfloor s/2 \rfloor} f_k\, x^{s-2k} \qquad \text{and} \qquad g(x) = \sum_{k=0}^{\lfloor t/2 \rfloor} g_k\, x^{t-2k}$$

where $f_0 = g_0 = 0$, $(-1)^k f_k \geq 0$ $(1 \leq k \leq \lfloor s/2 \rfloor)$ and $(-1)^k g_k \geq 0$ $(1 \leq k \leq \lfloor t/2 \rfloor)$. If

$$\Pi(x) = \sum_{k=0}^{\lfloor (s+t)/2 \rfloor} \pi_k\, x^{s+t-2k} = f(x)\, g(x)$$

then $\pi_0 = 0$ and $(-1)^k \pi_k \geq 0$ $(1 \leq k \leq \lfloor (s+t)/2 \rfloor)$. $\blacksquare$

Lemma 4.12. *If T' is obtained from T by Operation I, then $\mathscr{E}(T') < \mathscr{E}(T)$.*

Proof. Let A_l and B_l be the trees shown in Fig. 4.9. By Theorems 1.2, 1.4, and Corollary 1.1,

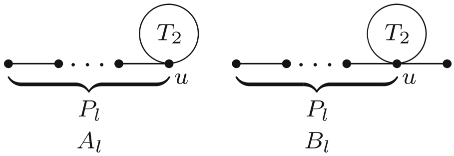

Fig. 4.9 The trees A_l and B_l

$$\begin{aligned}\phi(T) &= \phi(T - uv) - \phi(T - u - v)\\ &= \phi(T_1)\,\phi(A_s) - \phi(T_1 - v)\,\phi(T_2 - u)\,\phi(P_{s-1})\\ &= x\,\phi(T_1)\,\phi(A_{s-1}) - \phi(T_1)\,\phi(A_{s-2}) - \phi(T_1 - v)\,\phi(T_2 - u)\,\phi(P_{s-1})\end{aligned}$$

and

$$\begin{aligned}\phi(T') &= \phi(T' - v'v) - \phi(T' - v' - v)\\ &= \phi(T_1)\,\phi(B_{s-1}) - \phi(T_1 - v)\,\phi(B_{s-2})\\ &= x\,\phi(T_1)\,\phi(A_{s-1}) - \phi(T_1)\,\phi(T_2 - u)\,\phi(P_{s-2}) - x\,\phi(T_1 - v)\,\phi(A_{s-2})\\ &\quad + \phi(T_1 - v)\,\phi(T_2 - u)\,\phi(P_{s-3})\,.\end{aligned}$$

Since $T_1, T_2 \not\cong P_1$, it is $\phi(P_0) \equiv 1$, $\phi(P_1) \equiv x$, and $\phi(P_n) = x\,\phi(P_{n-1}) - \phi(P_{n-2})$ for $n \geq 2$. Then by Theorem 1.4,

$$\begin{aligned}\phi(T) - \phi(T') &= [\phi(T_1) - x\,\phi(T_1 - v)][\phi(T_2 - u)\,\phi(P_{s-2}) - \phi(A_{s-2})]\\ &= -\left(\sum_{vv_i \in E(T_1)} \phi(T_1 - v - v_i)\right)\left(\sum_{uu_i \in E(T_2)} \phi(T_2 - u - u_i)\right)\phi(P_{s-3})\,.\end{aligned}$$

Let $\phi(T) - \phi(T') = f(x)\,g(x)\,h(x)$, where

$$f(x) = -\sum_{vv_i \in E(T_1)} \phi(T_1 - v - v_i) = \sum_{k=0}^{\lfloor n_1/2 \rfloor} f_k\, x^{n_1 - 2k}$$

$$g(x) = -\sum_{uu_i \in E(T_2)} \phi(T_2 - u - u_i) = \sum_{j=0}^{\lfloor n_2/2 \rfloor} g_j\, x^{n_2 - 2j}$$

$$h(x) = -\phi(P_{s-3}) = \sum_{\ell=0}^{\lfloor (s-1)/2 \rfloor} h_\ell\, x^{s-1-2\ell}$$

and let n_1, n_2 be the orders of T_1, T_2, respectively. Since $T_1 - v - v_i$, $T_2 - u - u_i$, and P_{s-3} ($s \geq 3$) are forests, we have $f_0 = g_0 = h_0 = 0$, $(-1)^k f_k \geq 0$, $(-1)^j g_j \geq 0$, and $(-1)^\ell h_\ell \geq 0$ for any $1 \leq k \leq \lfloor n_1/2 \rfloor, 1 \leq j \leq \lfloor n_2/2 \rfloor$, and $1 \le \ell \le \lfloor (s-1)/2 \rfloor$. By Lemma 4.11, $T' \preceq T$. Note that $\phi(T) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k m(T,k) x^{n-2k}$ and $\phi(T') = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k m(T',k) x^{n-2k}$, and therefore $m(T',k) \le m(T,k)$ for any k $(1 \le k \le \lfloor n/2 \rfloor)$. By Lemma 4.10,

$$\sum_{k=0}^{\lfloor n/2 \rfloor} m(T',k) < \sum_{k=0}^{\lfloor n/2 \rfloor} m(T,k) .$$

Hence, $m(T',k) \le m(T,k)$ for any k $(1 \le k \le \lfloor n/2 \rfloor)$, and there is a k $(1 \le k \le \lfloor n/2 \rfloor)$, such that $m(T',k) < m(T,k)$. We thus have $T' \prec T$, and then $\mathscr{E}(T') < \mathscr{E}(T)$. ■

Lemma 4.13. *If T' is obtained from T by Operation II, then $\mathscr{E}(T') < \mathscr{E}(T)$.*

Proof. Let u_1, v_1 be pendent vertices, such that $d(u_1, v_1) = \max\{d(u,v) : u, v \in V(T)\}$. If $d(u_1, v_1) \ge 4$, then without loss of generality, we may suppose that $u_1 u, v_1 v, uw \in E(T)$ and $d_T(w) \ge 2$. Then $w \ne v$. Without loss of generality, we suppose that $T' \cong T - \{uu_2, \ldots, uu_s\} + \{vu_2, \ldots, vu_s\}$. Then T and T' are the trees depicted in Fig. 4.8.

Denote $A = \sum_{v'v \in E(T_1)} \phi(T_1 - v' - v)$ and $B = \sum_{v'v \in E(T_1 - w)} \phi(T_1 - v' - v - w)$. By Theorems 1.2, 1.4, and Corollary 1.1,

$$\begin{aligned}\phi(T) &= \phi(T - uw) - \phi(T - u - w) \\ &= x^{s+t-2} \big[(x^2 - s)(x^2 - t)\phi(T_1 - v) - x(x^2 - s)A \\ &\qquad - x(x^2 - t)\phi(T_1 - w - v) + x^2 B \big]\end{aligned}$$

$$\begin{aligned}\phi(T') &= \phi(T' - uw) - \phi(T' - u - w) \\ &= x^{s+t-2} \big[(x^2 - s - t + 1)(x^2 - 1)\phi(T_1 - v) - x(x^2 - 1)A \\ &\qquad - x(x^2 - s - t + 1)\phi(T_1 - w - v) + x^2 B \big] .\end{aligned}$$

It is easy to see that

$$\begin{aligned}\phi(T) - \phi(T') &= (s-1)x^{s+t-2} [(t-1)\,\phi(T_1 - v) - x\,\phi(T_1 - w - v) + x\,A] \\ &= (s-1)x^{s+t-2} [(t-1)\,\phi(T_1 - v) - \phi((T_1 - w - v) \cup w) + x\,A] .\end{aligned}$$

Let

$$(t-1)\,\phi(T_1 - v) - \phi((T_1 - w - v) \cup w) = \sum_{k=0}^{\lfloor (n_1 - 1)/2 \rfloor} f_k\, x^{n_1 - 1 - 2k}$$

$$x\,A = \sum_{k=0}^{\lfloor (n_1 - 1)/2 \rfloor} g_k\, x^{n_1 - 1 - 2k}$$

where n_1 is the order of T_1. Thus

$$\phi(T) - \phi(T') = \sum_{\ell=0}^{\lfloor n/2 \rfloor} (a_\ell - a'_\ell)\, x^{n-2\ell} = \sum_{k=0}^{\lfloor (n_1-1)/2 \rfloor} (s-1)(f_k + g_k)\, x^{n_1+s+t-3-2k}$$
$$= \sum_{k=0}^{\lfloor (n_1-1)/2 \rfloor} (s-1)(f_k + g_k)\, x^{n-2(2+k)}\ .$$

Note that for $2 \leq \ell \leq \lfloor (n_1-1)/2 \rfloor + 2$, $(-1)^\ell\,(a_\ell - a'_\ell) = (-1)^{k+2}\,(a_{k+2} - a'_{k+2}) = (-1)^{k+2}\,(s-1)(f_k + g_k) = (-1)^k (s-1)\,(f_k + g_k)$ $(0 \leq k \leq \lfloor (n_1-1)/2 \rfloor)$ and for the other values of ℓ, $a_\ell - a'_\ell = 0$.

Since $(T_1 - w - v) \cup w$ is a proper spanning subgraph of $T_1 - v$ and $t \geq 2$, by Lemma 4.5, we have $(-1)^k\, f_k \geq 0$ for $0 \leq k \leq \lfloor (n_1-1)/2 \rfloor$, and there is a k $(0 < k \leq \lfloor (n_1-1)/2 \rfloor)$, such that $(-1)^k\, f_k > 0$. Recall that $A = \sum_{v'v \in E(T_1)} \phi(T_1 - v' - v)$. We have $(-1)^k\, g_k \geq 0$ for $0 \leq k \leq \lfloor (n_1-1)/2 \rfloor$. Thus, $a_0 - a'_0 = 0$, $(-1)^\ell\,(a_\ell - a'_\ell) \geq 0$ for $1 \leq \ell \leq \lfloor n/2 \rfloor$, and there is an ℓ $(1 \leq \ell \leq \lfloor n/2 \rfloor)$, such that $(-1)^\ell\,(a_\ell - a'_\ell) > 0$. We have $T \succ T'$, which implies $\mathscr{E}(T) > \mathscr{E}(T')$.

If $d(u_1, v_1) = 3$, then $\phi(T) - \phi(T') = (s-1)(t-1)x^{s+t-2} = (s-1)(t-1)x^{n-4}$. Noting that $s, t \geq 2$, $T' \prec T$, we arrive at $\mathscr{E}(T') < \mathscr{E}(T)$. ■

Let $V_3(T)$ be the set of vertices of T with degrees greater than 2, and let $p(T)$ be the number of pendent paths in T with length greater than 1. If T is a tree of order n with k pendent vertices $(3 \leq k \leq n-2)$, T is not isomorphic to the comet $P_{n,k}$ and $p(T) \neq 0$, then T is the tree depicted in Fig. 4.7. It is easy to see that T' is a tree of order n with k pendent vertices. From Lemma 4.12, we immediately get the following result:

Lemma 4.14. *Let T be a tree of order n with k pendent vertices* $(3 \leq k \leq n-2)$, *$T \ncong P_{n,k}$ and $p(T) \neq 0$.*

(1) If $|V_3(T)| = 1$, a tree T' is obtained by Operation I, such that $\mathscr{E}(T') < \mathscr{E}(T)$ and $p(T') = 1$. Furthermore, $T' \cong P_{n,k}$.
(2) If $|V_3(T)| \geq 2$, a tree T' is obtained by Operation I, such that $\mathscr{E}(T') < \mathscr{E}(T)$, $|V_3(T')| = |V_3(T)|$, and $p(T') = 0$. ■

As an example of application of the two operations, we prove the following results. At first, we prove that $P_{n,k}$ is the tree with minimal energy among all trees of order n with k pendent vertices [511].

Theorem 4.15. *Let T be a tree of order n with k pendent vertices. Then $\mathscr{E}(T) \geq \mathscr{E}(P_{n,k})$, with equality holding if and only if $T \cong P_{n,k}$.*

Proof. Since P_n is the only tree of order n with 2 pendent vertices and $P_n \cong P_{n,2}$, S_n is the only tree of order n with $n-1$ pendent vertices and $S_n \cong P_{n,n-1}$, we may assume that $3 \leq k \leq n-2$, and it is sufficient to show that $\mathscr{E}(T) > \mathscr{E}(P_{n,k})$ for any T of order n with k pendent vertices and $T \ncong P_{n,k}$.

For all T of order n with k pendent vertices ($3 \leq k \leq n-2$) and $T \ncong P_{n,k}$, we know that $1 \leq |V_3(T)| \leq n-k$. We now verify that $\mathscr{E}(T) > \mathscr{E}(P_{n,k})$ by induction on $|V_3(T)|$. When $|V_3(T)| = 1$, noticing that $T \ncong S_n, P_n, P_{n,k}$, by Lemma 4.14 (1), we have $\mathscr{E}(T) > \mathscr{E}(P_{n,k})$. Let $|V_3(T)| = s \geq 2$. Suppose that the result holds for any tree T' with $|V_3(T')| = s-1$. If $p(T) \neq 0$, then by Lemma 4.14 (2), we get a tree T_1, which is also a tree of order n with k pendent vertices, such that $p(T_1) = 0$, $|V_3(T_1)| = s$, and $\mathscr{E}(T) > \mathscr{E}(T_1)$. By Lemma 4.13, we can get a tree T_2 from T_1, which is also a tree of order n with k pendent vertices, such that $p(T_2) = 1$, $|V_3(T_2)| = s-1$, and $\mathscr{E}(T_1) > \mathscr{E}(T_2)$. Hence, $\mathscr{E}(T) > \mathscr{E}(T_1) > \mathscr{E}(T_2)$. By the induction hypothesis, we have $\mathscr{E}(T) > \mathscr{E}(T_1) > \mathscr{E}(T_2) > \mathscr{E}(P_{n,k})$. Therefore, if T is a tree of order n with k pendent vertices, then $\mathscr{E}(T) \geq \mathscr{E}(P_{n,k})$, with equality holding if and only if $T \cong P_{n,k}$. ■

A tree in which there is exactly one vertex of degree greater than 2 is said to be *starlike*. Otherwise, it is *nonstarlike*. Obviously, the number of pendent vertices in a nonstarlike tree of order n is at least 4 and at most $n-2$. Let $\mathbb{T}_{n,k}$ be the class of nonstarlike trees of order n with k pendent vertices, where $4 \leq k \leq n-2$.

For integers n and k, such that $4 \leq k \leq n-2$, let $P_{n,k}^{r,s}(a,b)$ be the tree obtained from the path $P_{n-k+2} = v_1 v_2 \ldots v_{n-k+2}$ by attaching a pendent vertices to vertex v_r and b pendent vertices to v_s, where $2 \leq r < s \leq n-k+1$, $a, b \geq 1$ and $a+b = k-2$. Let $S_n(a+1, b+1) = P_{n,k}^{2,n-k+1}(a,b)$, i.e., $S_n(a+1,b+1)$ is the tree obtained from the path with $n-a-b-2$ vertices by attaching $a+1$ and $b+1$ pendent vertices to its two end vertices, respectively. Let $X_{n,k} = P_{n,k}^{2,n-k+1}(k-3,1) = S_n(k-2,2)$. In the following, we consider the trees in $\mathbb{T}_{n,k}$ [524] and determine the trees with minimal and second-minimal energy for $4 \leq k \leq n-2$ and $n \geq 8$:

Lemma 4.15. *For* $n \geq 9$, $\mathscr{E}\left(P_{n,n-3}^{2,3}(n-6,1)\right) > \mathscr{E}\left(P_{n,n-3}^{2,4}(n-7,2)\right)$.

Proof. Let $T_1 \cong P_{n,n-3}^{2,3}(n-6,1)$ and $T_2 \cong P_{n,n-3}^{2,4}(n-7,2)$. It is easily seen that $m(T_1,2) = 3n-13$, $m(T_1,3) = n-5$, and $m(T_1,i) = 0$ for $i \geq 4$, as well as $m(T_2,2) = 4n-21$ and $m(T_2,j) = 0$ for $j \geq 3$. Note that the eigenvalues of a tree T with n vertices are the n roots of its characteristic polynomial. In our case,

$$\phi(T_1,x) = x^{n-6}\left[x^6 - (n-1)x^4 + (3n-13)x^2 - (n-5)\right]$$
$$\phi(T_2,x) = x^{n-4}\left[x^4 - (n-1)x^2 + (4n-21)\right].$$

Let $\sqrt{a_1}, \sqrt{a_2}, \sqrt{a_3}$ be the positive eigenvalues of T_1, and $\sqrt{b_1}, \sqrt{b_2}$ be the positive eigenvalues of T_2. Then $a_1 + a_2 + a_3 = b_1 + b_2 = n-1$, $a_1 a_2 + a_2 a_3 + a_3 a_1 = 3n-13$, $a_1 a_2 a_3 = n-5$, and $b_1 b_2 = 4n-21$. We have

$$\left[\frac{\mathscr{E}(T_1)}{2}\right]^2 = \left(\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3}\right)^2$$
$$= a_1 + a_2 + a_3 + 2\left(\sqrt{a_1 a_2} + \sqrt{a_2 a_3} + \sqrt{a_3 a_1}\right)$$

$$= n - 1 + 2\sqrt{a_1 a_2 + a_2 a_3 + a_3 a_1 + 2\sqrt{a_1 a_2 a_3}\left(\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3}\right)}$$
$$= n - 1 + 2\sqrt{3n - 13 + \sqrt{n-5}\,\mathscr{E}(T_1)}$$

$$\left[\frac{\mathscr{E}(T_2)}{2}\right]^2 = \left(\sqrt{b_1} + \sqrt{b_2}\right)^2 = b_1 + b_2 + 2\sqrt{b_1 b_2} = n - 1 + 2\sqrt{4n-21}.$$

It is now easily seen that $\mathscr{E}(T_1) > \mathscr{E}(T_2)$ is equivalent to $n - 8 < \sqrt{n-5}\,\mathscr{E}(T_1)$, i.e., $\mathscr{E}(T_1) > (n-8)/\sqrt{n-5}$, which is obviously true because by Theorem 4.6, $\mathscr{E}(T_1) > \mathscr{E}(S_n) = 2\sqrt{n-1} > (n-8)/\sqrt{n-5}$. ■

For integers n and k with $3 \leq k \leq n-2$, let $P^r_{n,k}$ be the tree formed from the path $P_{n-k+2} = v_1 v_2 \ldots v_{n-k+2}$ by attaching $k-2$ pendent vertices to vertex v_r, where $2 \leq r \leq \lfloor (n-k+2)/2 \rfloor$.

For a tree T with diameter at least 3, if Operation I cannot be applied to T, then Operation II may be applied, resulting in a tree T'. When the diameter of T' is at least 4 and $|V_3(T')| \geq 2$, then Operation II may be applied to T'.

Theorem 4.16. *For integers n and k with* $4 \leq k \leq n-2$, $X_{n,k}$ *is the unique tree with minimal energy in* $\mathbb{T}_{n,k}$.

Proof. Let $T \in \mathbb{T}_{n,k}$ with $T \ncong X_{n,k}$. We prove that $T \succ X_{n,k}$.

Note that $|V_3(T)| \geq 2$. If $|V_3(T)| \geq 3$ or $|V_3(T)| = 2$ and $p(T) \geq 1$, then by applying Operations I and II to T and by Lemma 4.13, we get a tree $T' \in \mathbb{T}_{n,k}$, such that $|V_3(T')| = 2$, $p(T') = 0$, and $T \succ T'$. Assume that $|V_3(T)| = 2$ and $p(T) = 0$. Then T is a tree $S_n(a,b)$ with $a \geq b \geq 3$ and $a + b = k$.

Claim. $S_n(a,b) \succ S_n(a+1, b-1)$ for $a \geq b \geq 3$.

If $a + b = n - 2$, then this follows easily. Suppose that $a + b \leq n - 3$. By Lemma 4.4, we have

$$m\left(S_n(a,b), i\right) = m\left(S_{n-1}(a,b-1), i\right) + m\left(P^2_{n-b-1,a+1}, i-1\right)$$
$$m\left(S_n(a+1,b-1), i\right) = m\left(S_{n-1}(a,b-1), i\right) + m\left(P^2_{n-a-2,b}, i-1\right).$$

Since $P^2_{n-a-2,b}$ is a proper subgraph of $P^2_{n-b-1,a+1}$ for $a \geq b$,

$$m\left(P^2_{n-b-1,a+1}, i-1\right) \geq m\left(P^2_{n-a-2,b}, i-1\right)$$

and then $m\left(S_n(a,b), i\right) \geq m\left(S_n(a+1,b-1), i\right)$ for all $i \geq 0$, and it is strict for $i = 2$. This proves the Claim.

By the Claim, $T \succ S_n(k-2, 2) \cong X_{n,k}$. ■

By similar method, the tree with second-minimal energy in $\mathbb{T}_{n,k}$ for $4 \leq k \leq n-2$ was also determined in [524]. Some similar operations of comparing the energies of graphs were considered by Shao et al. [432, 433]. We omit the details.

4.6 Method 6: Coalescence of Two Graphs

We first introduce Ky Fan's theorem on matrices, from which we will deduce two methods: the coalescence of two graphs and the edge deletion (outlined in the subsequent section).

Let $\mathbf{X}$ be an $n \times n$ complex matrix and denote its singular values by $s_1(\mathbf{X}) \geq s_2(\mathbf{X}) \geq \cdots \geq s_n(\mathbf{X}) \geq 0$. If $\mathbf{X}$ has real eigenvalues only, denote its eigenvalues by $\lambda_1(\mathbf{X}) \geq \lambda_2(\mathbf{X}) \geq \cdots \geq \lambda_n(\mathbf{X})$. Nikiforov [383] came to the important and far-reaching idea to define the energy of the matrix $\mathbf{X}$ as

$$\mathscr{E}(\mathbf{X}) = \sum_i s_i(\mathbf{X}) .$$

The Ky Fan's theorem is stated as follows. This inequality is well known, and there are at least four different proofs in the literature; for details, see [31, 60, 108, 459].

Theorem 4.17. *Let* $\mathbf{A}$, $\mathbf{B}$, *and* $\mathbf{C}$ *be square matrices of order* n, *such that* $\mathbf{A}+\mathbf{B}=\mathbf{C}$. *Then*

$$\sum_{i=1}^{n} s_i(\mathbf{A}) + \sum_{i=1}^{n} s_i(\mathbf{B}) \geq \sum_{i=1}^{n} s_i(\mathbf{C}) .$$

Equality holds if and only if there exists an orthogonal matrix $\mathbf{P}$, *such that* $\mathbf{PA}$ *and* $\mathbf{PB}$ *are both positive semidefinite.* ■

From Theorem 4.17, we immediately conclude that the energies of graphs $G_{\mathbf{A}}$, $G_{\mathbf{B}}$, and $G_{\mathbf{C}}$, whose adjacency matrices satisfy the condition $\mathbf{A}(G_{\mathbf{A}}) + \mathbf{A}(G_{\mathbf{B}}) = \mathbf{A}(G_{\mathbf{C}})$, are related as $\mathscr{E}(G_{\mathbf{A}}) + \mathscr{E}(G_{\mathbf{B}}) \geq \mathscr{E}(G_{\mathbf{C}})$. Some special cases of this inequality are stated in the following corollaries [441]:

Corollary 4.1. *Let* G *be a graph of order* n *and* $\overline{G}$ *be its complement. Then* $\mathscr{E}(G) + \mathscr{E}(\overline{G}) \geq 2(n-1)$. *Equality holds if and only if either* $G \cong K_n$ *or* $G \cong \overline{K_n}$.

Proof. The inequality follows by observing that $\mathbf{A}(G) + \mathbf{A}(\overline{G}) = \mathbf{A}(K_n)$ and $\mathscr{E}(K_n) = 2(n-1)$. In order to establish conditions for equality, assume that the eigenvalues of G are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and $m(G)$ is the number of edges of G. Then

$$\mathscr{E}(G) + \mathscr{E}(\overline{G}) \geq 2\lambda_1(G) + 2\lambda_1(\overline{G}) \geq 2\frac{2m(G)}{n} + 2\frac{2m(\overline{G})}{n} = \frac{4}{n}\binom{n}{2} = 2n-2 .$$

Equality is possible if and only if G is regular, $\mathscr{E}(G) = 2\lambda_1(G)$, and $\mathscr{E}(\overline{G}) = 2\lambda_1(\overline{G})$. If so, then it must be $\lambda_2(G) \leq 0$ and $\lambda_2(\overline{G}) \leq 0$ (because the energy of a graph is equal to twice the sum of the positive eigenvalues). In other words, equality is attained if and only if both G and $\overline{G}$ have at most one positive eigenvalue. Then we have to separately consider the following three cases:

(i) G has no positive eigenvalue, i.e., $G \cong \overline{K_n}$.
(ii) $\overline{G}$ has no positive eigenvalue, i.e., $\overline{G} \cong \overline{K_n}$, which implies $G \cong K_n$.
(iii) Both G and $\overline{G}$ have exactly one positive eigenvalue. Then, by Smith's theorem [439], both G and $\overline{G}$ would be complete multipartite graphs. This is impossible because complete multipartite graphs are connected, whereas their complements are disconnected. ■

Corollary 4.2. *Let B be a bipartite graph whose two partitions have a and b vertices, respectively, and $\overline{B}$ be its bipartite complement, i.e., $\mathbf{A}(B) + \mathbf{A}(\overline{B}) = \mathbf{A}(K_{a,b})$. Then $\mathscr{E}(B) + \mathscr{E}(\overline{B}) \geq 2\sqrt{ab}$. Equality holds if and only if either $B \cong K_{a,b}$ or $B \cong \overline{K_{a+b}}$.* ■

So et al. [441] proved the following result, from which one can construct some graphs whose energy has many interesting properties. Let G and H be two graphs with disjoint vertex sets, and $u \in G$ and $v \in H$. Construct a new graph $G \circ H$ from copies of G and H by identifying the vertices u and v. Thus $|V(G \circ H)| = |V(G)| + |V(H)| - 1$. The graph $G \circ H$ is known as the *coalescence* of G and H with respect to u and v.

The following lemma appears as an exercise in [265] (Sect. 7.1, Exercise 2):

Lemma 4.16. *If $\mathbf{A} = [a_{ij}]$ is a positive semidefinite matrix and $a_{ii} = 0$ for some i, then $a_{ji} = a_{ij} = 0$ for all j.* ■

Theorem 4.18. *Let G, H, and $G \circ H$ be graphs as specified above. Then*

$$\mathscr{E}(G \circ H) \leq \mathscr{E}(G) + \mathscr{E}(H) . \tag{4.29}$$

Equality is attained if and only if either u is an isolated vertex of G or v is an isolated vertex of H or both.

Proof. By an appropriate labeling of the vertices of the graphs G and H, the adjacency matrix of $G \circ H$ assumes the form

$$\mathbf{A} = \mathbf{A}(G \circ H) = \begin{bmatrix} \mathbf{R} & \mathbf{x} & \mathbf{0} \\ \mathbf{x}^{\mathrm{T}} & \mathbf{0} & \mathbf{y}^{\mathrm{T}} \\ \mathbf{0} & \mathbf{y} & \mathbf{S} \end{bmatrix} = \begin{bmatrix} \mathbf{R} & \mathbf{x} & \mathbf{0} \\ \mathbf{x}^{\mathrm{T}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{y}^{\mathrm{T}} \\ \mathbf{0} & \mathbf{y} & \mathbf{S} \end{bmatrix} = \mathbf{B} + \mathbf{C}$$

where $\mathbf{R} = \mathbf{A}(G - u)$ and $\mathbf{S} = \mathbf{A}(H - v)$ and where x is the column vector corresponding to the vertex u in G, and y is the column vector corresponding to the vertex v in H.

Inequality (4.29) follows now immediately from Theorem 4.17.

For the equality case, it is straightforward to check that the condition is sufficient because either $\mathbf{x}$ or $\mathbf{y}$ is a zero vector.

For the necessity part, the equality in (4.29) implies the equality in the singular value inequality. By the equality case of Theorem 4.17, there exists an orthogonal matrix $\mathbf{P}$, such that both $\mathbf{PB}$ and $\mathbf{PC}$ are positive semidefinite. Now let $\mathbf{P}$ be partitioned according to the matrix $\mathbf{A}(G \circ H)$ as follows:

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} & \mathbf{P}_{13} \\ \mathbf{P}_{21} & \mathbf{P}_{22} & \mathbf{P}_{23} \\ \mathbf{P}_{31} & \mathbf{P}_{32} & \mathbf{P}_{33} \end{bmatrix} .$$

Then $\mathbf{P}^{\mathrm{T}}\mathbf{P} = \mathbf{I}_n$ implies that

$$\mathbf{P}_{11}^{\mathrm{T}}\mathbf{P}_{11} + \mathbf{P}_{21}^{\mathrm{T}}\mathbf{P}_{21} + \mathbf{P}_{31}^{\mathrm{T}}\mathbf{P}_{31} = \mathbf{I} \tag{4.30}$$

$$\mathbf{P}_{13}^{\mathrm{T}}\mathbf{P}_{13} + \mathbf{P}_{23}^{\mathrm{T}}\mathbf{P}_{23} + \mathbf{P}_{33}^{\mathrm{T}}\mathbf{P}_{33} = \mathbf{I} \tag{4.31}$$

$$\mathbf{P}_{11}^{\mathrm{T}}\mathbf{P}_{13} + \mathbf{P}_{21}^{\mathrm{T}}\mathbf{P}_{23} + \mathbf{P}_{31}^{\mathrm{T}}\mathbf{P}_{33} = \mathbf{0} \tag{4.32}$$

where $\mathbf{I}$ denotes an identity matrix of appropriate size. Note that both

$$\mathbf{PB} = \begin{bmatrix} \mathbf{P}_{11}\mathbf{R} + \mathbf{P}_{12}\mathbf{x}^{\mathrm{T}} & \mathbf{P}_{11}\mathbf{x} & \mathbf{0} \\ \mathbf{P}_{21}\mathbf{R} + \mathbf{P}_{22}\mathbf{x}^{\mathrm{T}} & \mathbf{P}_{21}\mathbf{x} & \mathbf{0} \\ \mathbf{P}_{31}\mathbf{R} + \mathbf{P}_{32}\mathbf{x}^{\mathrm{T}} & \mathbf{P}_{31}\mathbf{x} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \mathbf{PC} = \begin{bmatrix} \mathbf{0} & \mathbf{P}_{13}\mathbf{y} & \mathbf{P}_{12}\mathbf{y}^{\mathrm{T}} + \mathbf{P}_{13}\mathbf{S} \\ \mathbf{0} & \mathbf{P}_{23}\mathbf{y} & \mathbf{P}_{22}\mathbf{y}^{\mathrm{T}} + \mathbf{P}_{23}\mathbf{S} \\ \mathbf{0} & \mathbf{P}_{33}\mathbf{y} & \mathbf{P}_{32}\mathbf{y}^{\mathrm{T}} + \mathbf{P}_{33}\mathbf{S} \end{bmatrix}$$

are positive semidefinite, and so by symmetry $\mathbf{P}_{31}\mathbf{x} = \mathbf{0}$ and $\mathbf{P}_{13}\mathbf{y} = \mathbf{0}$. Now, multiplying Eq. (4.32) by $\mathbf{x}^{\mathrm{T}}$ from the left and $\mathbf{y}$ from the right, we obtain

$$(\mathbf{P}_{21}\mathbf{x})^{\mathrm{T}}(\mathbf{P}_{23}\mathbf{y}) = \mathbf{x}^{\mathrm{T}}\mathbf{P}_{11}^{\mathrm{T}}\mathbf{P}_{13}\mathbf{y} + \mathbf{x}^{\mathrm{T}}\mathbf{P}_{21}^{\mathrm{T}}\mathbf{P}_{23}\mathbf{y} + \mathbf{x}^{\mathrm{T}}\mathbf{P}_{31}^{\mathrm{T}}\mathbf{P}_{33}\mathbf{y} = \mathbf{0} .$$

Hence, one of the two scalars $(\mathbf{P}_{21}\mathbf{x})^{\mathrm{T}}$ and $(\mathbf{P}_{23}\mathbf{y})$ must be zero.

Case 1. $\mathbf{P}_{21}\mathbf{x} = \mathbf{0}$.

Note that $\mathbf{P}_{21}\mathbf{x}$ is a diagonal entry of the positive semidefinite matrix $\mathbf{PB}$. It follows that the entire column where $\mathbf{P}_{21}\mathbf{x}$ belongs is zero, and so $\mathbf{P}_{11}\mathbf{x} = \mathbf{0}$. Finally, from Eq. (4.30), $\mathbf{x}^{\mathrm{T}}\mathbf{x} = \mathbf{x}^{\mathrm{T}}\mathbf{P}_{11}^{\mathrm{T}}\mathbf{P}_{11}\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{P}_{21}^{\mathrm{T}}\mathbf{P}_{21}\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{P}_{31}^{\mathrm{T}}\mathbf{P}_{31}\mathbf{x} = 0 + 0 + 0 = 0$, i.e., $\mathbf{x} = \mathbf{0}$. This means that u is an isolated vertex of G.

Case 2. $\mathbf{P}_{23}\mathbf{y} = 0$.

Similarly as in Case 1, we prove that v is an isolated vertex of H. ∎

Corollary 4.3. *Let G, H, and $G \circ H$ be graphs as specified above. If G is strongly hypoenergetic and H is hypoenergetic (or vice versa), then $G \circ H$ is hypoenergetic.* ∎

4.7 Method 7: Edge Deletion

In this section we are concerned with the problem of how the energy of a graph changes when some of its edges are deleted. Day and So [94, 95] first studied this topic (see also [223, 432, 433]).

We start with some preparations.

The inequality in the next lemma is a special case of a more general inequality from [458]. The equality case is elaborated in [95]. More details are found in [31, 265].

Lemma 4.17. *For a partitioned matrix* $\mathbf{C} = \begin{bmatrix} \mathbf{A} & \mathbf{X} \\ \mathbf{Y} & \mathbf{B} \end{bmatrix}$ *where both* $\mathbf{A}$ *and* $\mathbf{B}$ *are square matrices, we have*

$$\sum_j s_j(\mathbf{A}) + \sum_j s_j(\mathbf{B}) \leq \sum_j s_j(\mathbf{C}) .$$

Equality holds if and only if there exist unitary matrices $\mathbf{U}$ *and* $\mathbf{V}$*, such that the matrix* $\begin{bmatrix} \mathbf{UA} & \mathbf{UX} \\ \mathbf{VY} & \mathbf{VB} \end{bmatrix}$ *is positive semidefinite.* ■

Corollary 4.4. *For a partitioned matrix* $\mathbf{C} = \begin{bmatrix} \mathbf{A} & \mathbf{X} \\ \mathbf{Y} & \mathbf{B} \end{bmatrix}$ *where both* $\mathbf{A}$ *and* $\mathbf{B}$ *are square matrices, we have*

$$\sum_j s_j(\mathbf{A}) \leq \sum_j s_j(\mathbf{C}) .$$

Equality holds if and only if $\mathbf{X}$, $\mathbf{Y}$, *and* $\mathbf{B}$ *are all zero matrices.* ■

Theorem 4.19. *Let* H *be an induced subgraph of a simple graph* $G = (V(G), E(G))$*. Then, (1)* $\mathscr{E}(H) \leq \mathscr{E}(G)$*, and equality holds if and only if* $E(H) = E(G)$*. (2)* $\mathscr{E}(G) - \mathscr{E}(H) \leq \mathscr{E}(G - E(H)) \leq \mathscr{E}(G) + \mathscr{E}(H)$*. Moreover, (i) if* H *is nonsingular (the adjacency matrix of* H *is nonsingular), then the left equality holds if and only if* $G = H \cup (G - H)$*; (ii) the right equality holds if and only if* $E(H) = \emptyset$*.*

Proof. For (1), apply Corollary 4.4 to the adjacency matrix

$$\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{X} \\ \mathbf{X}^{\mathrm{T}} & \mathbf{A}(G - H) \end{bmatrix}$$

where $\mathbf{X}$ represents edges connecting H and $G - H$.

For (2), note that

$$\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G - H) \end{bmatrix} = \begin{bmatrix} \mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G - H) \end{bmatrix} \tag{4.33}$$

where X represents the edges connecting H and $G - H$. By applying Theorem 4.17 to Eq. (4.33), we have $\mathscr{E}(G) \leq \mathscr{E}(H) + \mathscr{E}(G - E(H))$, which gives the left inequality. On the other hand,

$$\mathbf{A}(G - E(H)) = \mathbf{A}(G) + \begin{bmatrix} -\mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}. \tag{4.34}$$

Again, by applying Theorem 4.17 to Eq. (4.34), we have $\mathscr{E}(G - E(G)) \leq \mathscr{E}(G) + \mathscr{E}(H)$, which gives the right inequality.

(i) Assume that $\mathbf{A}(H)$ is a nonsingular matrix. For the sufficiency part, let $G \cong H \cup (G - H)$. Then $\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{A}(G-H) \end{bmatrix}$, which gives $\mathscr{E}(G) = \mathscr{E}(H) + \mathscr{E}(G - H)$. On the other hand, if the left inequality becomes equality then, by applying Theorem 4.17 to Eq. (4.33), there exists an orthogonal matrix $\mathbf{P} = \begin{bmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} \\ \mathbf{P}_{21} & \mathbf{P}_{22} \end{bmatrix}$ such that both $\mathbf{P}\begin{bmatrix} \mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$ and $\mathbf{P}\begin{bmatrix} \mathbf{0} & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G-H) \end{bmatrix}$ are positive semidefinite. The symmetry of

$$\begin{bmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} \\ \mathbf{P}_{21} & \mathbf{P}_{22} \end{bmatrix}\begin{bmatrix} \mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{P}_{11}\mathbf{A}(H) & \mathbf{0} \\ \mathbf{P}_{21}\mathbf{A}(H) & \mathbf{0} \end{bmatrix}$$

gives $\mathbf{P}_{21}\mathbf{A}(H) = \mathbf{0}$, and so $\mathbf{P}_{21} = \mathbf{0}$ because of the nonsingularity of $\mathbf{A}(H)$. Since $\mathbf{P}$ is an orthogonal matrix, it follows that $\mathbf{P}_{12} = \mathbf{0}$, and so $\mathbf{P}_{11}$ is nonsingular. Therefore,

$$\mathbf{P}\begin{bmatrix} \mathbf{0} & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G-H) \end{bmatrix} = \begin{bmatrix} \mathbf{P}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{P}_{22} \end{bmatrix}\begin{bmatrix} \mathbf{0} & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G-H) \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{P}_{11}\mathbf{X}^{\mathrm{T}} \\ \mathbf{P}_{22}\mathbf{X} & \mathbf{P}_{22}\mathbf{A}(G-H) \end{bmatrix}.$$

Since this matrix is positive semidefinite with a zero diagonal block, by Lemma 4.16, $\mathbf{P}_{11}\mathbf{X}^{\mathrm{T}} = \mathbf{0}$. Hence, $\mathbf{X}^{\mathrm{T}} = \mathbf{0}$ because of the nonsingularity of $\mathbf{P}_{11}$. Finally $\mathbf{X} = \mathbf{0}$ implies that $G \cong H \cup (G - H)$.

(ii) For the sufficiency part, let $E(H) = \emptyset$. Then $G - E(H) \cong G$ and $\mathscr{E}(H)$=0. Hence, $\mathscr{E}(G - E(H)) = \mathscr{E}(G) = \mathscr{E}(G) + \mathscr{E}(H)$. For the necessity part, assume that the right-hand-sided inequality becomes an equality, i.e., $\mathscr{E}(G - E(H)) = \mathscr{E}(G) + \mathscr{E}(H)$. By applying Theorem 4.17 to Eq. (4.34), there exists an orthogonal matrix $\mathbf{Q} = \begin{bmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} \end{bmatrix}$ such that both $\mathbf{Q}\begin{bmatrix} -\mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$ and $\mathbf{Q}\begin{bmatrix} \mathbf{A}(H) & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G-H) \end{bmatrix}$ are positive semidefinite. We want to show that $E(H) = \emptyset$. Suppose that the opposite is true, i.e., that $\mathbf{A}(H)$ is nonzero.

Case 3. Suppose that $\mathbf{A}(H)$ is nonsingular. As in the proof of (i), it follows that $\mathbf{Q}_{21} = \mathbf{0}$ because $\mathbf{A}(H)$ is nonsingular, and then $\mathbf{Q}_{12} = \mathbf{0}$ because $\mathbf{Q}$ is orthogonal. Hence, $\mathbf{Q}$ is block diagonal. Therefore, $\mathbf{Q}_{11}\mathbf{A}(H)$ and $-\mathbf{Q}_{11}\mathbf{A}(H)$ are both positive semidefinite, so $\mathbf{Q}_{11}\mathbf{A}(H)$ must be $\mathbf{0}$. This, however, implies $\mathbf{A}(H) = \mathbf{0}$ since $\mathbf{Q}_{11}$ is orthogonal. This leads to a contradiction because $\mathbf{A}(H)$ is nonsingular.

Case 4. Suppose that $\mathbf{A}(H)$ is singular (but nonzero). Since it is symmetric and nonzero, there exist an orthogonal $\mathbf{R}_1$ and a nonsingular symmetric $\mathbf{A}_1$ such that $\mathbf{A}(H) = \mathbf{R}_1 \begin{bmatrix} \mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{R}_1^{\mathrm{T}}$. Let $\mathbf{A}(H)$ be $(n-p)\times(n-p)$ and define $\mathbf{R} = \begin{bmatrix} \mathbf{R}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_p \end{bmatrix}$. Since both

$$\mathbf{Q}\begin{bmatrix} -\mathbf{A}(H) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \qquad \text{and} \qquad \mathbf{Q}\begin{bmatrix} \mathbf{A}(H) & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{A}(G-H) \end{bmatrix}$$

are positive semidefinite, it follows that both

$$\mathbf{R}^{\mathrm{T}}\mathbf{Q}\mathbf{R}\begin{bmatrix} -\mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \qquad \text{and} \qquad \mathbf{R}^{\mathrm{T}}\mathbf{Q}\mathbf{R}\begin{bmatrix} \mathbf{A}_1 & \mathbf{X}_1^{\mathrm{T}} \\ \mathbf{X}_1 & \mathbf{Y}_1 \end{bmatrix}$$

are also positive semidefinite. This cannot happen, by Case 3, because $\mathbf{A}_1$ is nonsingular and $\mathbf{R}^{\mathrm{T}}\mathbf{Q}\mathbf{R}$ is orthogonal. ■

Example 4.3. Let C_4 be the cycle with four vertices. Deleting any edge leaves the path P_4. P_4 is not an induced subgraph of C_4, and $\mathscr{E}(C_4) = 4 < 2\sqrt{5} = \mathscr{E}(P_4)$. ■

This example shows that the conclusion of Theorem 4.19(1) may not be true if H is not an induced subgraph.

Theorem 4.20. *(1) If F is an edge cut of a simple graph G, then $\mathscr{E}(G-F) \leq \mathscr{E}(G)$. (2) Let H be a subgraph of G and F, the edge cut between $G-H$ and H. Suppose that F is not empty and that all edges in F are incident to one and only one vertex in H, i.e., the edges in F form a star. Then $\mathscr{E}(G-F) < \mathscr{E}(G)$.*

Proof. For (1), since F is an edge cut of G, $G - F \cong H \cup K$, where H and K are two complementary induced subgraphs of G. Apply Lemma 4.17 to $\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{X} \\ \mathbf{X}^{\mathrm{T}} & \mathbf{A}(K) \end{bmatrix}$ to obtain the desired conclusion.

For (2), note that $G - F \cong H \cup K$ and that the edges of G can be ordered so that $\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{X} \\ \mathbf{X}^{\mathrm{T}} & \mathbf{A}(K) \end{bmatrix}$, where $\mathbf{A}(H)$ is of dimension $r \times r$, $\mathbf{A}(K)$ is of dimension $(n-r)\times(n-r)$, and $\mathbf{X}$ is of dimension $r \times (n-r)$ with all entries equal to 0 except the first column x_1 of $\mathbf{X}$, which is nonzero. By the above point (1), $\mathscr{E}(G-F) \leq \mathscr{E}(G)$.

Suppose that $\mathscr{E}(G-F) = \mathscr{E}(G)$. According to the equality case of Lemma 4.17, there exist orthogonal matrices $\mathbf{U}$ and $\mathbf{V}$, such that

$$\begin{bmatrix} \mathbf{U}\mathbf{A}(H) & \mathbf{U}\mathbf{X} \\ \mathbf{V}\mathbf{X}^{\mathrm{T}} & \mathbf{V}\mathbf{A}(K) \end{bmatrix} \tag{4.35}$$

is positive semidefinite. From (4.35), symmetry implies $(\mathbf{UX})^{\mathrm{T}} = \mathbf{VX}^{\mathrm{T}}$. Using the special structure of $\mathbf{X}$, it follows that $\mathbf{V} = \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_1 \end{bmatrix}$ where $\mathbf{V}_1$ is orthogonal and α is a scalar with $|\alpha| = 1$. Again, from (4.35), it follows that $\mathbf{VA}(K)$ is positive semidefinite. Write $\mathbf{A}(K) = \begin{bmatrix} \mathbf{0} & \mathbf{y}^{\mathrm{T}} \\ \mathbf{y} & \mathbf{K}_1 \end{bmatrix}$. Then $\mathbf{VA}(K) = \begin{bmatrix} \mathbf{0} & \alpha\mathbf{y}^{\mathrm{T}} \\ \mathbf{V}_1\mathbf{y} & \mathbf{V}_1\mathbf{K}_1 \end{bmatrix}$. Because the $(1,1)$-entry of $\mathbf{VA}(K)$ is zero and α is not zero, as in the proof of Corollary 4.4, we have $\alpha\mathbf{y}^{\mathrm{T}} = \mathbf{0}$, and hence $\mathbf{y} = \mathbf{0}$. Consequently, $\mathbf{A}(K) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_1 \end{bmatrix}$; hence, $\mathbf{A}(G) = \begin{bmatrix} \mathbf{A}(H) & \mathbf{x}_1 & \mathbf{0} \\ \mathbf{x}_1^{\mathrm{T}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K}_1 \end{bmatrix}$. Now calculate

$$\begin{aligned} \sum_j s_j(\mathbf{A}(H)) + \sum_j s_j(\mathbf{K}_1) &= \sum_j s_j(\mathbf{A}(H)) + \sum_j s_j(\mathbf{A}(K)) = \mathscr{E}(H) + \mathscr{E}(K) \\ &= \mathscr{E}(G - F) = \mathscr{E}(G) \\ &= \sum_j s_j\left(\begin{bmatrix} \mathbf{A}(H) & \mathbf{x}_1 \\ \mathbf{x}_1^{\mathrm{T}} & \mathbf{0} \end{bmatrix}\right) + \sum_j s_j(\mathbf{K}_1)\,. \end{aligned}$$

Hence, $\sum_j s_j\left(\begin{bmatrix} \mathbf{A}(H) & \mathbf{x}_1 \\ \mathbf{x}_1^{\mathrm{T}} & \mathbf{0} \end{bmatrix}\right) = \sum_j s_j(\mathbf{A}(H))$. By Corollary 4.4, $\mathbf{x}_1 = \mathbf{0}$, and therefore F would be empty, a contradiction. ■

It is interesting to characterize the equality case of Theorem 4.20(1). Using (4.35), it is equivalent to the existence of orthogonal matrices $\mathbf{U}$ and $\mathbf{V}$ for which $\mathbf{A}(G) = \begin{bmatrix} \mathbf{UA}(H) & \mathbf{UX} \\ \mathbf{VX}^{\mathrm{T}} & \mathbf{VA}(K) \end{bmatrix}$ is positive semidefinite. Unfortunately, this condition does not correspond to any known graph theoretical interpretation. Nonetheless, we give a sufficient (but not necessary) condition and a necessary (but not sufficient) condition.

Example 4.4. For $n \geq 2$, let $G(n,n)$ be the graph consisting of two copies of the complete graph K_n on n vertices with n parallel edges between them. If F is the set of the n parallel edges, then F is an edge cut of $G(n,n)$. Note that $\mathrm{Spec}(G(n,n)) = \{n, n-2, 0^{n-1}, (-2)^{n-1}\}$. Hence, $\mathscr{E}(G(n,n)) = 4n - 4 = E(K_n \cup K_n) = \mathscr{E}(G(n,n) - F)$. ■

In the following, by using Theorems 4.19 and 4.20, we give some bounds for graph energy and some further results. Actually, some approaches to find a graph G and an edge set F satisfying $\mathscr{E}(G) = \mathscr{E}(G - F)$ are discussed in Chap. 8.

Since G has at least one edge, the complete graph K_2 on two vertices is an induced subgraph of G. Then Theorem 4.19 implies $\mathscr{E}(G) \geq \mathscr{E}(K_2) = 2$, which improves a result in [26, Corollary 5.6]: $\mathscr{E}(G) > 1$ for any graph G with at least one edge.

Corollary 4.5. *For any simple graph G with at least one edge, $\mathscr{E}(G) \geq 2$.* ■

The following corollary gives a sufficient condition for graph energy to decrease when an edge is deleted. By taking $F = \{e\}$ in Theorem 4.20 (2), we get:

Corollary 4.6. *If $\{e\}$ is a cut edge (or a bridge) of a simple graph G, then $\mathscr{E}(G - e) < \mathscr{E}(G)$. In particular, for any edge e of a tree T, $\mathscr{E}(T - e) < \mathscr{E}(T)$.* ■

By Theorems 4.19 and 4.20 (1), we have:

Corollary 4.7. *Let e be an edge of a graph G. Then the subgraph with the edge set $\{e\}$ is induced and nonsingular. Hence, $\mathscr{E}(G) - 2 \leq \mathscr{E}(G - \{e\}) \leq \mathscr{E}(G) + 2$. Moreover, (i) the left equality holds if and only if e is an isolated edge of G, (ii) equality on the right-hand side never holds.* ■

By a repeated application of Corollary 4.7 to all edges of an (n, m)-graph, one arrives at [441]

$$\mathscr{E}(G) \leq 2m$$

with equality if and only if G consists of m isolated edges and $n - 2m$ isolated vertices, which is also a well-known upper bound (see Theorem 5.2). Similarly, by a repeated application of Corollary 4.7 to all edges of an (n, m)-graph, except to those that are incident to a vertex with maximum degree, we obtain [441]:

Corollary 4.8. *Let Δ be the maximum degree of an (n, m)-graph G. Then*

$$\mathscr{E}(G) \leq 2m - 2\left(\Delta - \sqrt{\Delta}\right). \tag{4.36}$$

Equality in (4.36) holds if and only if G is a union of the star $S_{\Delta+1}$, $m - \Delta$ isolated edges, and $n - 2m + \Delta - 1$ isolated vertices. ■

In an analogous manner, we also get the following upper bounds for energy [441]:

Corollary 4.9. *If G is a connected (n, m)-graph and T is its spanning tree, then $\mathscr{E}(G) \leq 2(m - n + 1) + \mathscr{E}(T)$. If $G \not\cong T$, then the inequality is strict.* ■

Corollary 4.10. *If G is a Hamiltonian (n, m)-graph, then $\mathscr{E}(G) \leq 2(m - n) + \mathscr{E}(C_n)$, where C_n stands for a Hamiltonian cycle of G. If $G \not\cong C_n$, then the inequality is strict.* ■

Some other results on energy related to the existence of Hamiltonian paths and cycles are reported in [321].

Corollary 4.11. *If d is the diameter of a connected graph G, then $\mathscr{E}(G) \leq 2(m - d) + \mathscr{E}(P_{d+1})$. If $G \not\cong P_{d+1}$, then the inequality is strict.* ■

In connection with Theorem 4.19, Yan and Zhang [499] obtained an interesting result. Given two graphs G and H whose vertex and edge sets need not be disjoint, denote $\Delta(G,H) = |E(G)| + |E(H)| - 2|E(G) \cap E(H)|$. In other words, $\Delta(G,H)$ is equal to the number of edges in the symmetric difference of $E(G)$ and $E(H)$.

Theorem 4.21. *Suppose that* $\{G_n\}$ *and* $\{H_n\}$ *are two sequences of graphs such that* $\lim_{n\to\infty} \frac{\Delta(G_n,H_n)}{\mathscr{E}(G_n)} = 0$. *Then*

$$\lim_{n\to\infty} \frac{\mathscr{E}(H_n)}{\mathscr{E}(G_n)} = 1 .$$

Proof. Let F_n be the subgraph of G_n or H_n induced by $E(G_n) \cap E(H_n)$. Note that

$$\left|\frac{\mathscr{E}(H_n)}{\mathscr{E}(G_n)} - 1\right| = \left|\frac{\mathscr{E}(H_n) - \mathscr{E}(G_n)}{\mathscr{E}(G_n)}\right| = \left|\frac{\mathscr{E}(H_n) - \mathscr{E}(F_n) + \mathscr{E}(F_n) - \mathscr{E}(G_n)}{\mathscr{E}(G_n)}\right|$$
$$\leq \left|\frac{\mathscr{E}(G_n) - \mathscr{E}(F_n)}{\mathscr{E}(G_n)}\right| + \left|\frac{\mathscr{E}(H_n) - \mathscr{E}(F_n)}{\mathscr{E}(G_n)}\right| .$$

Since $\mathscr{E}(G) \leq 2|E(G)|$, by Theorem 4.19, $\mathscr{E}(G_n) - \mathscr{E}(F_n) \leq \mathscr{E}(G_n - E(F_n)) \leq 2(|E(G_n)| - |E(F_n)|)$ and $\mathscr{E}(H_n) - \mathscr{E}(F_n) \leq \mathscr{E}(H_n - E(F_n)) \leq 2(|E(H_n)| - |E(F_n)|)$. Hence,

$$\left|\frac{\mathscr{E}(H_n)}{\mathscr{E}(G_n)} - 1\right| \leq \frac{2\Delta(G_n,H_n)}{\mathscr{E}(G_n)}$$

which implies the theorem. ■

Concluding this section, we answer to several open questions on graph energy:

Question 1 ([50]). (a) Do there exist graphs such that removing any one edge increases the energy? (b) If e is an edge of a connected graph G, such that $\mathscr{E}(G) = \mathscr{E}(G - \{e\}) + 2$, then is it true that $G \cong K_2$?

Answer. (a) The complete bipartite graph $K_{n,n}$ ($n \geq 1$), which includes the cycle with four vertices C_4 , possesses this property. It would be interesting to characterize all such graphs. (b) Yes. By (i) of Corollary 4.7, e is an isolated edge. Since G is connected, $G \cong K_2$.

Question 2 ([50]). Let G'' be a spanning subgraph of a graph G. When does the inequality $\mathscr{E}(G'') \leq \mathscr{E}(G)$ hold?

Answer. See Theorem 4.20 for a sufficient condition.

Question 3 ([7]). Are there any graphs G such that $\mathscr{E}(G - \{e\}) = \mathscr{E}(G) + 2$?

Answer. No. By (ii) of Corollary 4.7.

Question 4 ([173]). Characterize the graphs G and their edges e for which $\mathscr{E}(G - e) \leq \mathscr{E}(G)$.

Answer. See Corollary 4.6 for a sufficient condition that $\mathscr{E}(G - e) < \mathscr{E}(G)$.

Chapter 5
Bounds for the Energy of Graphs

5.1 Preliminary Bounds

A graph G of order n and size m is called an (n,m)-graph. In what follows we assume that the graph eigenvalues are labeled in a nonincreasing manner, i.e., $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. If G is connected, then $\lambda_1 > \lambda_2$ [81]. Because $\lambda_1 \geq |\lambda_i|$, $i = 2,\ldots,n$, the eigenvalue λ_1 is referred to as the *spectral radius* of G. Three well-known relations for the eigenvalues are

$$\sum_{i=1}^{n} \lambda_i = 0 \tag{5.1}$$

$$\sum_{i=1}^{n} \lambda_i^2 = 2m \tag{5.2}$$

$$\sum_{i<j} \lambda_i \lambda_j = -m\ . \tag{5.3}$$

The following lemma [81] will be frequently used in the proofs:

Lemma 5.1. *G has only one eigenvalue if and only if G is an empty graph. G has two distinct eigenvalues $\mu_1 > \mu_2$ with multiplicities m_1 and m_2 if and only if G is the direct sum of m_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $m_2 = m_1\mu_1$.* ■

Some simplest and longest standing bounds [53, 173, 368] for the energy of graphs are given below.

Theorem 5.1 (McClelland [368]). *For an (n,m)-graph G,*

$$\mathscr{E}(G) \leq \sqrt{2mn} \tag{5.4}$$

with equality if and only if G is either an empty graph or a regular graph of degree 1, i.e., $G \cong (n/2)K_2$.

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_5,

Proof. By Cauchy–Schwarz inequality, $\left(\sum_{i=1}^{n}|\lambda_i|\right)^2 \le n\sum_{i=1}^{n}|\lambda_i|^2 = 2mn$. Inequality (5.4) follows directly. Equality holds if and only if $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$. ■

In fact, McClelland [368] proved that Ineq. (5.4) is true for any Hermitian matrix A of order n , provided $m = \frac{1}{2}\sum_{k,\ell}|A_{k\ell}|$.

Theorem 5.2. *For a graph G with m edges,*

$$2\sqrt{m} \le \mathscr{E}(G) \le 2m \, .$$

Equality $\mathscr{E}(G) = 2\sqrt{m}$ *holds if and only if G consists of a complete bipartite graph* $K_{a,b}$ *such that* $a \cdot b = m$ *and arbitrarily many isolated vertices. Equality* $\mathscr{E}(G) = 2m$ *holds if and only if G consists of m copies of* K_2 *and arbitrarily many isolated vertices.*

Proof. If G has isolated vertices, then each isolated vertex results in an eigenvalue equal to zero. Adding isolated vertices to G will thus not change either m or $\mathscr{E}(G)$. From the definition of the energy of graph G, we have

$$\mathscr{E}(G)^2 = \sum_{i=1}^{n}|\lambda_i|^2 + 2\sum_{i<j}|\lambda_i\lambda_j| \, . \tag{5.5}$$

Because of Eq. (5.2), the first sum of the right-hand side of Eq. (5.5) is equal to $2m$. In view of Eq. (5.3),

$$\sum_{i<j}|\lambda_i||\lambda_j| \ge \left|\sum_{i<j}\lambda_i\,\lambda_j\right| = m \, . \tag{5.6}$$

Consequently, $\mathscr{E}(G)^2 \ge 4m$, that is,

$$\mathscr{E}(G) \ge 2\sqrt{m} \, . \tag{5.7}$$

From Ineq. (5.6), we see that equality in Ineq. (5.7) will occur if and only if the graph G has exactly one positive and exactly one negative eigenvalue. This, in turn, is the case if and only if one component of G is a complete bipartite graph and all its other components are isolated vertices (see [81], p. 163).

Consider, for a moment, graphs having m edges and no isolated vertices. The maximum number of vertices of such graphs is $2m$, which happens if $G \cong mK_2$, i.e., if the graph G consists of m isolated edges. For all other graphs, $n < 2m$. Bearing this in mind, we have

$$\sqrt{2mn} \le \sqrt{(2m)^2} = 2m \tag{5.8}$$

which combined with Ineq. (5.4) yields

$$\mathscr{E}(G) \le 2m \, . \tag{5.9}$$

The spectrum of mK_2 consists of numbers $+1$ (m times) and -1 (m times); hence, the absolute values of all eigenvalues are equal. Therefore, for $G \cong mK_2$, we have equality in both Ineqs. (5.4) and (5.8), and therefore, we have equality also in (5.9). Clearly, equality in Ineq. (5.9) will hold also if in addition to m isolated edges, the graph G contains any number of isolated vertices. By this, we have proved the theorem. ■

More bounds of this kind can be found in [179, 318, 376, 377].

5.2 Upper Bounds

5.2.1 Upper Bounds for General Graphs

Suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. By the Cauchy–Schwarz inequality, $\left(\sum_{i=2}^{n} |\lambda_i|\right)^2 \leq (n-1)\sum_{i=2}^{n} |\lambda_i|^2$ which by $\sum_{i=2}^{n} \lambda_i^2 = 2m - \lambda_1^2$ immediately implies Theorem 5.3, first reported by Koolen and Moulton [305].

Theorem 5.3. *Suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. Then,*

$$\mathscr{E}(G) \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} \,. \tag{5.10}$$

In this subsection, we will use the above inequality and some lower bounds of λ_1 to arrive at some upper bounds of graph energy.

Since $F(x) := x + \sqrt{(n-1)(2m - x^2)}$ is a decreasing function in the variable $x \in (\sqrt{2m/n}, \sqrt{2m})$, for any given lower bound ξ of λ_1 (e.g., lower bounds in [382]), one obtains an upper bound for energy. In particular, for $\lambda_1 \geq \xi \geq \sqrt{2m/n}$, one arrives at $\mathscr{E}(G) \leq \xi + \sqrt{(n-1)(2m - \xi^2)}$.

Since the spectral radius obeys the inequality $\lambda_1 \geq 2m/n$ [81], Koolen and Moulton [305] gave the following theorem:

Theorem 5.4. *Let G be an (n, m)-graph. If $2m \geq n$, then*

$$\mathscr{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \,. \tag{5.11}$$

Moreover, equality holds in (5.11) if and only if G consists of $n/2$ copies of K_2, or $G \cong K_n$ or G is a noncomplete connected strongly regular graph with two nontrivial eigenvalues both having absolute values equal to $\sqrt{(2m - (2m/n)^2)/(n-1)}$.

Proof. Suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. Since $F(x) := x + \sqrt{(n-1)(2m - x^2)}$ is a decreasing function in the variable $x \in (\sqrt{2m/n}, \sqrt{2m})$, by Ineq. (5.10) and $\lambda_1 \geq 2m/n$, we obtain Ineq. (5.11).

We now consider what happens when equality holds in (5.11). Since the eigenvalues of $(n/2)K_2$ are ± 1 (both with multiplicity $n/2$) and the eigenvalues of K_n are $n-1$ (multiplicity 1) and -1 (multiplicity $n-1$), it is easy to check that if G is one of the graphs specified in the second part of the theorem, then the equality holds.

Conversely, if equality holds in (5.11), we see that $\lambda_1 = 2m/n$ must hold. It follows that G is regular with degree $2m/n$ [81]. Now, since equality must also hold in the Cauchy–Schwarz inequality given above, we have

$$|\lambda_i| = \sqrt{(2m - (2m/n)^2)/(n-1)}$$

for $2 \leq i \leq n$. Hence, we are reduced to three possibilities: either G has two eigenvalues with equal absolute values, in which case $G \cong (n/2)\,K_2$, or G has two eigenvalues with distinct absolute values, in which case $G \cong K_n$, or G has three eigenvalues with distinct absolute values equal to $2m/n$ or $\sqrt{(2m - (2m/n)^2)/(n-1)}$, in which case G must be a noncomplete connected strongly regular graph (see [81]), as required. ■

A graph is said to be *semiregular bipartite* if it is bipartite and each vertex in the same part has the same degree. Among known bounds for λ_1, we need here Hofmeister's fundamental inequality [262, 527]:

Lemma 5.2. *Let G be the graph with n vertices and degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}\,. \tag{5.12}$$

Equality holds if and only if G is either regular or semiregular bipartite. ■

By means of Ineqs. (5.12) and (5.10), one obtains Ineq. (5.13) [528]:

Theorem 5.5. *If G is a graph with n vertices, m edges, and vertex degree sequence $d_1, d_2, \ldots, d_n$, then*

$$\mathcal{E}(G) \leq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} + \sqrt{(n-1)\left[2m - \left(\sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}\right)^2\right]}\,. \tag{5.13}$$

Moreover, equality in (5.13) holds if and only if G is either $(n/2)K_2$ $(n = 2m)$, K_n $(m = n(n-1)/2)$, a noncomplete connected strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{(2m - (2m/n)^2)/(n-1)}$, or nK_1 $(m = 0)$.

Proof. It is easy to check that if G is one of the graphs given in the second part of the theorem, then the equality in Ineq. (5.13) holds.

Conversely, if the equality in Ineq. (5.13) holds, then by Lemma 5.2, we see that $\lambda_1 = \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}$ and G is a regular graph or a semiregular bipartite graph. If G is regular and $m > 0$, then $\lambda_1 = \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} = 2m/n$, and hence by Theorem 5.4, G is either $(n/2)K_2$, K_n or a noncomplete connected strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{(2m - (2m/n)^2)/(n-1)}$. If $m = 0$, then $G \cong n\,K_1$. Now suppose that G is a semiregular bipartite graph. Since equality holds in the Cauchy–Schwarz inequality given above, we have

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} = \lambda_1 = -\lambda_n = \sqrt{\frac{2m - \lambda_1^2}{n-1}}$$

from which we have $\sum_{i=1}^{n} d_i^2 = 2m$, and hence, $d_i = 1$ or 0 for $1 \le i \le n$. Thus, G is either $(n/2)K_2$ or nK_1. ■

For $v_i \in V(G)$, the 2-*degree* of v_i, denoted by t_i, is defined as the sum of degrees of the vertices adjacent to v_i. The *average 2-degree* of v_i, denoted by m_i, is the average of the degrees of the vertices adjacent to v_i. Then $t_i = d_i\, m_i$. Furthermore, denote by σ_i the sum of the 2-degrees of vertices adjacent to v_i. A graph G is said to be *pseudoregular* if there exists a constant p, such that each vertex of G has an average 2-degree equal to p. Such a graph is also said to be *p-pseudoregular*. A bipartite graph $G = (X, Y)$ is *pseudo-semiregular* if there exist two constants p_x and p_y, such that each vertex in X has an average 2-degree p_x and each vertex in Y has an average 2-degree p_y. Such a graph is also said to be (p_x, p_y)-*pseudo-semiregular*. Obviously, any r-regular graph is an r-pseudoregular graph, and any (a, b)-semiregular bipartite graph is a (b, a)-pseudo-semiregular bipartite graph. Conversely, a pseudoregular graph may not be a regular graph, such as $S(K_{1,3})$, and a pseudo-semiregular bipartite graph may not be a semiregular bipartite graph, such as $S(K_{1,n-1})$, $n \ge 5$, where $S(K_{1,t})$ is the graph obtained by subdividing each edge of $K_{1,t}$ once.

For any nonempty connected graph G, Yu et al. [509] obtained a lower bound of $\lambda_1(G)$.

Lemma 5.3. *Let G be a nonempty connected graph with degree sequence $d_1, d_2, \ldots, d_n$ and 2-degree sequence $t_1, t_2, \ldots, t_n$. Then*

$$\lambda_1(G) \ge \sqrt{\sum_{i=1}^{n} t_i^2 \Big/ \sum_{i=1}^{n} d_i^2} \tag{5.14}$$

with equality if and only if G is a pseudoregular graph or a pseudo-semiregular bipartite graph. ■

By Ineqs. (5.10) and (5.14), one obtains Ineq. (5.15) [510]:

Theorem 5.6. *Let G be a nonempty graph with n vertices, m edges, degree sequence $d_1, d_2, \ldots, d_n$, and 2-degree sequence $t_1, t_2, \ldots, t_n$. Then*

$$\mathscr{E}(G) \le \sqrt{\sum_{i=1}^{n} t_i^2 \Big/ \sum_{i=1}^{n} d_i^2} + \sqrt{(n-1)\left(2m - \sum_{i=1}^{n} t_i^2 \Big/ \sum_{i=1}^{n} d_i^2\right)}\,. \tag{5.15}$$

Equality holds if and only if one of the following statements holds:

(1) $G \cong (n/2)K_2$; (2) $G \cong K_n$; (3) G is a nonbipartite connected p-pseudoregular graph with three distinct eigenvalues $\left(p, \sqrt{\frac{2m-p^2}{n-1}}, -\sqrt{\frac{2m-p^2}{n-1}}\right)$, where $p > \sqrt{2m/n}$.

Proof. If G is one of the three graphs specified in the second part of the theorem, it is easy to check that the equality in Ineq. (5.15) holds.

Conversely, if the equality in Ineq. (5.15) holds, according to Lemma 5.3, we have $\lambda_1(G) = \sqrt{\sum_{i=1}^{n} t_i^2 \Big/ \left(\sum_{i=1}^{n} d_i^2\right)}$, which implies that G is a pseudoregular graph or a pseudo-semiregular bipartite graph. Moreover, for $2 \le i \le n$, $|\lambda_i| = \sqrt{(2m - \lambda_1^2)/(n-1)}$. Note that G has only one eigenvalue if and only if G is an empty graph. We are reduced to the following two possibilities:

(1) G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = |\lambda_i| = \sqrt{(2m - \lambda_1^2)/(n-1)}$ for $2 \le i \le n$. By Lemma 5.1, $|\lambda_i| = \sqrt{(2m - \lambda_1^2)/(n-1)} = 1$ for $2 \le i \le n$. Hence, $2m = n$, which implies $G \cong (n/2)K_2$.

If the two eigenvalues of G have different absolute values, then, by Lemma 5.1, $\lambda_i = -1$ $(2 \le i \le n)$. Moreover, G is a complete graph of order n, i.e., $G \cong K_n$.

(2) G has three distinct eigenvalues.

In this case, $\lambda_1(G) = \sqrt{\sum_{i=1}^{n} t_i^2 \Big/ \left(\sum_{i=1}^{n} d_i^2\right)}$ and $|\lambda_i| = \sqrt{(2m - \lambda_1^2)/(n-1)}$ for $2 \le i \le n$. Moreover, $\lambda_1 > \lambda_i$ and $\lambda_i \ne 0$. Combining the fact that G is a pseudoregular graph or a pseudo-semiregular bipartite graph, we have that G is a nonbipartite connected p-pseudoregular graph with three distinct eigenvalues

$$\left(p\,,\ \sqrt{\frac{2m-p^2}{n-1}}\,,\ -\sqrt{\frac{2m-p^2}{n-1}}\right) \tag{5.16}$$

where $p = \lambda_1(G) = \sqrt{\sum_{i=1}^{n} t_i^2 \Big/ \left(\sum_{i=1}^{n} d_i^2\right)} = t_i/d_i > \sqrt{2m/n}$ $(1 \le i \le n)$. ∎

For any nonempty simple graph G, Hong and Zhang [264] obtained a lower bound of $\lambda_1(G)$.

Lemma 5.4. *Let G be a nonempty simple graph of order n, and let σ_i be the sum of the 2-degrees of vertices adjacent to vertex v_i. Then*

$$\lambda_1(G) \geq \sqrt{\frac{\sum_{i=1}^{n} \sigma_i^2}{\sum_{i=1}^{n} t_i^2}} \tag{5.17}$$

with equality if and only if

$$\frac{\sigma_1}{t_1} = \frac{\sigma_2}{t_2} = \cdots = \frac{\sigma_n}{t_n}$$

or G is a bipartite graph with $V = \{v_1, v_2, \ldots, v_s\} \cup \{v_{s+1}, v_{s+2}, \ldots, v_n\}$, such that $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \sigma_{s+2}/t_{s+2} = \cdots = \sigma_n/t_n$. ■

Similarly, by Ineqs. (5.10) and (5.17), one arrives at Ineq. (5.18) [348], whose proof is analogous to the above and is omitted.

Theorem 5.7. *Let G be a nonempty simple graph with n vertices and m edges. Then*

$$\mathscr{E}(G) \leq \sqrt{\frac{\sum_{i=1}^{n} \sigma_i^2}{\sum_{i=1}^{n} t_i^2}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} \sigma_i^2}{\sum_{i=1}^{n} t_i^2}\right)}. \tag{5.18}$$

Equality holds if and only if one of the following statements holds: (1) $G \cong (n/2)K_2$; (2) $G \cong K_n$; (3) G is a nonbipartite connected graph satisfying $\sigma_1/t_1 = \cdots = \sigma_n/t_n$ and has three distinct eigenvalues as in (5.16), where $p = \sigma_1/t_1 = \cdots = \sigma_n/t_n > \sqrt{2m/n}$. ■

The *k-degree $d_k(v)$* of a vertex $v \in G$ is defined as the number of walks of length k starting at v. The following upper bound on the k-degree is obtained in [271]:

Theorem 5.8. *Let G be a connected graph with n ($n \geq 2$) vertices and m edges. Then*

$$\mathscr{E}(G) \leq \sqrt{\frac{\sum_{v \in V(G)} d_{k+1}^2(v)}{\sum_{v \in V(G)} d_k^2(v)}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v \in V(G)} d_{k+1}^2(v)}{\sum_{v \in V(G)} d_k^2(v)}\right)}. \tag{5.19}$$

Equality holds if and only if G is the complete graph K_n or G is a strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$. ■

Using routine calculus, it can be shown that the right-hand side of Ineq. (5.11) becomes maximal when $m = \left(n^2 + n\sqrt{n}\right)/4$. It thus follows [305] that:

Theorem 5.9. *Let G be a graph on n vertices. Then*

$$\mathscr{E}(G) \le \frac{n}{2}(\sqrt{n}+1) \tag{5.20}$$

with equality if and only if G is a strongly regular graph with parameters

$$\left(n\,,\ \frac{n+\sqrt{n}}{2}\,,\ \frac{n+2\sqrt{n}}{4}\,,\ \frac{n+2\sqrt{n}}{4}\right).$$

Proof. Suppose that G is a graph with n vertices and m edges.

If $2m \ge n$, then using routine calculus, it is seen that the right-hand side of Ineq. (5.11) (considered as a function of m) is maximized when $m = (n^2 + n\sqrt{n})/4$ holds. Inequality (5.20) now follows by substituting this value of m into Ineq. (5.11). Moreover, it follows by Theorem 5.4 and Eq. (1.3) that equality holds in Ineq. (5.20) if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$.

If $2m \le n$, then by Theorem 5.2, $\mathscr{E}(G) \le n$. The proof of the theorem now follows immediately. ■

Remark 5.1. The graphs for which the equality is attained in Theorem 5.9 are strongly regular with parameter $\mu = r(r+1)$ and therefore strongly regular graphs of negative Latin square type.

Obviously, if such a graph with property $\mathscr{E} = n(\sqrt{n}+1)/2$ does exist, then n must be a square of a positive even integer r. Haemers [252] conjectured that $n = r^2$ is a necessary and sufficient condition for the existence of such graphs. He also tried to construct such strongly regular graphs and proved:

Theorem 5.10. *There are strongly regular graphs with parameters*

$$\left(n\,,\ \frac{n+\sqrt{n}}{2}\,,\frac{n+2\sqrt{n}}{4}\,,\ \frac{n+2\sqrt{n}}{4}\right)$$

for (i) $n = 4^p\,,\ p \ge 1$*; (ii)* $n = 4^p q^4,\ p,q \ge 1$*; and (iii)* $n = 4^{p+1} q^2\,,\ p \ge 1$*, and* $4q-1$ *is a prime power, or* $2q-1$ *is a prime power, or* q *is a square, or* $q < 167$. ■

As explained above, the graphs specified in Theorem 5.10 have maximal energy. Haemers also found that for $n = 4, 16, 36$, the above extremal graphs are unique, whereas for $n = 64, 100, 144$, these are not unique.

Xiang proved that the construction by him and Muzychuk (see [380]) can be modified so that the Hadamard matrices become graphical of negative type. This shows that maximal energy graphs of order $n = 4m^4$ exist for all m. These are the strongly regular graphs with parameters $(4m^4, 2m^4+m^2, m^4+m^2, m^4+m^2)$, which exist for all $m > 1$ [253].

A completely different approach to estimating graph energy was elaborated by Wagner [474]. He demonstrated that within the set of all graphs with cyclomatic number c (which includes, as special cases, trees, $c = 0$, or unicyclic graphs, $c = 1$),

$$\mathscr{E} \le \frac{4n}{\pi} + \gamma_c$$

for a constant γ_c that only depends on c. He also showed how to construct graphs G of arbitrary cyclomatic number, whose energy satisfies the relation

$$\mathscr{E}(G) = \frac{4n}{\pi} + O(1)\,.$$

5.2.2 Upper Bounds for Bipartite Graphs

For any (n,m)-graph G, Theorem 5.4 gives an upper bound of $\mathscr{E}(G)$. For special classes of graphs, one can obtain better bounds. We now consider bipartite graph G with n vertices and m edges. The results look very similar to the corresponding results of the above section. However, because of the special property of bipartite graphs, their proofs are somewhat different, especially in the analysis of equality cases, and so we prefer to give the details for some of them.

Suppose that $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ are the eigenvalues of G. Since G is bipartite, $\lambda_1 = -\lambda_n$ and $\sum\limits_{i=2}^{n-1} {\lambda_i}^2 = 2m - 2{\lambda_1}^2$ holds. By similar arguments as those used in the proof of Theorem 5.4, we obtain

$$\mathscr{E}(G) \le 2\lambda_1 + \sqrt{(n-2)(2m-2\lambda_1^2)} \tag{5.21}$$

which again is a result by Koolen and Moulton [306]. Thus, by replacing λ_1 by a lower bound for λ_1, we obtain further upper bounds for $\mathscr{E}(G)$. Such are those stated in Theorems 5.11 and 5.13–5.15.

Recall [256] that a 2-(ν,k,λ)-*design* is a collection of k-subsets or blocks of a set of ν points, such that each 2-set of points lies in exactly λ blocks. The design is called *symmetric* (or *square*) in case the number of blocks b equals ν. The *incidence matrix* $\mathbf{B}$ of a 2-(ν,k,λ)-design is the $\nu \times b$ matrix defined so that for each point x and block S, $B_{x,S} = 0$ if $x \notin S$ and $B_{x,S} = 1$ otherwise. The *incidence graph* of a design is defined to be the graph with adjacency matrix $\begin{bmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{0} \end{bmatrix}$. Note that the incidence graph of a symmetric 2-(ν,k,λ)-design with $\nu > k > \lambda > 0$ has eigenvalues k, $\sqrt{k-\lambda}$ (with multiplicity $\nu-1$), $-\sqrt{k-\lambda}$ (with multiplicity $\nu-1$), and $-k$. Infinite families of symmetric 2-(ν,k,λ)-designs are known to exist. For example, the symmetric designs with $\lambda = 1$ are exactly the projective planes. However, it is not known for fixed $\lambda > 1$ whether or not there are infinitely many symmetric 2-(ν,k,λ)-designs. The following result is presented in [306]:

Theorem 5.11. *If $2m \ge n$ and G is a bipartite graph with $n > 2$ vertices and m edges, then the inequality*

$$\mathscr{E}(G) \le 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left[2m - 2\left(\frac{2m}{n}\right)^2\right]} \tag{5.22}$$

holds. Moreover, equality holds if and only if at least one of the following statements holds: (i) $n = 2m$ and $G \cong mK_2$; (ii) $n = 2t, m = t^2$, and $G \cong K_{t,t}$; and (iii) $n = 2\nu$, $2\sqrt{m} < n < 2m$, and G is the incidence graph of a symmetric 2-(ν, k, λ)-design with $k = 2m/n$ and $\lambda = k(k-1)/(\nu-1)$.

Proof. Inequality (5.22) is immediately obtained from Ineq. (5.21).

It is straightforward to check that if G is one of the graphs specified in $(i)-(iii)$, then the equality in (5.22) must hold.

Conversely, if the equality in Ineq. (5.22) holds, then by the previous discussion on the function $F(x)$, we see that $\lambda_1 = 2m/n$ must hold. It follows that G is regular with degree $2m/n$ [81]. Now, we have $|\lambda_i| = \sqrt{\left[2m - 2\,(2m/n)^2\right]/(n-2)}$, for $2 \le i \le n-1$. Hence, by the pairing theorem, we are reduced to three possibilities: either G has two eigenvalues with equal absolute values, in which case G must be equal to mK_2 so that (i) holds; G has three distinct eigenvalues, i.e., $|\lambda_i| = 0$ for $2 \le i \le n-1$, and hence, $n = 2\sqrt{m}$ and $G \cong K_{\sqrt{m},\sqrt{m}}$ so that (ii) holds; or G has four distinct eigenvalues in which case G is connected, $2m/n > \sqrt{\left[2m - 2\left(\frac{2m}{n}\right)^2\right]/(n-2)}$ holds, and G is the incidence graph of a symmetric 2-$(\nu, 2m/n, \lambda)$-design [81] so that (iii) holds. ■

We now give an upper bound for the energy of a bipartite graph G in terms of the number of its vertices and characterize those graphs for which this bound is sharp [306].

Theorem 5.12. *Let G be a bipartite graph on $n > 2$ vertices. Then*

$$\mathscr{E}(G) \le \frac{n}{\sqrt{8}}(\sqrt{n} + \sqrt{2}) \tag{5.23}$$

with equality holding if and only if $n = 2\nu$ and if G is the incidence graph of a 2-$(\nu, \frac{\nu+\sqrt{\nu}}{2}, \frac{\nu+2\sqrt{\nu}}{4})$-design.

Proof. Suppose that G is a graph with n vertices and m edges.

If $2m > n$, then using routine calculus, it is seen that the right-hand side of Ineq. (5.22) (considered as a function of m) is maximized when $m = [n^2 + n\sqrt{2n}]/8$. Ineq. (5.23) now follows by substituting this value of m into Ineq. (5.22).

Observe now that $m = [n^2 + n\sqrt{2n}]/8 < n^2/4$ holds if $n > 2$. Thus, it follows from Theorem 5.11 that equality holds in Ineq. (5.23) if and only if $n = 2\nu$ and G is the incidence graph of a 2-$(\nu, \frac{\nu+\sqrt{\nu}}{2}, \frac{\nu+2\sqrt{\nu}}{4})$-design.

If $2m \le n$, then by Theorem 5.4, $\mathscr{E}(G) \le n$. Since $n < \frac{n}{\sqrt{8}}(\sqrt{n} + \sqrt{2})$ for $n > 2$, the theorem follows. ■

In the following, an upper bound for the energy of bipartite graph with n vertices, m edges, and degree sequence $d_1, d_2, \ldots, d_n$ is given, and those graphs for which this bound is best possible are determined [528]. First, we need the following easy and well-known [90, 91, 97] result:

Lemma 5.5. *Let G be a connected bipartite graph with n vertices and m edges, and let $d_1, d_2, \ldots, d_n$ be the degree sequence of G. Then $d_1^2 + d_2^2 + \cdots + d_n^2 \leq mn$, with equality holding if and only if G is a complete bipartite graph.*

Proof. It is sufficient to require that the graph G be triangle-free [388]. Then for any edge uv of G, $d_u + d_v \leq n$ implying $\sum\limits_{i=1}^{n} d_i^2 = \sum\limits_{uv} (d_u + d_v) \leq mn$. The equality holds if and only if $d_u + d_v = n$ for each edge uv of G, i.e., if G is complete bipartite. ■

Note that $4m^2 = \left(\sum_{i=1}^{n} d_i\right)^2 \leq n \sum_{i=1}^{n} d_i^2$, i.e., $2m/n \leq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}$, which together with Ineq. (5.21) yields:

Theorem 5.13. *If G is a bipartite graph with $n > 2$ vertices, m edges, and degree sequence $d_1, d_2, \ldots, d_n$, then*

$$\mathscr{E}(G) \leq 2\sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} + \sqrt{(n-2)\left(2m - \frac{2}{n}\sum_{i=1}^{n} d_i^2\right)}\,. \tag{5.24}$$

Moreover, equality holds if and only if G is either $(n/2)K_2$ ($n = 2m$), $K_{r,n-r}$ with $1 \leq r \leq n/2$ ($m = r(n-r)$), the incidence graph of a symmetric 2-(ν, k, λ)-design with $\nu > k$, $k = 2m/n$ and $\lambda = k(k-1)/(\nu-1)$, ($n = 2\nu$), or $n\,K_1$ ($m = 0$).

Proof. It is easy to check that if G is one of the graphs specified in the second part of the theorem, then equality in Ineq. (5.24) holds.

Conversely, if equality in Ineq. (5.24) holds, then by the above argument and Lemma 5.2, we see that $\lambda_1 = \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}$ and G is a semiregular bipartite graph. Now, we have $|\lambda_i| = \sqrt{(2m - 2\lambda_1^2)/(n-2)}$ for $2 \leq i \leq n-1$. Hence, we have the following possibilities: G has two eigenvalues with equal absolute values, and hence, $G \cong m\,K_2$; G has three distinct eigenvalues, i.e., $\lambda_i = 0$ for $2 \leq i \leq n-1$, and hence, $(\sum_{i=1}^{n} d_i^2)/n = \lambda_1^2 = m$ and by Lemma 5.5 $G \cong K_{r,n-r}$ with $1 \leq r \leq n/2$; G has four distinct eigenvalues in which case G is regular (since 0 is not an eigenvalue and G is a semiregular bipartite graph) and connected, $\lambda_1 = 2m/n > \sqrt{(2m - 2\lambda_1^2)/(n-2)}$, and hence, G is the incidence graph of a symmetric 2-$(\nu, 2m/n, \lambda)$-design [102]; or $G \cong n\,K_1$ ($m = 0$). ■

By Ineq. (5.21) and Lemma 5.3, we have the following result, whose proof is similar to the above and is omitted:

Theorem 5.14 [510]. *Let $G = (X, Y)$ be a nonempty bipartite graph with $n > 2$ vertices, m edges, degree sequence $d_1, d_2, \ldots, d_n$, and 2-degree sequence $t_1, t_2, \ldots, t_n$. Then*

$$\mathscr{E}(G) \le 2\sqrt{\sum_{i=1}^{n} t_i^2 / \sum_{i=1}^{n} d_i^2 + \sqrt{(n-2)\left(2m - 2\sum_{i=1}^{n} t_i^2 / \sum_{i=1}^{n} d_i^2\right)}}\,. \tag{5.25}$$

Equality holds if and only if one of the following statements holds: (1) $G \cong (n/2)K_2$; (2) $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1 r_2 = m$; (3) G is a connected (p_x, p_y)-pseudo-semiregular bipartite graph with four distinct eigenvalues

$$\left(\sqrt{p_x p_y}\,,\ \sqrt{\frac{2m - 2p_x\,p_y}{n-2}}\,,\ -\sqrt{\frac{2m - 2p_x\,p_y}{n-2}}\,,\ -\sqrt{p_x\,p_y}\right) \tag{5.26}$$

where p_x denotes the average degree of each vertex in X, p_y denotes the average degree of each vertex in Y, and $\sqrt{p_x\,p_y} > \sqrt{2m/n}$. ■

Similarly, by Ineq. (5.21), the following two upper bounds are given in [271,348]:

Theorem 5.15. *Let $G = (X, Y)$ be a nonempty bipartite graph with $n > 2$ vertices and m edges. Then*

$$\mathscr{E}(G) \le 2\sqrt{\sum_{i=1}^{n} \sigma_i^2 \Big/ \sum_{i=1}^{n} t_i^2 + \sqrt{(n-2)\left(2m - 2\sum_{i=1}^{n} \sigma_i^2 \Big/ \sum_{i=1}^{n} t_i^2\right)}}\,. \tag{5.27}$$

Equality holds if and only if one of the following statements holds: (1) $G \cong (n/2)K_2$; (2) $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1 r_2 = m$; (3) G is a connected bipartite graph with $V = \{v_1, v_2, \ldots, v_s\} \cup \{v_{s+1}, v_{s+2}, \ldots, v_n\}$, such that $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \sigma_{s+2}/t_{s+2} = \cdots = \sigma_n/t_n$, and has four distinct eigenvalues as in (5.26), where $p_x = \sigma_1/t_1 = \cdots = \sigma_s/t_s$, $p_y = \sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n$ and $\sqrt{p_x\,p_y} > \sqrt{2m/n}$. ■

Theorem 5.16. *Let G be a connected bipartite graph with n ($n \ge 2$) vertices and m edges. Then*

$$\mathscr{E}(G) \le 2\sqrt{\frac{\sum_{v \in V(G)} d_{k+1}^2(v)}{\sum_{v \in V(G)} d_k^2(v)} + \sqrt{(n-2)\left(2m - 2\frac{\sum_{v \in V(G)} d_{k+1}^2(v)}{\sum_{v \in V(G)} d_k^2(v)}\right)}}\,. \tag{5.28}$$

Equality holds if and only if G is a complete bipartite graph or G is the incidence graph of a symmetric 2-(ν, k, λ)-design with $k = 2m/n$, $n = 2\nu$, and $\lambda = k(k-1)/(\nu - 1)$. ■

More upper bounds of the same kind are found in [140, 320, 347, 515, 516, 544]. As a special class of bipartite graphs, trees (and forests) have also been investigated. The following two lemmas are reported in [93] and [81], respectively:

Lemma 5.6. *Let T be a tree of order n ($n \geq 2$), and suppose that there exists a vertex $v_i \in T$ such that the eccentricity $\epsilon(v_i) \leq 2$. Then*

$$\lambda_1(T) \geq \sqrt{d_i + m_i - 1} \tag{5.29}$$

where $d_i = d(v_i)$ and m_i is the average 2-degree of v_i. Moreover, equality holds if and only if the degree of the neighbors of v_i is equal. ■

Lemma 5.7. *Let G be a connected graph and G' a subgraph of G. Then $\lambda_1(G') \leq \lambda_1(G)$ and equality holds if and only if $G' \cong G$.* ■

Let T_{d_i,d_j} ($d_j \geq 2$) be a tree obtained by joining the centers of d_i copies of K_{1,d_j-1} to a new vertex v_i. Then $T_{1,n-1} \cong K_{1,n-1}$. In the following, the proof of our main result is carried out by means of Lemma 5.8.

Lemma 5.8. *Let T be a tree with order n, degree sequence $d_1, d_2, \ldots, d_n$, and average 2-degree sequence $m_1, m_2, \ldots, m_n$. Then*

$$\lambda_1(T) \geq max\{\sqrt{d_i + m_i - 1} : 1 \leq i \leq n\} . \tag{5.30}$$

Moreover, equality holds if and only if T is isomorphic to some T_{d_i,d_j}.

Proof. We know that if H is a subgraph of G, then $\lambda_1(H) \leq \lambda_1(G)$. Thus, by Lemma 5.6, we have

$$\lambda_1(T) \geq \sqrt{d_i + m_i - 1}\ ,\ 1 \leq i \leq n\ . \tag{5.31}$$

By Ineq. (5.31), (5.30) holds immediately.

Now suppose that equality holds in (5.30), that is, for some $v_i \in V(T)$,

$$\lambda_1(T) = \sqrt{d_i + m_i - 1}\ .$$

Note that if $T' \subset T$, then by Lemma 5.7, $\lambda_1(T') < \lambda_1(T)$. Therefore, by Lemma 5.6, $T \cong T_{d_i,d_j}$. Conversely, let $T \cong T_{d_i,d_j}$. It is easy to check that then equality holds in (5.30). ■

From Lemma 5.8 and Ineq. (5.21), by a similar discussion as the proof of Theorem 5.15, we have

Theorem 5.17. *Let T be a forest with n vertices, m edges, vertex degree sequence $d_1, d_2, \ldots, d_n$, and average 2-degree sequence $m_1, m_2, \ldots, m_n$. Then*

$$\mathscr{E}(T) \leq 2\sqrt{s} + \sqrt{(n-2)(2m-2s)}$$

where $s = max\{d_i + m_i - 1 : 1 \leq i \leq n\}$. Equality holds if and only if one of the following statements holds: (1) $T \cong (n/2)K_2$; (2) $T \cong K_{1,m} \cup$

$(n-1-m)K_1$; (3) $T \cong T_{d_i,d_j}$ ($d_j \geq 2$) with four distinct eigenvalues $\left(\sqrt{s}, \sqrt{\frac{2m-2s}{n-2}}, -\sqrt{\frac{2m-2s}{n-2}}, -\sqrt{s}\right)$. ■

Theorem 5.18 presents an application of the Lagrange multiplier method, to obtain bounds for the energy of bipartite graphs. We only give the result here, for details see [400]. In what follows, G denotes a bipartite graph with $n = 2N$ vertices ($N \geq 2$) and m edges. The case $n = 2N + 1$ will be considered separately. It is well known that the spectrum of G is symmetric with respect to the origin of $\mathbb{R}$, and so, the eigenvalues of G can be labeled so as $\pm\lambda_1, \ldots, \pm\lambda_N$, where

$$\lambda_1 \geq \cdots \geq \lambda_N \geq 0 \tag{5.32}$$

In particular, the energy of G is given by $\mathscr{E}(G) = 2(\lambda_1 + \cdots + \lambda_N)$. For an even integer $k \geq 2$, the k-th spectral moment of G is defined as $M_k = 2\sum_{i=1}^{N} \lambda_i^k$. By setting $q = M_4/2$, we have the following relations:

$$m = \sum_{i=1}^{N} \lambda_i^2 \qquad \text{and} \qquad q = \sum_{i=1}^{N} \lambda_i^4 \,. \tag{5.33}$$

We assume that $m > 0$ in order to avoid the trivial case. Note also that $m^2 \geq q$. Moreover, using the Cauchy–Schwarz inequality, we have $m^2 \leq Nq$. Set $P = Nq - m^2$.

Recall [256] that a *balanced incomplete block design* (BIBD) is a family of b blocks of a set of v elements, such that (1) each element is contained in r blocks, (ii2) each block contains k elements, and (3) each pair of elements is simultaneously contained in λ blocks. The integers (v, b, r, k, λ) are called the parameters of the design. In the particular case $r = k$, the design is said to be symmetric. The graph of a design is formed in the following way: The $b + v$ vertices of the graph correspond to the blocks and elements of the design with two vertices adjacent if and only if one corresponds to a block and the other corresponds to an element contained in that block.

Theorem 5.18. *Let G be a bipartite graph with $2N$ vertices.*

(1) $m^2 = Nq$ if and only if $G \cong N\,K_2$.
(2) $m^2 = q$ if and only if G is the direct sum of h isolated vertices and a copy of a complete bipartite graph $K_{r,s}$, such that $rs = m$ and $h + r + s = 2N$.
(3) If $1 < m^2/q < N$, then $\mathscr{E}(G) \leq \varepsilon(G)$, where

$$\varepsilon(G) = \frac{2}{\sqrt{N}}\left[\left(m + \sqrt{(N-1)P}\right)^{1/2} + (N-1)\left(m - \sqrt{P/(N-1)}\right)^{1/2}\right]. \tag{5.34}$$

Equality holds if G is the graph of a symmetric $BIBD$. Conversely, if equality holds and G is regular, then G is the graph of a symmetric $BIBD$. ■

Assume that G has $n = 2N + 1$ vertices and that the eigenvalues of G are labeled according to (5.32).

Theorem 5.19. *Let G be a bipartite graph with $2N + 1$ vertices.*

(1) $P \geq 0$ and the equality holds if and only if G is the direct sum of an isolated vertex with NK_2.
(2) Inequality in part (3) of Theorem 5.18 remains true if $1 < m^2/q < N$, and the equality holds if G consists of an isolated vertex and a copy of the graph of a symmetric $BIBD$. ■

5.2.3 Upper Bounds for Regular Graphs

From many aspects, regular graphs are the far best studied types of graphs. Yet, relatively little is known on their energy. In [14], the energy of the complement of regular line graphs was studied. In [247], lower and upper bounds for the energy of some special kinds of regular graphs were obtained. The paper [295] gives analytic expressions for the energy of two specially designed regular graphs. In [26, 35, 284, 411, 428], results were communicated for the energy of some very symmetric graphs: circulant graphs, Cayley graphs, and unitary Cayley graphs.

For an n-vertex regular graph G of degree k, an upper bound for the energy of G is readily deduced from the McClelland Ineq. (5.4), i.e., from $\mathscr{E}(G) \leq \sqrt{2mn}$, namely, $\mathscr{E}(G) \leq n\sqrt{k}$. From Theorem 5.4, we have $\mathscr{E}(G) \leq \mathscr{E}_0$, where $\mathscr{E}_0 = k + \sqrt{k(n-1)(n-k)}$. Balakrishnan [26] showed that for any $\varepsilon > 0$, there exist infinitely many n, for which there are n-vertex regular graphs of degree k, $k < n-1$, such that $\mathscr{E}(G)/\mathscr{E}_0 < \varepsilon$.

Before proceeding to the main results, we make some observations on circulant graphs; for details see [125]. Let $S \subseteq \{1, 2, \dots, n\}$ with the property that if $i \in S$, then $n - i \in S$. The graph G with vertex set $V = \{v_0, v_1, \dots, v_{n-1}\}$ in which v_i is adjacent to v_j if and only if $i - j \pmod{n} \in S$ is called a *circulant graph*, since the adjacency matrix $\mathbf{A}(G)$ of G is a circulant of order n with 1 in $(i+1)$-th position of its first row if and only if $i \in S$ (and 0 in the remaining positions). Clearly G is $|S|$-regular. If $S = \{\alpha_1, \dots, \alpha_k\} \subset \{1, 2, \dots, n\}$, then the first row of $\mathbf{A}(G)$ has 1 in the $(\alpha_i + 1)$-th position, $1 \leq i \leq k$, and 0 in the remaining positions. Hence, the eigenvalues of G are given by

$$\{\omega^{j\alpha_1} + \omega^{j\alpha_2} + \cdots + \omega^{j\alpha_k} : 1 \leq j \leq n\}$$

with ω being a primitive n-th root of unity.

Theorem 5.20. *For each $\varepsilon > 0$, there exist infinitely many n, such that there exists a k-regular graph G of order n with $k < n - 1$ and*

$$\frac{\mathscr{E}(G)}{\mathscr{E}_0} < \varepsilon \,. \tag{5.35}$$

Proof. Let $\alpha_1, \alpha_2, \ldots, \alpha_k$ be the numbers less than n and prime to n so that $k = \psi(n)$, where ψ is the Eulerian ψ-function. Let G be the circulant graph of order n with $S = \{\alpha_1, \ldots, \alpha_k\}$. Let $\lambda_j = \omega^{j\alpha_1} + \omega^{j\alpha_2} + \cdots + \omega^{j\alpha_k}$, $1 \le j \le n$, where ω is a primitive n-th root of unity. Then the eigenvalues of G are $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$. We now want to compute $\mathscr{E}(G) = \sum |\lambda_i|$, the energy of G. Set $Q_i = \omega^{\alpha_i}$, $1 \le i \le k$. Then $\lambda_j = \sum_{i=1}^k Q_i^j$. Now $Q_1, \ldots, Q_k$ are the roots of the cyclotomic polynomial [309].

$$\Phi_n(X) = (X - Q_1)(X - Q_2) \cdots (X - Q_k) = X^k + a_1 X^{k-1} + \cdots + a_k \tag{5.36}$$

where $a_1 = -\sum_{i=1}^k Q_i$, etc., and as is well known, the coefficients a_i are all integers.

We apply Newton's interpolation method [30] to compute the eigenvalues λ_j. Consider

$$\begin{aligned}(1-Q_1\, y)(1-Q_2\, y)\cdots(1-Q_k\, y) &= 1-\left(\sum_i Q_i\right) y+\left(\sum_{i<j} Q_i\, Q_j\right) y^2-\cdots \\ &= 1 + a_1\, y + a_2\, y^2 + \cdots + a_k\, y^k .\end{aligned}$$

By means of logarithmic differentiation (with respect to y), we get

$$\sum_{i=1}^k \frac{-Q_i}{1 - Q_i\, y} = \frac{a_1 + 2a_2\, y + 3a_3\, y^2 + \cdots + ka_k\, y^{k-1}}{1 + a_1\, y + a_2\, y^2 + \cdots + a_k\, y^k} .$$

This gives

$$\begin{aligned}&\sum_{i=1}^k -Q_i \left(\sum_{j=0}^\infty Q_i^j\, y^j\right)(1 + a_1 y + a_2 y^2 + \cdots + a_k y^k) \\ &= a_1 + 2a_2\, y + 3a_3\, y^2 + \cdots + ka_k\, y^{k-1} \\ &\Rightarrow \left[\sum_{j=0}^\infty \left(\sum_{i=1}^k -Q_i^{j+1}\right) y^j\right](1 + a_1\, y + a_2\, y^2 + \cdots + a_k\, y^k) \\ &= \left[\sum_{j=0}^\infty -\lambda_{j+1}\, y^j\right](1 + a_1\, y + a_2\, y^2 + \cdots + a_k\, y^k) \\ &= (-\lambda_1 - \lambda_2\, y - \lambda_3\, y^2 - \cdots)(1 + a_1\, y + a_2\, y^2 + \cdots + a_k\, y^k) \\ &= a_1 + 2a_2\, y + 3a_3\, y^2 + \cdots + ka_k\, y^{k-1} .\end{aligned} \tag{5.37}$$

Equation (5.37) implies the following recurrence equations:

$$-\lambda_r - \lambda_{r-1} a_1 - \lambda_{r-2} a_2 - \cdots - \lambda_1 a_{r-1} = r\, a_r \ \text{ or } \ 0 \tag{5.38}$$

depending on whether $r \leq k$ or $r > k$.

Hence, if we know the a_i's (that is, if we know the cyclotomic polynomial $\Phi_n(X)$), then the λ_i's can be computed recursively.

We now take $n = p^r$, $r \geq 1$, and p a prime. Then $k = \psi(n) = p^r - p^{r-1}$. Now the cyclotomic polynomial $\Phi_n(X)$ is given by [309]

$$\Phi_n(X) = \prod_{d|n} (X^d - 1)^{\mu(n|d)} \tag{5.39}$$

where μ stands for the Möbius function defined by

$$\mu(m) = \begin{cases} 1 & \text{if } m = 1 \\ 0 & \text{if } m \text{ contains a square greater than 1} \\ (-1)^r & \text{if } m \text{ is a product of } r \text{ distinct primes .} \end{cases}$$

Hence,

$$\begin{aligned} \Phi_{p^r}(X) &= \prod_{d|n} (X^d - 1)^{\mu(p^r|d)} = (X^{p^r} - 1)^{\mu(1)} (X^{p^{r-1}} - 1)^{\mu(p)} \\ &= (X^{p^r} - 1)/(X^{p^{r-1}} - 1) \\ &= X^{(p-1)p^{r-1}} + X^{(p-2)p^{r-1}} + \cdots + X^{p^{r-1}} + 1 \,. \end{aligned} \tag{5.40}$$

From Eq. (5.36), recalling that $k = \psi(p^r) = (p-1)p^{r-1}$,

$$\begin{aligned} \Phi_{p^r}(X) = {} & X^{(p-1)p^{r-1}} + a_1 X^{(p-1)p^{r-1}-1} + a_2 X^{(p-1)p^{r-1}-2} \\ & + \cdots + a_{p^{r-1}} X^{(p-2)p^{r-1}} + \cdots + a_{2p^{r-1}} X^{(p-3)p^{r-1}} \\ & + \cdots + a_{(p-2)p^{r-1}} X^{p^{r-1}} + \cdots + a_{(p-1)p^{r-1}} \,. \end{aligned} \tag{5.41}$$

From Eqs. (5.40) and (5.41), we have $a_{p^{r-1}} = a_{2p^{r-1}} = \cdots = a_{(p-1)p^{r-1}} = 1$, whereas the remaining a_j's are zero. These, when substituted in Eq. (5.38), yield $\lambda_{p^{r-1}} = \lambda_{2p^{r-1}} = \cdots = \lambda_{(p-1)p^{r-1}} = -p^{r-1}$, while

$$\lambda_{p^r} = \sum_{j=1}^{k} Q_j^{p^r} = \sum_{j=1}^{k} (\omega^{\alpha_j})^{p^r} = \sum_{j=1}^{k} (\omega^{p^r})^{\alpha_j} = \sum_{j=1}^{k} 1 = k = (p-1)p^{r-1}. \tag{5.42}$$

Thus, from Eq. (5.42),

$$\mathscr{E}(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{i=1}^{p-1} |\lambda_{i\,p^{r-1}}| + |\lambda_{p^r}|$$
$$= (p-1)p^{r-1} + (p-1)p^{r-1} = 2(p-1)p^{r-1} .$$

Now the bound $\mathscr{E}_0$ for $\mathscr{E}(G)$ is given by

$$\mathscr{E}_0 = k + \sqrt{k(n-1)(n-k)}, \text{ (where } n = p^r \text{ and } k = (p-1)p^{r-1})$$
$$= (p-1)p^{r-1} + \sqrt{(p-1)p^{r-1}(p^r-1)(p^r-(p^r-p^{r-1}))} .$$

Hence,

$$\frac{\mathscr{E}(G)}{\mathscr{E}_0} = \frac{2}{1+\sqrt{1+p+p^2+\cdots+p^{r-1}}} \to 0$$

either as $p \to \infty$ or as $r \to \infty$.

This proves that there are $\psi(n)$-regular graphs of order n for infinitely many n, whose energies are much smaller than the bound $\mathscr{E}_0$. ∎

In [332], another class of graphs was constructed, which also support the above assertion. Let $q > 2$ be a positive integer. We take q copies of the complete graph K_q. Denote by $v_1, \ldots, v_q$ the vertices of K_q and the corresponding vertices in each copy by $v_1[i], \ldots, v_q[i]$, for $1 \leq i \leq q$. Let G_{q^2} be a graph consisting of q copies of K_q and q^2 edges by joining vertices $v_j[i]$ and $v_j[i+1]$, $(1 \leq i < q)$, $v_j[q]$, and $v_j[1]$ where $1 \leq j \leq q$. Obviously, the graph G_{q^2} is the Cartesian product $K_q \times C_q$ and is $q+1$-regular. Employing Corollary 4.7, deleting all the q^2 edges joining two copies of K_q, we have $\mathscr{E}(G_{q^2}) \leq \mathscr{E}(qK_q) + 2q^2$. Thus, $\mathscr{E}(G_{q^2}) \leq 2q(q-1) + 2q^2$. Then, it follows that

$$\frac{\mathscr{E}(G_{q^2})}{\mathscr{E}_0} \leq \frac{4q^2-2q}{q+1+\sqrt{(q+1)(q^2-1)(q^2-q-1)}}$$

$$\leq \frac{4q^2-2q}{(q^2-q-1)\sqrt{q+1}} \to 0 \quad \text{as } q \to \infty .$$

Thus, for any $\varepsilon > 0$, when q is large enough, the graph G_{q^2} satisfies the required condition (5.35).

In the same paper, Balakrishnan [26] proposed the following open problem:

Problem 5.1. Given a positive integer $n \geq 3$ and $\varepsilon > 0$, does there exist a k-regular graph G of order n, such that $\mathscr{E}(G)/\mathscr{E}_0 > 1 - \varepsilon$ for some $k < n-1$? ∎

In [332], the following theorem was proven:

Theorem 5.21. *For any $\varepsilon > 0$, there exist infinitely many n for which there exists a k-regular graph of order n with $k < n-1$ and $\mathscr{E}(G)/\mathscr{E}_0 > 1-\varepsilon$.*

Proof. It suffices to verify that an infinite sequence of graphs satisfies the condition. To this end, we focus on the Paley graphs (for details see [125]). Let $p \geq 11$ be a prime and $p \equiv 1 (\text{mod } 4)$. The Paley graph G_p of order p has the elements of the finite field $GF(p)$ as vertex set and two vertices are adjacent if and only if their difference is a nonzero square in $GF(p)$. It is well known that the Paley graph G_p is a $(p-1)/2$-regular graph and that its eigenvalues are $(p-1)/2$ (with multiplicity 1) and $(-1 \pm \sqrt{p})/2$ (both with multiplicity $(p-1)/2$). Consequently, we have

$$\begin{aligned} \mathscr{E}(G_p) &= \frac{p-1}{2} + \frac{-1+\sqrt{p}}{2} \cdot \frac{p-1}{2} + \frac{1+\sqrt{p}}{2} \cdot \frac{p-1}{2} \\ &= (p-1)\frac{1+\sqrt{p}}{2} > \frac{p^{3/2}}{2} \,. \end{aligned} \tag{5.43}$$

Moreover, $\mathscr{E}_0 = \frac{p-1}{2} + \sqrt{\frac{p-1}{2}(p-1)(p-\frac{p-1}{2})}$, and we deduce that

$$\mathscr{E}(G_p)/\mathscr{E}_0 > \frac{\frac{1}{2}\,p^{3/2}}{\frac{p-1}{2}(\sqrt{p+1}+1)} > \frac{\frac{1}{2}\,p^{3/2}}{\frac{p}{2}(\sqrt{p}+2)} \to 1 \text{ as } p \to \infty \,.$$

Therefore, for any $\varepsilon > 0$ and some integer N, if $p > N$, then it follows that $\mathscr{E}(G_p)/\mathscr{E}_0 > 1-\varepsilon$. Hence, the theorem is proved. ■

5.3 Lower Bounds

In [247], it was shown that for all regular graphs G with degree $k > 0$, the energy is not less than the number of vertices, i.e., $\mathscr{E}(G) \geq n$. Equality is attained if G consists of $n/(2p)$ components isomorphic to the complete bipartite graph $K_{p,p}$.

Eventually, several other classes of graphs were characterized for which $\mathscr{E} \geq n$ holds [177]. Among these are the hexagonal systems (representing benzenoid hydrocarbons [183]).

A trivial lower bound $\mathscr{E}(G) \geq 2\lambda_1$ is reported in [53]. Another lower bound for $\mathscr{E}$ was obtained by McClelland [368]. Start with

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} \lambda_i^2 + \sum_{i \neq j} |\lambda_i||\lambda_j| \,.$$

Since the geometric mean of positive numbers is not greater than their arithmetic mean,

$$\frac{1}{n(n-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| \geq \prod_{i \neq j} (|\lambda_i||\lambda_j|)^{1/n(n-1)} = \prod_{i=1}^{n} (|\lambda_i|)^{2/n} = |\det(\mathbf{A})|^{2/n} .$$

Hence,

$$\mathscr{E}(G)^2 \geq \sum_{i=1}^{n} \lambda_i^2 + n(n-1)|\det(\mathbf{A})|^{2/n} .$$

Theorem 5.22. $\mathscr{E}(G) \geq \sqrt{2m + n(n-1)|\det \mathbf{A}|^{2/n}}$. ■

If $\det A \neq 0$, which is equivalent to the condition that no graph eigenvalue is equal to zero, then from Theorem 5.22 follows that $\mathscr{E}(G) \geq n$. For bipartite graphs, a similar argument yields [142]

$$\mathscr{E}(G) \geq \sqrt{4m + n(n-2)|\det \mathbf{A}|^{2/n}} .$$

From Theorem 5.1, we know that $\mathscr{E}(G) \leq \sqrt{2mn}$ holds for all graphs. For particular classes of graphs, it is possible to find a constant g, such that $g\sqrt{2mn}$ is a lower bound for $\mathscr{E}(G)$. In the following, we list a result of this kind, valid for quadrangle-free graphs [530]. Some other lower bounds of this type are found in the papers [24, 158, 167, 467, 530].

Theorem 5.23. *Let G be a quadrangle-free (n, m)-graph with minimum degree $\delta \geq 1$ and maximum degree Δ. Then*

$$\mathscr{E}(G) > \frac{2\sqrt{2\delta\Delta}}{2(\delta + \Delta) - 1} \sqrt{2mn} .$$

Proof. If $\Delta = 1$, then $G \cong m\, K_2$ and the result follows easily.

Suppose that $\Delta > 1$. Note that $M_4^*(G) = \sum_{i=1}^{n} |\lambda_i|^4 = 2 \sum_{i=1}^{n} d_i^2 - 2m + 8Q$, where Q is the number of quadrangles in G. The equality in Ineq. (4.2) holds if and only if G is the disjoint union of complete bipartite graphs $K_{a_1,b_1}, \ldots, K_{a_k,b_k}$ such that $a_1\, b_1 = \cdots = a_k\, b_k$ for some $k \geq 1$.

Recall that $\sum_{i=1}^{n} d_i^2 \leq 2m(\delta + \Delta) - n\delta\Delta$, with equality if and only if all the vertex degrees of G are equal to either δ or to Δ [535].

Since G is quadrangle-free,

$$\mathscr{E}(G) \geq \sqrt{\frac{(2m)^3}{2[2m(\delta + \Delta) - n\delta\Delta] - 2m}}$$

with equality if and only if G is the disjoint union of k copies of the complete bipartite graph $K_{1,\Delta}$ for some $k \geq 1$.

To find a constant g, such that $\mathscr{E}(G) \geq g\sqrt{2mn}$, it is sufficient that g satisfies the condition

$$\sqrt{\frac{(2m)^3}{2[2m(\delta + \Delta) - n\delta\Delta] - 2m}} \geq g\sqrt{2mn}$$

i.e., we may choose g as $g = \min_{G \in \mathscr{G}} \gamma(G)$, where

$$\gamma(G) = \sqrt{\frac{2m^2}{n[2m(\delta + \Delta) - n\delta\Delta] - mn}}$$

and where $\mathscr{G}$ is the set of all quadrangle-free graphs with n vertices, m edges, minimum degree δ, and maximum degree Δ.

It is easy to see that when $[2(\delta + \Delta) - 1]m = 2\delta\Delta n$, then $\gamma(G)$ attains its minimal value $2\sqrt{2\delta\Delta}/[2(\delta + \Delta) - 1]$. But if G is the disjoint union of k copies of the complete bipartite graph $K_{1,\Delta}$ for $k \geq 1$, then $[2(\delta+\Delta)-1]m = 2\delta\Delta n$ becomes $[2(1 + \Delta) - 1]k\Delta = 2\Delta k(\Delta + 1)$, which is obviously impossible. Therefore, $\mathscr{E}(G) > g\sqrt{2mn}$ with $g = 2\sqrt{2\delta\Delta}/[2(\delta + \Delta) - 1]$, which proves the theorem. ■

It is easy to obtain the following corollary from Theorem 5.23, which was first stated in [168]:

Corollary 5.1. *For a quadrangle-free (n, m)-graph G with maximum degree 2 and no isolated vertices, $\mathscr{E}(G) > \frac{4}{5}\sqrt{2mn}$. If the maximum vertex degree is 3, then $\mathscr{E}(G) > \frac{2\sqrt{6}}{7}\sqrt{2mn}$.* ■

The authors of [305] expressed the opinion that for a given $\varepsilon > 0$ and almost all $n \geq 1$, there exists a graph G on n vertices for which $\mathscr{E}(G) \geq (1-\varepsilon)(n/2)(\sqrt{n}+1)$. Nikiforov [383, 384] arrived at a stronger result, valid for sufficiently large n.

We write $M_{m,n}$ for the set of $m \times n$ matrices and A^* for the Hermitian adjoint of $\mathbf{A}$. As we have defined, let $s_1(\mathbf{A}) \geq s_2(\mathbf{A}) \geq \cdots$ be the singular values of a matrix $\mathbf{A}$. Note that if $\mathbf{A} \in M_{n,n}$ is a Hermitian matrix with eigenvalues $\mu_1(\mathbf{A}) \geq \cdots \geq \mu_n(\mathbf{A})$, then $s_1(\mathbf{A}), s_2(\mathbf{A}), \ldots, s_n(\mathbf{A})$ are the moduli of $\mu_i(\mathbf{A})$ taken in descending order, for details see [265]. For any $\mathbf{A} \in M_{m,n}$, call $\mathscr{E}(\mathbf{A}) = s_1(\mathbf{A}) + \cdots + s_m(\mathbf{A})$ the energy of $\mathbf{A}$.

Theorem 5.24. *(i) For all sufficiently large n, there exists a graph G of order n with $\mathscr{E}(G) \geq \frac{1}{2}n^{3/2} - n^{11/10}$.*

(ii) For almost all graphs,

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

Moreover, $\mathscr{E}(G) = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2}$ for almost all graphs G.

Proof. (i) Note first that for any graph G of order n and size m, it is $\sum_{i=1}^{n} s_i^2(G) = tr(A^2(G)) = 2m$, and so

$$2m - s_1^2(G) = s_2^2(G) + \cdots + s_n^2(G) \leq s_2(G)\big[\mathscr{E}(G) - s_1(G)\big] .$$

Hence, if $m > 0$, then

$$\mathscr{E}(G) \geq s_1(G) + \frac{2m - s_1^2(G)}{s_2(G)} . \tag{5.44}$$

Let $p \geq 11$ be a prime, $p \equiv 1(\mathrm{mod}\ 4)$, and G_p be the Paley graph of order p. It is known that G_p is a regular graph of degree $(p-1)/2$ and $s_2(G_p) = (\sqrt{p}+1)/2$. From Ineq. (5.43), we see that $\mathscr{E}(G_p) > \frac{1}{2}\, p^{3/2}$. Hence, if n is a prime and $n \equiv 1(\mathrm{mod}\ 4)$, then the theorem holds. In order to prove the theorem for any n, recall that for n sufficiently large, there exists a prime p, such that $p \equiv 1(\mathrm{mod}\ 4)$ and $p \leq n + n^{11/20} + \varepsilon$. Suppose that n is large and fix some prime $p \leq n + \frac{1}{2}\, n^{3/5}$. The average number of edges induced by a set of size n in G_p is

$$\frac{n(n-1)}{p(p-1)}\, m(G_p) = \frac{n(n-1)}{4} .$$

Therefore, there exists a set $X \subset V(G_p)$ with $|X| = n$ and $m(X) \geq n(n-1)/4$. Write G_n for $G_p[X]$-the graph induced by X. The Cauchy interlacing theorem implies that $s_2(G_n)s_2(G_p)$ and $s_1(G_n) \leq s_1(G_p)$. Therefore, in Ineq. (5.44), we see that

$$\mathscr{E}(G_n) \geq s_1(G_n) + \frac{2m(G_n) - s_1^2(G_n)}{s_2(G_n)} \geq \frac{n-1}{2} + \frac{\frac{n(n-1)}{2} - s_1^2(G_p)}{s_2(G_p)}$$

$$> \frac{n-1}{2} + \frac{\frac{n(n-1)}{2} - \frac{1}{4}\left(n + \frac{1}{2}n^{3/5}\right)^2}{\frac{1}{2}\left(\sqrt{n + \frac{1}{2}n^{3/5}} + 1\right)} > \frac{n^{3/2}}{2} - n^{11/10}$$

which completes the proof.

(ii) From Theorem 5.9, $\mathscr{E}(G) \leq \frac{n}{2}(1+\sqrt{n})$. For every $\mathbf{A}$, we have $s_1^2(\mathbf{A}) + s_2^2(\mathbf{A}) + \cdots = tr(\mathbf{A}\mathbf{A}^*) = \|\mathbf{A}\|_2^2$, and so $\|\mathbf{A}\|_2^2 - s_1^2(\mathbf{A}) = s_2^2(\mathbf{A}) + \cdots + s_m^2(\mathbf{A}) \leq s_2(\mathbf{A})(\mathscr{E}(\mathbf{A}) - s_1(\mathbf{A}))$. Thus, if $\mathbf{A}$ is a nonconstant matrix, then

$$\mathscr{E}(\mathbf{A}) \geq s_1(\mathbf{A}) + \frac{\|\mathbf{A}\|_2^2 - s_1^2(\mathbf{A})}{s_2(\mathbf{A})} .$$

If $\mathbf{A}$ is the adjacency matrix of a graph, this inequality is tight up to a factor of 2 for almost all graphs. To see this, recall that the adjacency matrix $\mathbf{A}(n, 1/2)$ of the random graph $G(n, 1/2)$ is a symmetric matrix with zero diagonal, whose entries a_{ij} are independent random variables and the expectation of a_{ij} is $1/2$, the variance of a_{ij}^2 is $\sigma^2 = 1/4$, and the expectation of a_{ij}^{2k} is $1/4^k$ for all $1 \le i < j \le n, k \ge 1$. A result of Füredi and Komlós [120] implies that, with probability tending to 1,

$$s_1(G(n,1/2)) = \left(\frac{1}{2} + o(1)\right) n$$

$$s_2(G(n,1/2)) < (2\sigma + o(1))\, n^{1/2} = (1 + o(1))\, n^{1/2} .$$

Hence, the above conclusion implies that

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

for almost all graphs G.

Moreover, the Wigner semicircle law (for details, we refer to Theorem 6.1) implies

$$\mathcal{E}(G(n,1/2))\, n^{-1/2} = n \left(\frac{2}{\pi} \int_{-1}^{1} |x| \sqrt{1 - x^2}\, \mathrm{d}x + o(1) \right) = \left(\frac{4}{3\pi} + o(1)\right) n$$

and so $\mathcal{E}(G) = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2}$ for almost all graphs G. ■

Chapter 6
The Energy of Random Graphs

In the previous chapter, several lower and upper bounds have been established for various classes of graphs, among which bipartite graphs are of particular interest. But only a few graphs attain the equalities in these bounds. In [105], an exact estimate of the energy of random graphs $G_n(p)$ was established, by using the Wigner semicircle law for any probability p. Furthermore, in [105], the energy of random multipartite graphs was investigated, by considering a generalization of the Wigner matrix, and some estimates of the energy of random multipartite graphs were obtained.

6.1 The Energy of $G_n(p)$

In this section, we formulate an exact estimate of the energy of almost all graphs by means of the Wigner semicircle law.

We start by recalling the Erdős–Rényi's random graph model $\mathcal{G}_n(p)$ (see [38]), consisting of all graphs with vertex set $[n] = \{1, 2, \ldots, n\}$ in which the edges are chosen independently with probability $p = p(n)$. Evidently, the adjacency matrix $\mathbf{A}(G_n(p))$ of the random graph $G_n(p) \in \mathcal{G}_n(p)$ is a random matrix, and thus, one readily evaluates the energy of $G_n(p)$ once the spectral distribution of the random matrix $\mathbf{A}(G_n(p))$ is known.

In fact, the study on the spectral distributions of random matrices is rather abundant and active and can be traced back to [493]. We refer the readers to [25, 100, 369] for an overview and some spectacular progress in this field. One important achievement in that field is the Wigner semicircle law which characterizes the limiting spectral distribution of the empirical spectral distribution of eigenvalues for a type of random matrices.

In order to characterize the statistical properties of the wave functions of quantum mechanical systems, Wigner in the 1950s investigated the spectral distribution for a class of random matrices, so-called *Wigner matrices*,

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$$\mathbf{X}_n := (x_{ij}) \ , \ 1 \le i, j \le n$$

which satisfy the following conditions:

- The x_{ij}'s are independent random variables with $x_{ij} = x_{ji}$.
- The x_{ii}'s have the same distribution F_1, whereas the x_{ij}'s $(i \ne j)$ have the same distribution F_2 .
- $\mathbb{V}\mathrm{ar}(x_{ij}) = \sigma_2^2 < \infty$ for all $1 \le i < j \le n$.

We denote the eigenvalues of $\mathbf{X}_n$ by $\lambda_{1,n}, \lambda_{2,n}, \ldots, \lambda_{n,n}$ and their empirical spectral distribution (ESD) by

$$\Phi_{\mathbf{X}_n}(x) = \frac{1}{n} \cdot \#\{\lambda_{i,n} \mid \lambda_{i,n} \le x, \ i = 1, 2, \ldots, n\} \ .$$

Wigner [491, 492] considered the limiting spectral distribution (LSD) of $\mathbf{X}_n$ and obtained his semicircle law as follows:

Theorem 6.1. *Let $\mathbf{X}_n$ be a Wigner matrix. Then*

$$\lim_{n\to\infty} \Phi_{n^{-1/2}\mathbf{X}_n}(x) = \Phi(x) \quad a.s.$$

i.e., with probability 1, the ESD $\Phi_{n^{-1/2}\mathbf{X}_n}(x)$ converges weakly to a distribution $\Phi(x)$ as n tends to infinity, where $\Phi(x)$ has the density

$$\phi(x) = \frac{1}{2\pi\sigma_2^2}\sqrt{4\sigma_2^2 - x^2}\, \mathbf{1}_{|x|\le 2\sigma_2} . \qquad \blacksquare$$

Remark 6.1. One of the classical methods to prove the above theorem is the moment approach. Employing this method, we get more information about the LSD of the Wigner matrix. Set $\mu_i = \int x \, \mathrm{d}F_i \ (i = 1, 2)$ and $\overline{\mathbf{X}}_n = \mathbf{X}_n - \mu_1 \mathbf{I}_n - \mu_2 (\mathbf{J}_n - \mathbf{I}_n)$, where $\mathbf{I}_n$ is the unit matrix of order n and $\mathbf{J}_n$ is the matrix of order n in which all entries are equal to 1. It is easily seen that the random matrix $\overline{\mathbf{X}}_n$ is also a Wigner matrix. By means of Theorem 6.1, we have

$$\lim_{n\to\infty} \Phi_{n^{-1/2}\overline{\mathbf{X}}_n}(x) = \Phi(x) \quad \text{a.s.} \tag{6.1}$$

Evidently, each entry of $\overline{\mathbf{X}}_n$ has mean 0. Furthermore, using the moment approach, Wigner [491, 492] showed that for each positive integer k,

$$\lim_{n\to\infty} \int x^k \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{X}}_n}(x) = \int x^k \, \mathrm{d}\Phi(x) \quad \text{a.s.} \tag{6.2}$$

It is interesting that the existence of the second moment of the off-diagonal entries is the necessary and sufficient condition for the semicircle law, but there is no moment requirement on the diagonal elements. For further comments on the moment approach and the Wigner semicircle law, we refer the readers to the seminal survey by Bai [25].

We say that *almost every (a.e.)* graph in $\mathscr{G}_n(p)$ has a certain property Q (see [38]) if the probability that a random graph $G_n(p)$ has the property Q converges to 1 as n tends to infinity. Occasionally, we write *almost all* instead of almost every. It is easy to see that if F_1 is a *point mass at 0*, i.e., $F_1(x) = 1$ for $x \geq 0$ and $F_1(x) = 0$ for $x < 0$, and F_2 is the *Bernoulli distribution with mean* p, then the Wigner matrix $\mathbf{X}_n$ coincides with the adjacency matrix $\mathbf{A}(G_n(p))$ of the random graph $G_n(p)$. Obviously, $\sigma_2 = \sqrt{p(1-p)}$ in this case.

In order to establish the exact estimate of the energy $\mathscr{E}(G_n(p))$ for a.e. graph $G_n(p)$, we first present some notions. In what follows, for convenience we use $\mathbf{A}$ to denote the adjacency matrix $\mathbf{A}(G_n(p))$. Set

$$\overline{\mathbf{A}} = \mathbf{A} - p(\mathbf{J}_n - \mathbf{I}_n) .$$

It is easy to check that each entry of $\overline{\mathbf{A}}$ has mean 0. We define the *energy* $\mathscr{E}(\mathbf{M})$ *of a matrix* $\mathbf{M}$ as the sum of absolute values of the eigenvalues of $\mathbf{M}$ (for details, see Sect. 11.3). By virtue of the following two lemmas, we shall formulate an estimate of the energy $\mathscr{E}(\overline{\mathbf{A}})$ and then establish the exact estimate of $\mathscr{E}(\mathbf{A}) = \mathscr{E}(G_n(p))$ by using Theorem 4.17 (the Ky Fan's theorem). Let I be the interval $[-1, 1]$.

Lemma 6.1. *Let I^c be the set $\mathbb{R} \setminus I$. Then*

$$\lim_{n\to\infty} \int_{I^c} x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \int_{I^c} x^2 \,\mathrm{d}\Phi(x) \quad \textit{a.s.}$$

Proof. Suppose that $\phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$ is the density of $\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$. According to Eq. (6.1), with probability 1, $\phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$ converges to $\phi(x)$ almost everywhere as n tends to infinity. Since $\phi(x)$ is bounded on I, it follows that with probability 1, $x^2\phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$ is bounded almost everywhere on I. Then the bounded convergence theorem yields

$$\lim_{n\to\infty} \int_{I} x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \int_{I} x^2 \,\mathrm{d}\Phi(x) \quad \text{a.s.}$$

Combining the above fact with Eq. (6.2), we get

$$\begin{aligned}
\lim_{n\to\infty} \int_{I^c} x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) &= \lim_{n\to\infty} \left(\int x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) - \int_I x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) \right) \\
&= \lim_{n\to\infty} \int x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) - \lim_{n\to\infty} \int_I x^2 \,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) \\
&= \int x^2 \,\mathrm{d}\Phi(x) - \int_I x^2 \mathrm{d}\Phi(x) \quad \text{a.s.} \\
&= \int_{I^c} x^2 \,\mathrm{d}\Phi(x) \quad \text{a.s.}
\end{aligned}$$

■

Lemma 6.2 ([34, p. 219]). *Let μ be a measure. Suppose that the functions a_n, b_n, and f_n converge almost everywhere to functions a, b, and f, respectively, and that $a_n \le f_n \le b_n$ almost everywhere. If $\int a_n \, \mathrm{d}\mu \to \int a \, \mathrm{d}\mu$ and $\int b_n \, \mathrm{d}\mu \to \int b \, \mathrm{d}\mu$, then $\int f_n \, \mathrm{d}\mu \to \int f \, \mathrm{d}\mu$.* ■

We now turn to the estimate of the energy $\mathscr{E}(\overline{\mathbf{A}})$. To this end, we first investigate the convergence of $\int |x| \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$. According to Eq. (6.1) and the bounded convergence theorem, by an argument similar to the first part of the proof of Lemma 6.1, we deduce that

$$\lim_{n\to\infty} \int_I |x| \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \int_I |x| \, \mathrm{d}\Phi(x) \quad \text{a.s.}$$

Obviously, $|x| \le x^2$ if $x \in I^c := \mathbb{R} \setminus I$. Set $a_n(x) = 0$, $b_n(x) = x^2 \, \phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$, and $f_n(x) = |x| \, \phi_{n^{-1/2}\overline{\mathbf{A}}}(x)$. Employing Lemmas 6.1 and 6.2, we have

$$\lim_{n\to\infty} \int_{I^c} |x| \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \int_{I^c} |x| \, \mathrm{d}\Phi(x) \quad \text{a.s.}$$

Consequently,

$$\lim_{n\to\infty} \int |x| \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \int |x| \, \mathrm{d}\Phi(x) \quad \text{a.s.} \tag{6.3}$$

Suppose that $\overline{\lambda}_1, \ldots, \overline{\lambda}_n$ and $\overline{\lambda}'_1, \ldots, \overline{\lambda}'_n$ are the eigenvalues of $\overline{\mathbf{A}}$ and $n^{-1/2}\overline{\mathbf{A}}$, respectively. Clearly,

$$\sum_{i=1}^{n} |\overline{\lambda}_i| = n^{1/2} \sum_{i=1}^{n} |\overline{\lambda}'_i| \, .$$

By Eq. (6.3), we deduce that

$$\begin{aligned}
\mathscr{E}\left(\overline{\mathbf{A}}\right)/n^{3/2} &= \frac{1}{n^{3/2}} \sum_{i=1}^{n} |\overline{\lambda}_i| = \frac{1}{n} \sum_{i=1}^{n} |\overline{\lambda}'_i| = \int |x| \, \mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) \\
&\to \int |x| \, \mathrm{d}\Phi(x) \quad \text{a.s.} \quad (n \to \infty) \\
&= \frac{1}{2\pi\sigma_2^2} \int_{-2\sigma_2}^{2\sigma_2} |x| \sqrt{4\sigma_2^2 - x^2} \, \mathrm{d}x = \frac{8}{3\pi}\sigma_2 = \frac{8}{3\pi} \sqrt{p(1-p)} \, .
\end{aligned}$$

Therefore, the energy $\mathscr{E}\left(\overline{\mathbf{A}}\right)$ satisfies a.s. the equation

$$\mathscr{E}\left(\overline{\mathbf{A}}\right) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) .$$

By means of Theorem 4.17, it is not difficult to verify that the eigenvalues of the matrix $\mathbf{J}_n - \mathbf{I}_n$ are $n-1$ and -1 ($n-1$ times). Consequently, $\mathscr{E}(\mathbf{J}_n - \mathbf{I}_n) = 2(n-1)$. One readily sees that $\mathscr{E}\big(p(\mathbf{J}_n - \mathbf{I}_n)\big) = p\mathscr{E}(\mathbf{J}_n - \mathbf{I}_n)$. Thus, $\mathscr{E}\big(p(\mathbf{J}_n - \mathbf{I}_n)\big) = 2p(n-1)$. Since $\mathbf{A} = \overline{\mathbf{A}} + p(\mathbf{J}_n - \mathbf{I}_n)$, it follows from Theorem 4.17 that with probability 1,

$$\begin{aligned}\mathscr{E}(\mathbf{A}) &\leq \mathscr{E}\left(\overline{\mathbf{A}}\right) + \mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_n)) \\ &= n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) + 2p(n-1) .\end{aligned}$$

Consequently,

$$\lim_{n\to\infty} \frac{\mathscr{E}(\mathbf{A})}{n^{3/2}} \leq \frac{8}{3\pi}\sqrt{p(1-p)} \quad \text{a.s.} \tag{6.4}$$

On the other hand, since $\overline{\mathbf{A}} = \mathbf{A} + p\big(-(\mathbf{J}_n - \mathbf{I}_n)\big)$, by Theorem 4.17, we deduce that with probability 1,

$$\begin{aligned}\mathscr{E}(\mathbf{A}) &\geq \mathscr{E}\left(\overline{\mathbf{A}}\right) - \mathscr{E}\left(p\big(-(\mathbf{J}_n - \mathbf{I}_n)\big)\right) \\ &= \mathscr{E}\left(\overline{\mathbf{A}}\right) - \mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_n)) \\ &= n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) - 2p(n-1) .\end{aligned}$$

Consequently,

$$\lim_{n\to\infty} \frac{\mathscr{E}(\mathbf{A})}{n^{3/2}} \geq \frac{8}{3\pi}\sqrt{p(1-p)} \quad \text{a.s.} \tag{6.5}$$

Combining Ineq. (6.4) with Ineq. (6.5), we obtain

$$\mathscr{E}(\mathbf{A}) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) \quad \text{a.s.}$$

Recalling that $\mathbf{A}$ is the adjacency matrix of $G_n(p)$, we thus obtain:

Theorem 6.2. *Almost every graph G in $G_n(p)$ satisfies:*

$$\mathscr{E}(G) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right). \tag{6.6}$$

6.2 The Energy of the Random Multipartite Graph

We begin with the definition of the random multipartite graph. We use $K_{n;\nu_1,\ldots,\nu_m}$ to denote the complete m-partite graph with vertex set $[n]$ whose parts $V_1,\ldots,V_m$ ($m = m(n) \geq 2$) are such that $|V_i| = n\nu_i = n\nu_i(n)$, $i = 1,\ldots,m$. Let $\mathscr{G}_{n;\nu_1\ldots\nu_m}(p)$ be the set of random m-partite graphs with vertex set $[n]$ in which the edges are chosen independently with probability p from the set of edges of $K_{n;\nu_1,\ldots,\nu_m}$. We further introduce two classes of random m-partite graphs. Denote by $\mathscr{G}_{n,m}(p)$ and $\mathscr{G}'_{n,m}(p)$, respectively, the sets of random m-partite graphs satisfying, respectively, the following conditions:

$$\lim_{n\to\infty} \max\{\nu_1(n),\ldots,\nu_m(n)\} > 0, \qquad \lim_{n\to\infty} \frac{\nu_i(n)}{\nu_j(n)} = 1 \tag{6.7}$$

and

$$\lim_{n\to\infty} \max\{\nu_1(n),\ldots,\nu_m(n)\} = 0\,. \tag{6.8}$$

One can easily see that in order to obtain an estimate of the energy of the random multipartite graph $G_{n;\nu_1\ldots\nu_m}(p) \in \mathscr{G}_{n;\nu_1\ldots\nu_m}(p)$, we need to investigate the spectral distribution of the random matrix $\mathbf{A}(G_{n;\nu_1\ldots\nu_m}(p))$. It is not difficult to verify that $\mathbf{A}(G_{n;\nu_1\ldots\nu_m}(p))$ would be a special case of a random matrix $\mathbf{X}_n(\nu_1,\ldots,\nu_m)$ (or $\mathbf{X}_{n,m}$ for short) called a *random multipartite matrix* which has the following properties:

- The x_{ij}'s are independent random variables with $x_{ij} = x_{ji}$.
- The x_{ij}'s have the same distribution F_1 if i and $j \in V_k$, whereas the x_{ij}'s have the same distribution F_2 if $i \in V_k$ and $j \in [n] \setminus V_k$, where $V_1,\ldots,V_m$ are the parts of $K_{n;\nu_1,\ldots,\nu_m}$ and k is an integer such that $1 \leq k \leq m$.
- $|x_{ij}| \leq K$ for some constant K.

Evidently, if F_1 is a point mass at 0 and F_2 is a Bernoulli distribution with mean p, then the random matrix $\mathbf{X}_{n,m}$ coincides with the adjacency matrix $\mathbf{A}(G_{n;\nu_1\ldots\nu_m}(p))$. Thus, we can readily evaluate the energy $\mathscr{E}(G_{n;\nu_1\ldots\nu_m}(p))$ once we obtain the spectral distribution of $\mathbf{X}_{n,m}$. In fact, the random matrix $\mathbf{X}_{n,m}$ is a special case of the random matrix considered by Anderson and Zeitouni [19] in a more general setting called the band matrix model which may be regarded as a generalization of the Wigner matrix. We shall employ their results to deal with the spectral distribution of $\mathbf{X}_{n,m}$.

The rest of this section is divided into three parts. In the first part, we present, respectively, exact estimates of the energies of random graphs $G_{n,m}(p) \in \mathscr{G}_{n,m}(p)$ and $G'_{n,m}(p) \in \mathscr{G}'_{n,m}(p)$ by exploring the spectral distribution of the band matrix. In the second part, we establish lower and upper bounds of the energy of the random multipartite graph $G_{n;\nu_1\ldots\nu_m}(p)$. In the third part, we obtain an exact estimate of the energy of the random bipartite graph $G_{n;\nu_1,\nu_2}(p)$.

6.2.1 The Energy of $G_{n,m}(p)$ and $G'_{n,m}(p)$

Here we formulate exact estimates of the energy of the random graphs $G_{n,m}(p)$ and $G'_{n,m}(p)$. For this purpose, we establish the following theorem. In order to state our result, we first present some notation. Let $\mathbf{I}_{n,m} = (i_{p,q})_{n\times n}$ be a *quasi-unit matrix* such that

$$i_{p,q} = \begin{cases} 1 & \text{if } p,q \in V_k \\ 0 & \text{if } p \in V_k \text{ and } q \in [n] \setminus V_k \end{cases}$$

where $V_1, \ldots, V_m$ are the parts of $K_{n;\nu_1,\ldots,\nu_m}$ and k is an integer such that $1 \le k \le m$. Set $\mu_i = \int x \, \mathrm{d}F_i$ $(i = 1, 2)$ and

$$\overline{\mathbf{X}}_{n,m} = \mathbf{X}_{n,m} - \mu_1 \mathbf{I}_{n,m} - \mu_2(\mathbf{J}_n - \mathbf{I}_{n,m}) \, .$$

Evidently, $\overline{\mathbf{X}}_{n,m}$ is a random multipartite matrix as well, in which each entry has mean 0. In order to make our statement concise, we define $\Delta^2 = (\sigma_1^2 + (m-1)\sigma_2^2)/m$.

Theorem 6.3. (i) *If condition (6.7) holds, then*

$$\Phi_{n^{-1/2}\overline{\mathbf{X}}_{n,m}}(x) \to_P \Psi(x) \text{ as } n \to \infty$$

i.e., the ESD $\Phi_{n^{-1/2}\overline{\mathbf{X}}_{n,m}}(x)$ converges weakly to a probability distribution $\Psi(x)$ as n tends to infinity, where $\Psi(x)$ has the density

$$\psi(x) = \frac{1}{2\pi\Delta^2}\sqrt{4\Delta^2 - x^2}\, \mathbf{1}_{|x|\le 2\Delta} \, .$$

(ii) *If condition (6.8) holds, then $\Phi_{n^{-1/2}\overline{\mathbf{X}}_{n,m}}(x) \to_P \Phi(x)$ as $n \to \infty$.* ■

Our theorem can be proven by a result of Anderson and Zeitouni [19]. We begin with a brief introduction of the band matrix model, defined by Anderson and Zeitouni [19], from which one can readily see that a random multipartite matrix is a band matrix.

We fix a nonempty set $\mathscr{C} = \{c_1, c_2, \ldots, c_m\}$ which is finite or countably infinite. The elements of $\mathscr{C}$ are called *colors*. Let κ be a surjection from $[n]$ to the color set $\mathscr{C}$. Then we say that $\kappa(i)$ is the color of i. Naturally, we can obtain a partition $V_1, \ldots, V_m$ of $[n]$ according to the colors of its elements, i.e., two elements i and i' in $[n]$ belong to the same part V_j if and only if their colors are identical. We next define the probability measure θ_m on the color set as:

$$\theta_m(C) = \theta_{m(n)}(C) = |\kappa^{-1}(C)|/n \;\; , \;\; 1 \le i \le m = m(n)$$

where $C \subseteq \mathscr{C}$ and $\kappa^{-1}(C) = \{x \in [n] : \kappa(x) \in C\}$. Evidently, the probability space $(\mathscr{C}, 2^{\mathscr{C}}, \theta_m)$ is discrete. Set $\theta = \lim_{n\to\infty} \theta_m$. For each positive integer k, we fix a bounded nonnegative function $d^{(k)}$ on the color set and a symmetric bounded nonnegative function $s^{(k)}$ on the product of two copies of the color set. We make the following assumptions:

(1) $d^{(k)}$ is constant for $k \neq 2$.
(2) $s^{(k)}$ is constant for $k \notin \{2, 4\}$.

Let $\{\xi_{ij}\}_{i,j=1}^{n}$ be a family of independent real-valued mean zero random variables. Suppose that for all $1 \leq i, j \leq n$, and positive integers k,

$$\mathrm{e}(|\xi_{ij}|^k) \leq \begin{cases} s^{(k)}(\kappa(i), \kappa(j)) \text{ if } i \neq j \\ d^{(k)}(\kappa(i)) \qquad \text{ if } i = j, \end{cases}$$

and moreover, assume that equality holds above whenever one of the conditions (a) and (b) holds: (a) $k = 2$ (b) $i \neq j$ and $k = 4$.

In other words, the rule is to enforce equality whenever the not-necessarily-constant functions $d^{(2)}$, $s^{(2)}$, or $s^{(4)}$ are involved but otherwise merely to impose a bound.

We are now ready to present the random symmetric matrix $\mathbf{Y}_n$, called *band matrix*, in which the entries are the r.v. ξ_{ij}. Evidently, $\mathbf{Y}_n$ is the same as $\overline{\mathbf{X}}_{n,m}$ provided that

$$s^{(2)}(\kappa(i), \kappa(j)) = \begin{cases} \sigma_1^2 \text{ if } \kappa(i) = \kappa(j) \\ \sigma_2^2 \text{ if } \kappa(i) \neq \kappa(j) \end{cases} \text{ and } d^{(2)}(\kappa(i)) = \sigma_1^2, 1 \leq i, j \leq n \,. \tag{6.9}$$

So the random multipartite matrix $\overline{\mathbf{X}}_{n,m}$ is a special case of the band matrix $\mathbf{Y}_n$.

Define the standard semicircle distribution $\Phi_{0,1}$ of zero mean and unit variance to be the measure on the real set of compact support with density

$$\phi_{0,1}(x) = \frac{1}{2\pi}\sqrt{4 - x^2}\, \mathbf{1}_{|x| \leq 2} \,.$$

Anderson and Zeitouni investigated the LSD of $\mathbf{Y}_n$ and proved the following result (Theorem 3.5 in [19]):

Lemma 6.3. *If* $\int s^{(2)}(c, c')\theta(\mathrm{d}c') \equiv 1$, *then* $\Phi_{n^{-1/2}\mathbf{Y}_n}(x)$ *converges weakly to the standard semicircle probability distribution* $\Phi_{0,1}$ *as n tends to infinity.* ∎

Remark 6.2. The main approach employed by Anderson and Zeitouni to prove the assertion is a combinatorial enumeration scheme for different types of terms that contribute to the expectation of products of traces of powers of the matrices. It is worthwhile to point out that by an analogous method, called moment approach, one can readily obtain a stronger assertion for $\overline{\mathbf{X}}_{n,m}$ that the convergence could be valid with probability 1. Moreover, Anderson and Zeitouni [19] showed that for each positive integer k,

$$\lim_{n\to\infty}\int x^k\,\Phi_{n^{-1/2}\overline{\mathbf{X}}_n}(x)=\begin{cases}\displaystyle\int x^k\,\Psi(x)\quad\text{a.s. if condition (6.7) holds,}\\[2ex]\displaystyle\int x^k\,\Phi(x)\quad\text{a.s. if condition (6.8) holds.}\end{cases}\tag{6.10}$$

However, we shall not present the proof of Eq. (6.10) here since the arguments of the two methods are similar and the calculation of the moment approach is rather tedious. We refer the readers to Bai's survey [25] for details.

Using Lemma 6.3 to prove Theorem 6.3, we just need to verify that

$$\int s^{(2)}(c,c')\theta(\mathrm{d}c')\equiv 1\,.$$

For Theorem 6.3(i), we consider the matrix $\Delta^{-1}\overline{\mathbf{X}}_{n,m}$ where

$$\Delta^2=(\sigma_1^2+(m-1)\sigma_2^2)/m\,.$$

Note that condition (6.7) implies that $\theta_m(c_i)\to 1/m$ as $n\to\infty$, $1\le i\le m$. By means of condition (6.9), it is readily seen that for the random matrix $\Delta^{-1}\overline{\mathbf{X}}_{n,m}$,

$$\int s^{(2)}(c,c')\theta(\mathrm{d}c')=\frac{1}{\Delta^2}\left(\frac{\sigma_1^2}{m}+\frac{(m-1)\sigma_2^2}{m}\right)\equiv 1\,.$$

Consequently, Lemma 6.3 implies that

$$\Phi_{n^{-1/2}\,\Delta^{-1}\overline{\mathbf{X}}_{n,m}}\to_P\Phi_{0,1}\text{ as }n\to\infty\,.$$

Therefore,

$$\Phi_{n^{-1/2}\overline{\mathbf{X}}_{n,m}}\to_P\Psi(x)\text{ as }n\to\infty$$

and thus, the first part of Theorem 6.3 follows.

For the second part of Theorem 6.3, we consider the matrix $\sigma_2^{-1}\overline{\mathbf{X}}_{n,m}$. Note that condition (6.8) implies that $\theta(c_i)=\lim\limits_{n\to\infty}\theta_m(c_i)=\lim\limits_{n\to\infty}\nu_i(n)=0, 1\le i\le m$. By virtue of condition (6.9), if $c\neq c'$, then $s^{(2)}(c,c')=1$. Consequently, for the random matrix $\sigma_2^{-1}\overline{\mathbf{X}}_{n,m}$, we have

$$\begin{aligned}\int s^{(2)}(c,c')\theta(\mathrm{d}c')&=\int s^{(2)}(c,c')\chi_{\mathscr{C}\setminus\{c\}}\theta(\mathrm{d}c')\\&=\int\chi_{\mathscr{C}\setminus\{c\}}\theta(\mathrm{d}c')=\theta(\mathscr{C}\setminus\{c\})\equiv 1\,.\end{aligned}$$

As a result, Lemma 6.3 implies that

$$\Phi_{n^{-1/2}\,\sigma_2^{-1}\overline{\mathbf{X}}_{n,m}}\to_P\Phi_{0,1}\text{ as }n\to\infty\,.$$

Therefore,

$$\Phi_{n^{-1/2}\overline{\mathbf{X}}_{n,m}} \to_P \Phi(x) \text{ as } n \to \infty$$

and thus, the second part follows.

We now employ Theorem 6.3 to estimate the energy of $G_{n;\nu_1\ldots\nu_m}(p)$ under conditions (6.7) or (6.8). For convenience, we use $\mathbf{A}_{n,m}$ to denote the adjacency matrix $\mathbf{A}(G_{n,m}(p))$. One readily sees that if a random multipartite matrix $\mathbf{X}_{n,m}$ satisfies condition (6.7) and F_1 is a point mass at 0 and F_2 is a Bernoulli distribution with mean p, then $\mathbf{X}_{n,m}$ coincides with the adjacency matrix $\mathbf{A}_{n,m}$. Set

$$\overline{\mathbf{A}}_{n,m} = \mathbf{A}_{n,m} - p(\mathbf{J}_n - \mathbf{I}_{n,m}) \tag{6.11}$$

where $\mathbf{I}_{n,m}$ is the quasi-unit matrix whose parts are the same as $\mathbf{A}_{n,m}$. Evidently, each entry of $\overline{\mathbf{A}}_{n,m}$ has mean 0. It follows from the first part of Theorem 6.3 that

$$\Phi_{n^{-1/2}\overline{\mathbf{A}}_{n,m}} \to_P \Psi(x) \text{ as } n \to \infty\,.$$

Since the density of $\Psi(x)$ is bounded with the finite support, we can use a method similar as for obtaining Eq. (6.3), to prove that

$$\int |x|\,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}_{n,m}}(x) \to_P \int |x|\,\mathrm{d}\Psi(x) \text{ as } n \to \infty\,.$$

Consequently,

$$\begin{aligned}
\mathscr{E}\left(\overline{\mathbf{A}}_{n,m}\right)/n^{3/2} &= \int |x|\,\mathrm{d}\Phi_{n^{-1/2}\overline{\mathbf{A}}_{n,m}}(x) \\
&\to_P \int |x|\,\mathrm{d}\Psi(x) \text{ as } n \to \infty \\
&= \frac{\sigma m}{2\pi(m-1)\sigma_2^2} \int\limits_{-2\sqrt{\frac{m-1}{m}}\sigma_2}^{2\sqrt{\frac{m-1}{m}}\sigma_2} |x| \sqrt{4\frac{(m-1)\sigma_2^2}{m} - x^2}\,\mathrm{d}x \\
&= \frac{8}{3\pi}\sqrt{\frac{m-1}{m}}\,\sigma_2 = \frac{8}{3\pi}\sqrt{\frac{m-1}{m}\,p(1-p)}\,.
\end{aligned}$$

Therefore, a.e. random matrix $\overline{\mathbf{A}}_{n,m}$ satisfies:

$$\mathscr{E}\left(\overline{\mathbf{A}}_{n,m}\right) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{\frac{m-1}{m}\,p(1-p)} + o(1)\right).$$

We now turn to the estimate of the energy $\mathscr{E}(\mathbf{A}_{n,m}) = \mathscr{E}(G_{n,m}(p))$. Evidently,

$$\mathbf{J}_n - \mathbf{I}_{n,m} = (\mathbf{J}_n - \mathbf{I}_n) + (\mathbf{I}_n - \mathbf{I}_{n,m}) \,.$$

By virtue of Theorem 4.17, we arrive at

$$\mathscr{E}(\mathbf{J}_n - \mathbf{I}_{n,m}) \leq \mathscr{E}(\mathbf{J}_n - \mathbf{I}_n) + \mathscr{E}(\mathbf{I}_n - \mathbf{I}_{n,m}) \,.$$

Recalling the definition of the quasi-unit matrix $\mathbf{I}_{n,m}$ and the fact that $\mathscr{E}(\mathbf{J}_n - \mathbf{I}_n) = 2(n-1)$, we have $\mathscr{E}(\mathbf{J}_n - \mathbf{I}_{n,m}) \leq O(n)$. According to Eq. (6.11), we use a similar argument for the estimate of the energy $\mathscr{E}(\mathbf{A})$ from $\mathscr{E}(\overline{\mathbf{A}})$ to show that a.e. random matrix $\mathbf{A}_{n,m}$ satisfies the following equation:

$$\mathscr{E}(\mathbf{A}_{n,m}) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{\frac{m-1}{m}p(1-p)} + o(1)\right).$$

Since the random matrix $\mathbf{A}_{n,m}$ is the adjacency matrix of $G_{n,m}(p)$, we thus have:

Theorem 6.4. *Almost every graph G in $G_{n,m}(p)$, satisfying the condition* (6.7)*, obeys*

$$\mathscr{E}(G) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{\frac{m-1}{m}p(1-p)} + o(1)\right). \tag{6.12}$$

In what follows, we use $\mathbf{A}'_{n,m}$ to denote the adjacency matrix $\mathbf{A}(G'_{n,m}(p))$. It is easily seen that if a random multipartite matrix $\mathbf{X}_{n,m}$ satisfies the condition (6.8), if F_1 is a point mass at 0, and if F_2 is a Bernoulli distribution with mean p, then $\mathbf{X}_{n,m}$ coincides with the adjacency matrix $\mathbf{A}'_{n,m}$. Set

$$\overline{\mathbf{A}'}_{n,m} = \mathbf{A}'_{n,m} - p(\mathbf{J}_n - \mathbf{I}'_{n,m})$$

where $\mathbf{I}'_{n,m}$ is the quasi-unit matrix whose parts are the same as $\mathbf{A}'_{n,m}$. One can readily check that each entry in $\overline{\mathbf{A}'}_{n,m}$ has mean 0. It follows from the second part of Theorem 6.3 that

$$\Phi_{n^{-1/2}\overline{\mathbf{A}'}_{n,m}}(x) \to_P \Phi(x) \text{ as } n \to \infty \,.$$

Employing the argument analogous to the estimate of $\mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_{n,m}))$, $\mathscr{E}(\overline{\mathbf{A}}_{n,m})$, and $\mathscr{E}(\mathbf{A}_{n,m})$, one can evaluate, respectively, $\mathscr{E}(p(\mathbf{J}_n - \mathbf{I}'_{n,m}))$, $\mathscr{E}(\overline{\mathbf{A}'}_{n,m})$, and $\mathscr{E}(\mathbf{A}'_{n,m})$ and finally arrive at:

Theorem 6.5. *Almost every graph G in $G'_{n,m}(p)$, satisfying the condition (6.8), obeys the equation:*

$$\mathscr{E}(G) = n^{3/2}\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) \,. \tag{6.13}$$

6.2.2 The Energy of $G_{n;\nu_1\ldots\nu_m}(p)$

In this subsection we give an estimate of the energy of the random multipartite graph $G_{n;\nu_1\ldots\nu_m}(p)$ satisfying the condition:

$$\lim_{n\to\infty} \max\{\nu_1(n),\ldots,\nu_m(n)\} > 0 \text{ and there exist } \nu_i \text{ and } \nu_j\ ,\ \lim_{n\to\infty} \frac{\nu_i(n)}{\nu_j(n)} < 1\ . \tag{6.14}$$

Moreover, for random bipartite graphs $G_{n;\nu_1,\nu_2}(p)$ satisfying $\lim_{n\to\infty} \nu_i(n) > 0$ $(i = 1, 2)$, we formulate an exact estimate of the energy.

Anderson and Zeitouni [19] established the existence of the LSD of $\mathbf{X}_{n,m}$ with partitions satisfying condition (6.14). Unfortunately, they failed to get the exact form of the LSD, which appears to be a much harder and complicated task. However, we can establish lower and upper bounds for the energy $\mathscr{E}(G_{n;\nu_1\ldots\nu_m}(p))$ in another way.

Here, we still denote the adjacency matrix of the multipartite graph satisfying condition (6.14) by $\mathbf{A}_{n,m}$. Without loss of generality, we assume that for some $r \geq 1$, $|V_1|,\ldots,|V_r|$ are of order $O(n)$ while $|V_{r+1}|,\ldots,|V_m|$ are of order $o(n)$. Let $\mathbf{A}'_{n,m}$ be a random symmetric matrix such that

$$\mathbf{A}'_{n,m}(ij) = \begin{cases} \mathbf{A}_{n,m}(ij) & \text{if } i \text{ or } j \notin V_s, 1 \leq s \leq r \\ t_{ij} & \text{if } i, j \in V_s, 1 \leq s \leq r \text{ and } i > j \\ 0 & \text{if } i, j \in V_s\ (r+1 \leq s \leq m) \text{ or } i = j \end{cases}$$

where the t_{ij}'s are independent Bernoulli r.v. with mean p. Evidently, $\mathbf{A}'_{n,m}$ is a random multipartite matrix. By means of Eq. (6.13), we have

$$\mathscr{E}(\mathbf{A}'_{n,m}) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) n^{3/2}\ .$$

Set

$$\mathbf{D}_n = \mathbf{A}'_{n,m} - \mathbf{A}_{n,m} = \begin{pmatrix} \mathbf{K}_1 & & & & & & \\ & \mathbf{K}_2 & & & & & \\ & & \ddots & & & & \\ & & & \mathbf{K}_r & & & \\ & & & & \mathbf{0} & & \\ & & & & & \ddots & \\ & & & & & & \mathbf{0} \end{pmatrix}_{n\times n}\ . \tag{6.15}$$

Then one can readily see that $\mathbf{K}_i$ $(i = 1, \ldots, r)$ is a Wigner matrix, and thus, a.e. $\mathbf{K}_i$ satisfies:

$$\mathscr{E}(\mathbf{K}_i) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right)(\nu_i\, n)^{3/2} .$$

Consequently, for a.e. matrix $\mathbf{D}_n$, it holds:

$$\mathscr{E}(\mathbf{D}_n) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right)\left(\nu_1^{3/2} + \cdots + \nu_r^{3/2}\right) n^{3/2} .$$

By Eq. (6.15), $\mathbf{A}_{n,m} + \mathbf{D}_n = \mathbf{A}'_{n,m}$ and $\mathbf{A}'_{n,m} + (-\mathbf{D}_n) = \mathbf{A}_{n,m}$. Employing Theorem 4.17, we deduce

$$\mathscr{E}(\mathbf{A}'_{n,m}) - \mathscr{E}(\mathbf{D}_n) \le \mathscr{E}(\mathbf{A}_{n,m}) \le \mathscr{E}(\mathbf{A}'_{n,m}) + \mathscr{E}(\mathbf{D}_n) .$$

Recalling that $\mathbf{A}_{n,m}$ is the adjacency matrix of $G_{n;\nu_1\ldots\nu_m}(p)$, the following result is relevant:

Theorem 6.6. *Almost every graph G in $G_{n;\nu_1\ldots\nu_m}(p)$ satisfies the inequalities:*

$$\left(1 - \sum_{i=1}^{r} \nu_i^{3/2}\right) n^{3/2} \le \mathscr{E}(G)\left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right)^{-1}$$
$$\le \left(1 + \sum_{i=1}^{r} \nu_i^{3/2}\right) n^{3/2}. \qquad \blacksquare$$

Remark 6.3. Since $\nu_1, \ldots, \nu_r$ are positive real numbers with $\sum_{i=1}^{r} \nu_i \le 1$, we have $\sum_{i=1}^{r} \nu_i(1-\nu_i^{1/2}) > 0$. Therefore, $\sum_{i=1}^{r} \nu_i > \sum_{i=1}^{r} \nu_i^{3/2}$, and thus, $1 > \sum_{i=1}^{r} \nu_i^{3/2}$. Hence, the above theorem implies that a.e. random graph $G_{n;\nu_1\ldots\nu_m}(p)$ obeys:

$$\mathscr{E}(G_{n;\nu_1\ldots\nu_m}(p)) = O(n^{3/2}) .$$

6.2.3 *The Energy of Random Bipartite Graphs*

In this subsection, we investigate the energy of random bipartite graphs $G_{n;\nu_1,\nu_2}(p)$ satisfying $\lim_{n\to\infty} \nu_i(n) > 0$ $(i = 1, 2)$ and present the precise estimate of $\mathscr{E}(G_{n;\nu_1,\nu_2}(p))$ by employing the Marčenko–Pastur Law.

For convenience, set $n_1 = \nu_1\, n$ and $n_2 = \nu_2\, n$. Let $\mathbf{I}_{n,2}$ be a quasi-unit matrix with the same partition as $\mathbf{A}_{n,2}$. Set

$$\overline{\mathbf{A}}_{n,2} = \mathbf{A}_{n,2} - p(\mathbf{J}_n - \mathbf{I}_{n,2}) = \begin{bmatrix} \mathbf{O} & \mathbf{X}^{\mathrm{T}} \\ \mathbf{X} & \mathbf{O} \end{bmatrix} \tag{6.16}$$

where $\mathbf{X}$ is a random matrix of order $n_2 \times n_1$ in which the entries $\mathbf{X}(ij)$ are iid. with mean zero and variance $\sigma^2 = p(1-p)$. By

$$\begin{pmatrix} \lambda \mathbf{I}_{n_1} & \mathbf{0} \\ -\mathbf{X} & \lambda \mathbf{I}_{n_2} \end{pmatrix} \begin{pmatrix} \lambda \mathbf{I}_{n_1} & -\mathbf{X}^{\mathrm{T}} \\ \mathbf{0} & \lambda \mathbf{I}_{n_2} - \lambda^{-1}\mathbf{X}\mathbf{X}^{\mathrm{T}} \end{pmatrix} = \lambda \begin{pmatrix} \lambda \mathbf{I}_{n_1} & -\mathbf{X}^{\mathrm{T}} \\ -\mathbf{X} & \lambda \mathbf{I}_{n_2}, \end{pmatrix}$$

we have

$$\lambda^n \cdot \lambda^{n_1} |\lambda \mathbf{I}_{n_2} - \lambda^{-1}\mathbf{X}\mathbf{X}^{\mathrm{T}}| = \lambda^n |\lambda \mathbf{I}_n - \overline{\mathbf{A}}_{n,2}|$$

and, consequently,

$$\lambda^{n_1} |\lambda^2 \mathbf{I}_{n_2} - \mathbf{X}\mathbf{X}^{\mathrm{T}}| = \lambda^{n_2} |\lambda \mathbf{I}_n - \overline{\mathbf{A}}_{n,2}| \ .$$

Thus, the eigenvalues of $\overline{\mathbf{A}}_{n,2}$ are symmetric, and moreover, $\overline{\lambda}$ is the eigenvalue of $\frac{1}{\sqrt{n_1}} \overline{\mathbf{A}}_{n,2}$ if and only if $\overline{\lambda}^2$ is the eigenvalue of $\frac{1}{n_1} \mathbf{X}\mathbf{X}^{\mathrm{T}}$. Therefore, we can characterize the spectrum of $\overline{\mathbf{A}}_{n,2}$ by means of the spectrum of $\mathbf{X}\mathbf{X}^{\mathrm{T}}$. Bai formulated the LSD of $\frac{1}{n_1} \mathbf{X}\mathbf{X}^{\mathrm{T}}$ (Theorem 2.5 in [25]) by moment approach.

Lemma 6.4 Marčenko–Pastur Law [25]**.** *Suppose that the* $\mathbf{X}(ij)$*'s are iid. with mean zero and variance* $\sigma^2 = p(1-p)$ *and* $\nu_2/\nu_1 \to y \in (0,\infty)$. *Then, with probability 1, the ESD* $\Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^{\mathrm{T}}}$ *converges weakly to the Marčenko–Pastur Law* F_y *as* $n \to \infty$ *where* F_y *has the density*

$$f_y(x) = \frac{1}{2\pi p(1-p)xy} \sqrt{(b-x)(x-a)}\, \mathbf{1}_{a \le x \le b}$$

and has a point mass $1 - 1/y$ *at the origin if* $y > 1$, *where* $a = p(1-p)(1-\sqrt{y})^2$ *and* $b = p(1-p)(1+\sqrt{y})^2$. ■

By the symmetry of the eigenvalues of $\frac{1}{\sqrt{n_1}} \overline{\mathbf{A}}_{n,2}$, in order to evaluate the energy $\mathscr{E}(\frac{1}{\sqrt{n_1}} \overline{\mathbf{A}}_{n,2})$, we just need to consider the positive eigenvalues. Define $\Theta_{n_2}(x) = \frac{\sum 1_{\overline{\lambda} < x}}{n_2}$. One can see that the sum of the positive eigenvalues of $\frac{1}{\sqrt{n_1}} \overline{\mathbf{A}}_{n,2}$ is equal to $n_2 \int_0^{\infty} x \, \mathrm{d}\Theta_{n_2}(x)$. Suppose that $0 < x_1 < x_2$. Then we have

$$\Theta_{n_2}(x_2) - \Theta_{n_2}(x_1) = \Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^{\mathrm{T}}}(x_2^2) - \Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^{\mathrm{T}}}(x_1^2) \ .$$

It follows that

$$\int_0^{\infty} x \, \mathrm{d}\Theta_{n_2}(x) = \int_0^{\infty} \sqrt{x} \, \mathrm{d}\Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^{\mathrm{T}}}(x) \ .$$

Note that all eigenvalues of $\frac{1}{n_1} \mathbf{X}\mathbf{X}^{\mathrm{T}}$ are nonnegative. By the moment approach (see [25] for instance), we get

$$\begin{aligned}\int x^2\,\mathrm{d}\Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^\mathrm{T}}(x) &= \int_0^\infty x^2\,\mathrm{d}\Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^\mathrm{T}}(x)\\ &\to \int_0^\infty x^2\,\mathrm{d}F_y(x) \quad \text{a.s. } (n\to\infty)\\ &= \int x^2\,\mathrm{d}F_y(x)\;.\end{aligned}$$

Analogous to the proof of Eq. (6.3), we deduce that

$$\lim_{n\to\infty}\int_0^\infty \sqrt{x}\,\mathrm{d}\Phi_{\frac{1}{n_1}\mathbf{X}\mathbf{X}^\mathrm{T}}(x) = \int_0^\infty \sqrt{x}\,\mathrm{d}F_y(x) \quad \text{a.s.}$$

Therefore,

$$\lim_{n\to\infty}\int_0^\infty x\,\mathrm{d}\Theta_{n_2}(x) = \int_{\sqrt{a}}^{\sqrt{b}} \frac{1}{\pi p(1-p)y}\sqrt{(b-x^2)(x^2-a)}\,\mathrm{d}x \quad \text{a.s.}$$

Let

$$\Lambda = \int_{\sqrt{a}}^{\sqrt{b}} \frac{1}{\pi p(1-p)y}\sqrt{(b-x^2)(x^2-a)}\,\mathrm{d}x\;.$$

Then we obtain that for a.e. $\overline{\mathbf{A}}_{n,2}$, the sum of the positive eigenvalues is $(\Lambda + o(1))\,n_2\sqrt{n_1}$. Thus, a.e. $\mathscr{E}(\overline{\mathbf{A}}_{n,2})$ satisfies:

$$\mathscr{E}(\overline{\mathbf{A}}_{n,2}) = (2\Lambda + o(1))n_2\sqrt{n_1}\;.$$

Furthermore,

$$\Lambda = \frac{\sqrt{b}[(a+b)\,\mathrm{Ep}(1-a/b) - 2a\,\mathrm{Ek}(1-a/b)]}{3\pi p(1-p)y}$$

where Ek is the complete elliptic integral of the first kind and Ep is the complete elliptic integral of the second kind. For $t \in [0,1]$, these are defined as

$$\mathrm{Ek}(t) = \int_0^{\pi/2} \frac{\mathrm{d}\theta}{\sqrt{1-t\sin^2\theta}} \qquad \text{and} \qquad \mathrm{Ep}(t) = \int_0^{\pi/2}\sqrt{1-t\sin^2\theta}\,\mathrm{d}\theta\;.$$

For any t, the numerical values of $\mathrm{El}(t)$ and $\mathrm{Ep}(t)$ are readily computed by appropriate software.

Employing Eq. (6.16) and Theorem 4.17, we have

$$\mathscr{E}(\overline{\mathbf{A}}_{n,2}) - \mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_{n,2})) \leq \mathscr{E}(\mathbf{A}_{n,2}) \leq \mathscr{E}(\overline{\mathbf{A}}_{n,2}) + \mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_{n,2})) \; .$$

Together with the fact that $\mathscr{E}(p(\mathbf{J}_n - \mathbf{I}_{n,2})) = 2p\sqrt{\nu_1 \nu_2}\, n$ and $n_2\sqrt{n_1} = \nu_2\sqrt{\nu_1}\, n^{3/2}$, we get

$$\mathscr{E}(\mathbf{A}_{n,2}) = (2\nu_2\sqrt{\nu_1}\,\Lambda + o(1))n^{3/2} \; .$$

Therefore, the following theorem is relevant:

Theorem 6.7. *Almost every bipartite graph G in $G_{n;\nu_1,\nu_2}(p)$ with $\nu_2/\nu_1 \to y$ satisfies*

$$\mathscr{E}(G) = (2\nu_2\sqrt{\nu_1}\,\Lambda + o(1))n^{3/2} \; . \qquad \blacksquare$$

We now compare the above estimate of the energy $\mathscr{E}(G_{n;\nu_1,\nu_2}(p))$ with bounds obtained in Theorem 6.6 for $p = 1/2$. For the upper bound, Theorem 5.9 established an upper bound $\frac{n}{2}(\sqrt{n} + 1)$ of the energy $\mathscr{E}(G)$ for simple graphs G. It is easy to see that for $p = 1/2$, this upper bound is better than ours. So we turn our attention to comparing the estimate of $\mathscr{E}(G_{n;\nu_1,\nu_2}(1/2))$ in Theorem 6.7 with the lower bound in Theorem 6.6. By numerical computation (see the table below), the energy $\mathscr{E}(G_{n;\nu_1,\nu_2}(1/2))$ of a.e. random bipartite graphs $G_{n;\nu_1,\nu_2}(1/2)$ is found to be close to our lower bound.

y	real value of $\mathscr{E}(G_{n;\nu_1,\nu_2}(1/2))$	lower bound of $\mathscr{E}(G_{n;\nu_1,\nu_2}(1/2))$
1	$(0.3001 + o(1))n^{3/2}$	$(0.1243 + o(1))n^{3/2}$
2	$(0.2539 + o(1))n^{3/2}$	$(0.1118 + o(1))n^{3/2}$
3	$(0.2071 + o(1))n^{3/2}$	$(0.0957 + o(1))n^{3/2}$
4	$(0.1731 + o(1))n^{3/2}$	$(0.0828 + o(1))n^{3/2}$
5	$(0.1482 + o(1))n^{3/2}$	$(0.0727 + o(1))n^{3/2}$
6	$(0.1294 + o(1))n^{3/2}$	$(0.06470 + o(1))n^{3/2}$
7	$(0.1148 + o(1))n^{3/2}$	$(0.05828 + o(1))n^{3/2}$
8	$(0.1031 + o(1))n^{3/2}$	$(0.05301 + o(1))n^{3/2}$
9	$(0.09353 + o(1))n^{3/2}$	$(0.04862 + o(1))n^{3/2}$
10	$(0.08558 + o(1))n^{3/2}$	$(0.04491 + o(1))n^{3/2}$

Chapter 7
Graphs Extremal with Regard to Energy

One of the fundamental questions that is encountered in the study of graph energy is which graphs (from a given class) have greatest and smallest $\mathcal{E}$-values. The first such result was obtained for trees in [145], where it was demonstrated that the star has minimal and the path maximal energy. In the meantime, a remarkably large number of papers was published on such extremal problems: for general graphs [82,242,252, 253, 305, 306, 341, 416, 482], trees and chemical trees [141, 219, 268, 314, 316, 319, 324, 327, 339, 343, 344, 389, 390, 434, 435, 483, 487, 497, 498, 505, 506, 511, 517, 518, 543, 547], unicyclic [51, 58, 185, 191, 266, 270, 273–275, 277, 283, 312, 313, 330, 342, 480, 484–486, 488–490, 514], bicyclic [121, 267, 280, 340, 358, 500, 501, 522, 523], tricyclic [326, 329, 521], and tetracyclic graphs [325], as well as for benzenoid and related polycyclic systems [158, 243, 395, 399, 413–415, 519, 520, 526].

In this chapter we state a few of these results, selecting those that can be formulated in a simple manner or that otherwise deserve to be mentioned. We start with a few elementary results.

The n-vertex graph with minimal energy is $\overline{K_n}$, the graph consisting of isolated vertices, whose energy is zero. The minimal-energy n-vertex graph without isolated vertices is the complete bipartite graph $K_{1,n-1}$, also known as the star [53], whose energy is equal to $2\sqrt{n-1}$.

Finding the maximal-energy n-vertex graph(s) is a much more difficult task, and a complete solution of this problem is not known.

7.1 Trees with Extremal Energies

In the preceding chapter it was shown that $\mathcal{E}$ is a bounded quantity and various upper and lower bounds were derived [142, 368]. A related problem is which graphs (within a given class of graphs) have extremal (maximal and minimal) values of $\mathcal{E}$. Evidently, the answer to this question would provide the best possible bounds for $\mathcal{E}$ (within the class considered).

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_7,

Recall that among all n-vertex trees, the star S_n and the path P_n are the minimum- and maximum-energy tree, respectively. The second- and third-minimum-energy trees and the second-maximum-energy tree are also described in Sect. 4.3. The third- and fourth-maximum-energy trees are characterized in [319] and [219, 279, 327, 432, 434], respectively. Andriantiana [17] made a major breakthrough in this area, determining (for sufficiently large n) the first $3n - 84$ maximum-energy trees for odd n and the first $3n - 87$ maximum-energy trees for even n.

For more results on the ordering of the trees by minimal energies, we refer to [488].

In the following subsections, we will employ Method 3, "quasi-order," outlined in Sect. 4.3, to deal with extremal problems on some classes of trees. Exceptionally, in Sect. 7.1.3, the Method 4, "Coulson integral formula," and the Method 5, "graph operations," will be applied.

Lemma 7.1. *Let G and G' be two acyclic graphs. Suppose that u (resp. u') is a pendent vertex of G (resp. G') and uv (resp. $u'v'$) is the edge of G (resp. G') incident with u (resp. u'). If $G-u \succeq G'-u'$ and $G-u-v \succ G'-u'-v'$ or $G-u \succ G'-u'$ and $G-u-v \succeq G'-u'-v'$, then $G \succ G'$.*

Proof. Since uv is an edge of G with pendent vertex u, we have $\phi(G) = x\phi(G-u) - \phi(G-u-v)$, from which it follows that

$$m(G,k) = m(G-u,k) + m(G-u-v,k-1). \tag{7.1}$$

Similarly,

$$m(G',k) = m(G'-u',k) + m(G'-u'-v',k-1). \tag{7.2}$$

If $G-u \succeq G'-u'$ and $G-u-v \succ G'-u'-v'$, then by Eqs. (7.1) and (7.2), $m(G,k) \geq m(G',k)$ for all k and there is at least one k such that $m(G,k) > m(G',k)$, and so $G \succ G'$. Similarly, if $G-u \succ G'-u'$ and $G-u-v \succeq G'-u'-v'$, then $G \succ G'$. ■

7.1.1 Minimal Energy of Trees with a Given Maximum Degree

Given the maximum degree $\Delta(T)$, Lin et al. [344] characterized the trees with minimal energy among all trees T of order n and $\lceil \frac{n+1}{3} \rceil \leq \Delta(T) \leq n-2$. Heuberger and Wagner [260] completely characterized the trees with given maximum degree that minimize the energy for any $\Delta(T)$, which will be presented in this subsection.

In order to state our result, we use the notion of *complete d-ary trees*: The complete d-ary tree of height $h-1$ is denoted by CA_h, i.e., CA_1 is a single vertex and CA_h has d branches $CA_{h-1}, \ldots, CA_{h-1}$, as shown in Fig. 7.1. It is convenient to set CA_0 to be the null graph. For more properties of this class of trees, see [259–261]. We define a special tree $T^*_{n,d}$ as follows:

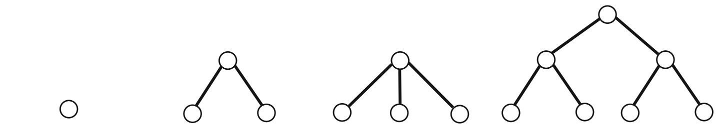


Fig. 7.1 Some small complete d-ary trees

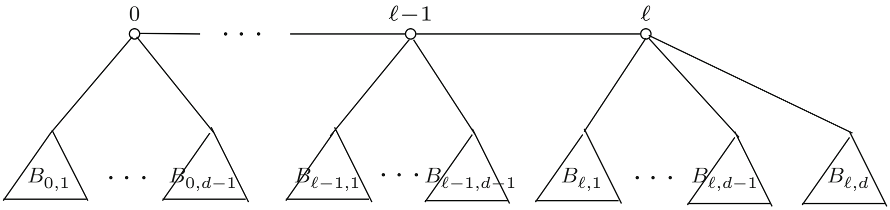


Fig. 7.2 Tree $T^*_{n,d}$

Definition 7.1. $T^*_{n,d}$ is the tree with n vertices that can be decomposed as in Fig. 7.2 with $B_{k,1}, \dots, B_{k,d-1} \in \{CA_k, CA_{k+2}\}$ for $0 \le k < \ell$ and either $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_{\ell-1}$ or $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_\ell$ or $B_{\ell,1}, \dots, B_{\ell,d} \in \{CA_\ell, CA_{\ell+1}, CA_{\ell+2}\}$, where at least two of $B_{\ell,1}, \dots, B_{\ell,d}$ equal $CA_{\ell+1}$. This representation is unique, and one has the "digital expansion"

$$(d-1)n + 1 = \sum_{k=0}^{\ell} a_k\, d^k \tag{7.3}$$

where $a_k = (d-1)[1 + (d+1)\, r_k]$ and $0 \le r_k \le d-1$ is the number of $B_{k,i}$ that is isomorphic to CA_{k+2} for $k < \ell$ and

- $a_\ell = 1$ if $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_{\ell-1}$
- $a_\ell = d$ if $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_\ell$
- or otherwise $a_\ell = d + (d-1)q_\ell + (d^2-1)r_\ell$ where $q_\ell \ge 2$ is the number of $B_{\ell,i}$ that is isomorphic to $CA_{\ell+1}$ and r_ℓ is the number of $B_{\ell,i}$ that is isomorphic to $CA_{\ell+2}$.

Denote by $\mathscr{T}_{n,d}$ the set of trees of order n with maximum degree $\Delta \le d+1$. Define the polynomial for all positive values of x,

$$M(T,x) = \sum_k m(T,k)\, x^k$$

where $m(T,k)$ denotes the number of matchings of T with cardinality k. Note that $M(T,x)$ is just another form of the *matching polynomial* [80, 111, 112, 124, 151], cf. Eq. (1.4).

We say that T is a *minimal tree* with respect to $x > 0$, if it minimizes $M(T,x)$ among all trees in $\mathscr{T}_{n,d}$, that is, for $x > 0$, $M(T^*_{n,d}, x) \le M(T,x)$ for any $T \in \mathscr{T}_{n,d}$.

Theorem 7.1. *Let n and d be positive integers and $x > 0$. Then $T^*_{n,d}$ is the unique (up to isomorphism) minimal tree in $\mathscr{T}_{n,d}$.* ■

The main theorem is an immediate consequence that follows from Eq. (4.7):

Theorem 7.2. *Let n and d be positive integers. Then $T^*_{n,d}$ is the unique (up to isomorphism) tree in $\mathscr{T}_{n,d}$ that minimizes the energy.* ■

Theorem 7.3. *The energy of $T^*_{n,d}$ is asymptotically $\mathscr{E}(T^*_{n,d}) = \alpha_d \cdot n + O(\log n)$, where*

$$\alpha_d = 2\sqrt{d}(d-1)^2 \left[\sum_{\substack{j \geq 1 \\ j \equiv 0 \pmod 2}} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) + \sum_{\substack{j \geq 1 \\ j \equiv 1 \pmod 2}} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right] \tag{7.4}$$

is a constant that only depends on d. ■

Let $x > 0$ be fixed. A typical way to determine $M(T, x)$ recursively is the formula

$$M(T, x) = M(T - e, x) + x\, M(T - v - w, x) \tag{7.5}$$

that holds for any edge $e = vw$ of T. For our purposes, it will be useful to introduce two auxiliary quantities first. We fix a root r of T and define $m_1(T, k)$ to be the number of matchings of cardinality k covering the root and $m_0(T, k)$ to be the number of matchings of cardinality k not covering the root.

Furthermore, we write $M_j(T, x) = \sum_k m_j(T, k)\, x^k$ for $j \in \{0, 1\}$. Obviously, we have $M(T, x) = M_0(T, x) + M_1(T, x)$. The ratio

$$\tau(T, x) = \frac{M_0(T, x)}{M(T, x)} \tag{7.6}$$

will be an important auxiliary quantity in our proofs. The following lemma summarizes important properties of all these quantities, for which we will provide short self-contained proofs as well (following the ideas used to prove Eq. (7.5)).

Lemma 7.2. *Let $T_1, \ldots, T_\ell$ be the branches of the rooted tree T. Then the following recursive formula holds:*

$$M_0(T, x) = \prod_{i=1}^{\ell} M(T_i, x) \tag{7.7}$$

$$M_1(T, x) = x \sum_{i=1}^{\ell} M_0(T_i, x) \prod_{\substack{j=1 \\ j \neq i}}^{\ell} M(T_j, x) \tag{7.8}$$

$$\tau(T, x) = \left[1 + x \sum_{i=1}^{\ell} \tau(T_i, x) \right]^{-1}. \tag{7.9}$$

Proof. A matching not covering the root corresponds to a selection of an arbitrary matching in each branch. If the matching of T is required to have cardinality k, then the cardinalities of the corresponding matchings in the branches must add up to k. This is exactly the coefficient of x^k in the product $\prod_{i=1}^{\ell} M(T_i, x)$. This proves Eq. (7.7).

Every matching of T covering the root contains exactly one edge between the root and some branch T_i. In this branch, a matching not covering the root of T_i may be chosen; in all other branches, arbitrary matchings are allowed. The cardinality of the matching of T is then the sum of the cardinalities of the matchings in the branches plus one for the edge incident to the root. This yields Eq. (7.8).

Finally, Eq. (7.9) is an immediate consequence of Eqs. (7.6)–(7.8). ∎

In the following, we will fix a positive integer d and consider only trees whose maximum degree is at most $d+1$. First of all, we study the behavior of the sequence $\tau(CA_h, x)$. It is convenient to set $M_0(CA_0, x) \equiv 0$ and $M_1(CA_0, x) \equiv 1$ for the polynomials associated to the empty tree. Note that this choice allows adding empty branches without disturbing the recursive formulas Eqs. (7.7)–(7.9). Then Eq. (7.9) translates into a the following recursion for $\tau(CA_h, k)$:

$$\tau(CA_h, x) = \frac{1}{1 + d \cdot x \cdot \tau(CA_{h-1}, x)}$$

with initial conditions $\tau(CA_0, x) = 0$ and $\tau(CA_1, x) = 1$.

It is an easy exercise to prove the following explicit formula for $\tau(CA_h, x)$ by means of induction:

Lemma 7.3. *For every $x > 0$,*

$$\tau(CA_h, x) = \frac{\left(\frac{1+\sqrt{1+4\mathrm{d}x}}{2}\right)^h - \left(\frac{1-\sqrt{1+4\mathrm{d}x}}{2}\right)^h}{\left(\frac{1+\sqrt{1+4\mathrm{d}x}}{2}\right)^{h+1} - \left(\frac{1-\sqrt{1+4\mathrm{d}x}}{2}\right)^{h+1}}. \qquad ∎$$

Now, the limit behavior of $\tau(CA_h, x)$ for positive x follows immediately.

Lemma 7.4. *For every $x > 0$, the subsequence $\tau(CA_{2h}, x)$ is strictly increasing, whereas the subsequence $\tau(CA_{2h+1}, x)$ is strictly decreasing. Both subsequences converge to the same limit $\frac{2}{1+\sqrt{1+4\mathrm{d}x}}$, and we have*

$$0 = \tau(CA_0, x) < \tau(CA_2, x) < \cdots < \frac{2}{1 + \sqrt{1 + 4\mathrm{d}x}}$$
$$< \cdots < \tau(CA_3, x) < \tau(CA_1, x) = 1. \qquad ∎$$

Lemma 7.5. *Let T be a rooted tree and $x > 0$. Then $\frac{1}{dx+1} \leq \tau(T, x) \leq 1$, unless T is empty, where $\tau(T, x) = 0$.*

Proof. It follows easily from induction and Lemma 7.2. ■

Definition 7.2. Let T be a rooted tree. We construct the *outline graph* of T by replacing all maximal subtrees isomorphic to some CA_k, $k \geq 0$, by a special leaf CA_k. In this process, we attach $d+1-r$ leaves CA_0 to internal vertices (nonleaves and nonroot) of degree r with $2 \leq r \leq d$. If T is a rooted tree with a root of degree r $(1 \leq r \leq d)$, then we also attach $d-r$ leaves CA_0 to it.

Lemma 7.6. *Let $j \geq 0$ be an integer and T a rooted tree whose outline does not contain any CA_k for $0 \leq k \leq j-3$ and $x > 0$. If either j is odd and $\tau(CA_j, x) \leq \tau(T, x)$ or j is even and $\tau(T, x) \leq \tau(CA_j, x)$, then $T \in \{CA_{j-2}, CA_j\}$.*

Proof. We first assume that $T \cong CA_\ell$ for some ℓ. Since the outline of T does not contain a CA_k for $k \leq j-3$, we conclude that $\ell \geq j-2$. The monotonicity properties of $\tau(CA_j, x)$ in Lemma 7.4 imply that $\ell \in \{j-2, j\}$ and we are done. Thus, we may assume that the outline of T is a d-ary rooted tree with more than one vertex.

We proceed by induction on j. If $j = 0$, the assumptions of the lemma imply that $\tau(T, x) \leq \tau(CA_0, x) = 0$, whence $T \cong CA_0$ by Lemma 7.5. Assume that $j \geq 1$. By our assumption, T is not empty and has (possibly empty) branches $T_1, T_2, \ldots, T_d$. Furthermore, there is no CA_k in the outlines of T_i for $k \leq j-3$.

Assume that j is even. Then

$$\frac{1}{1 + x \sum_{i=1}^{d} \tau(T_i, x)} = \tau(T, x) \leq \tau(CA_j, x) = \frac{1}{1 + d\, x\, \tau(CA_{j-1}, x)}$$

which is equivalent to

$$\sum_{i=1}^{d} \tau(T_i, x) \geq \mathrm{d}\tau(CA_{j-1}, x). \tag{7.10}$$

Without loss of generality, we may assume that $\tau(T_1, x) \geq \tau(T_2, x) \geq \cdots \geq \tau(T_d, x)$.

We claim that $T_i \cong CA_{j-1}$ for $1 \leq i \leq d$. We proceed by induction on i. Assume that the claim is proved up to $i-1$ for some $i \geq 1$. Then subtracting $(i-1)\tau(CA_{j-1}, x)$ from Ineq. (7.10) yields

$$(d-i+1)\tau(T_i, x) \geq \sum_{\ell=i}^{d} \tau(T_\ell, x) \geq (d-i+1)\tau(CA_{j-1}, x)$$

thus $\tau(T_i, x) \geq \tau(CA_{j-1}, x)$. By the (outer) induction hypothesis, we have $T_i \in \{CA_{j-1}, CA_{j-3}\}$. Since the outline of T_i does not contain any CA_k for $k \leq j-3$, we clearly have $T_i \ncong CA_{j-3}$ and therefore $T_i \cong CA_{j-1}$, as required.

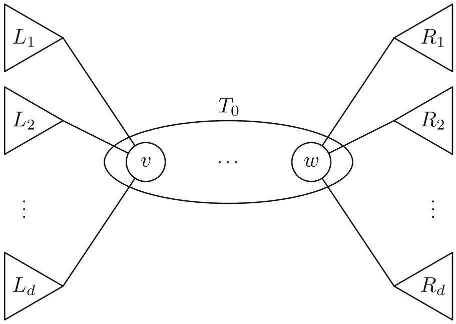


Fig. 7.3 The decomposition of T

Thus, $T_1 \cong \cdots \cong T_d \cong CA_{j-1}$, and therefore, $T \cong CA_j$, which has been handled earlier.

The proof for odd j follows by exchanging "odd" and "even" and reversing all inequality signs. ■

The key lemma is an exchange lemma which gives a local optimality criterion.

Lemma 7.7. *Let $x > 0$ and let T be a minimal tree with respect to x. If there are (possibly empty) rooted trees $L_1, \ldots, L_d, R_1, \ldots, R_d$ and a tree T_0 such that T can be decomposed as in Fig. 7.3 and such that $\tau(L_1, x) < \tau(R_1, x)$ (after appropriate reordering of the L_i's and the R_i's), then*

$$\max\{\tau(L_i, x) : 1 \le i \le d\} \le \min\{\tau(R_i, x) : 1 \le i \le d\}.$$

Proof. We need four auxiliary quantities:

(i) $m_{00}(T_0, k)$: the number of matchings of T_0 of cardinality k where neither v nor w is covered;
(ii) $m_{10}(T_0, k)$: the number of matchings of T_0 of cardinality k where v is covered, but w is not;
(iii) $m_{01}(T_0, k)$: the number of matchings of T_0 of cardinality k where w is covered, but v is not;
(iv) $m_{11}(T_0, k)$: the number of matchings of T_0 of cardinality k where both v and w are covered.

The corresponding polynomials are denoted by $M_{ij}(T_0, x) = \sum_k m_{ij}(T_0, k)\, x^k$. Define

$$G(L_1, \ldots, L_d, R_1, \ldots, R_d; x) := M_{00}(T_0, x)\left(1 + x\sum_{i=1}^{d}\tau(L_i, x)\right) \times \left(1 + x\sum_{i=1}^{d}\tau(R_i, x)\right)$$

$$+M_{10}(T_0,x)\left(1+x\sum_{i=1}^{d}\tau(R_i,x)\right)$$

$$+M_{01}(T_0,x)\left(1+x\sum_{i=1}^{d}\tau(L_i,x)\right)+M_{11}(T_0,x).$$

Then it is easily seen that

$$M(T,x)=G(L_1,\dots,L_d,R_1,\dots,R_d;x)\prod_{i=1}^{d}M(L_i,x)\prod_{i=1}^{d}M(R_i,x).$$

In view of the minimality of $M(T,x)$, we must have

$$G(L_1,\dots,L_d,R_1,\dots,R_d;x)\le G(\pi(L_1),\dots,\pi(L_d),\pi(R_1),\dots,\pi(R_d);x)$$

for all permutations π of $\{L_1,\dots,L_d,R_1,\dots,R_d\}$. Ignoring for the moment the assumption $\tau(L_1,x)<\tau(R_1,x)$, we see that the minimum of the first summand among all possible permutations is attained if

$$\max\{\tau(L_i,x):i=1,\dots,d\}\le\min\{\tau(R_i,x):i=1,\dots,d\}\quad\text{or}$$
$$\min\{\tau(L_i,x):i=1,\dots,d\}\ge\max\{\tau(R_i,x):i=1,\dots,d\}\qquad(7.11)$$

by standard arguments (note that the sum of the two factors does not depend on the permutation). The sum of the second and the third summand is minimized if $\max\{\tau(L_i,x):i=1,\dots,d\}\le\min\{\tau(R_i,x):i=1,\dots,d\}$ in the case $M_{10}(T_0,x)\le M_{01}(T_0,x)$ and is minimized if $\min\{\tau(L_i,x):i=1,\dots,d\}\ge\max\{\tau(R_i,x):i=1,\dots,d\}$ in the case that $M_{10}(T_0,x)\ge M_{01}(T_0,x)$. Therefore, the minimality of G yields (7.11). The assumption $\tau(L_1,x)<\tau(R_1,x)$ implies the first possibility. ■

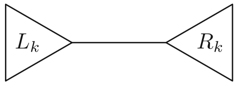
Lemma 7.8. *Let T be a minimal tree with respect to $x>0$, and let j be the least nonnegative integer such that the outline graph of T contains a CA_j. Then the outline graph of T contains CA_j at most $d-1$ times, and there is a vertex v of the outline graph of T which is adjacent to all copies of CA_j in the outline graph of T.*

Proof. Assume that there are two copies of CA_j in the outline graph of T that are adjacent to v and w, respectively, for different vertices v and w of the outline graph of T. For suitable rooted trees $L_2,\dots,L_d$ and $R_2,\dots,R_d$, the outline of T can be decomposed as in Fig. 7.3 with $L_1\cong R_1\cong CA_j$.

By our assumption, the outlines of these rooted trees do not contain a CA_ℓ for $\ell<j$.

Assume that j is even. We claim that there is an L_i with $2\le i\le d$, such that $\tau(L_i,x)>\tau(CA_j,x)$. Otherwise, all L_i satisfy $\tau(L_i,x)\le\tau(CA_j,x)$ and do not

Fig. 7.4 The decomposition of the outline graph of T in Lemma 7.9



contain a CA_ℓ for $\ell < j$, which by Lemma 7.6 implies that $L_i \cong CA_j$ for all $2 \le i \le d$. Thus, $CA_j, L_2, \ldots, L_d$, and v could be merged to a CA_{j+1}, which contradicts to the assumption that the outline graph of T has the form given above.

Therefore, there is an L_i with $\tau(L_i, x) > \tau(CA_j, x)$. By Lemma 7.7, we conclude that $\tau(R_i, x) \le \tau(CA_j, x)$ for all $2 \le i \le d$. As above, Lemma 7.6 implies that $R_2 \cong \cdots \cong R_d \cong CA_j$, again a contradiction.

Hence, all copies of CA_j in the outline of T are adjacent to the same vertex v. There cannot be d copies of CA_j, because these would be merged to a CA_{j+1}. Therefore, there are at most $d - 1$ copies of CA_j.

Once again, the proof for odd j follows by exchanging "odd" and "even" and reversing all inequality signs. ∎

The inductive step can be formulated as follows:

Lemma 7.9. *Let $x > 0$, T be a minimal tree with respect to x, and k be a nonnegative integer, and assume that the outline graph of T can be decomposed as in Fig. 7.4 for some rooted trees L_k (possibly empty) and R_k with*

$$k \text{ is even} \qquad \text{and} \qquad \tau(CA_k, x) < \tau(L_k, x) < \tau(CA_{k+2}, x) \tag{7.12}$$

or

$$k \text{ is odd} \qquad \text{and} \qquad \tau(CA_{k+2}, x) < \tau(L_k, x) < \tau(CA_k, x) \tag{7.13}$$

or

$$L_k \cong CA_k.$$

Assume that R_k is nonempty and the outline of R_k does not contain any CA_ℓ with $\ell < k$. Then exactly one of the following assertions is true:

(1) $R_k \in \{CA_k, CA_{k+1}, CA_{k+3}\}$.
(2) R_k consists of d branches $CA_{k+1}, CA_{k+1}, CA_{\ell_3}, \ldots, CA_{\ell_d}$ with $\ell_i \in \{k, k+1, k+2\}$ for $3 \le i \le d$.
(3) The outline of R_k can be decomposed as in Fig. 7.5 for $B_{k,1}, \ldots, B_{k,d-1} \in \{CA_k, CA_{k+2}\}$ and a nonempty rooted tree R_{k+1} whose outline does not contain any CA_ℓ for $\ell \le k$. Furthermore, if k is even, then

$$\tau(CA_{k+3}, x) < \tau(L_{k+1}, x) < \tau(CA_{k+1}, x) \tag{7.14}$$

or, if k is odd, then

$$\tau(CA_{k+1}, x) < \tau(L_{k+1}, x) < \tau(CA_{k+3}, x) \tag{7.15}$$

where L_{k+1} is defined as in Fig. 7.6.

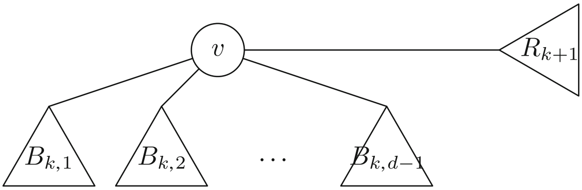


Fig. 7.5 The outline graph of R_k in assertion (3) of Lemma 7.9

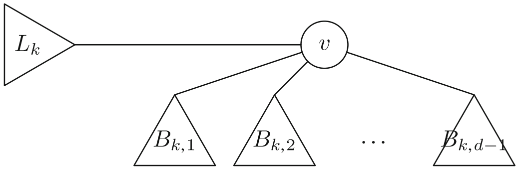


Fig. 7.6 L_{k+1} used in Ineqs. (7.14) and (7.15)

Proof. We first note that the three assertions are indeed mutually exclusive. In the second case, R_k has at least two branches CA_{k+1}. Thus, R_k contains more vertices than a CA_k or a CA_{k+1}, but we also have $R_k \ncong CA_{k+3}$; so we are not in the first case. In the third case, R_k has at most one branch CA_{k+1}, so the second and the third cases are mutually exclusive. Finally, the third and the first cases are mutually exclusive since the outline of R_k can be decomposed in the third case, but this cannot be done in the first case.

If $R_k \in \{CA_k, CA_{k+1}, CA_{k+3}\}$, there is nothing to prove. Thus, we assume that this is not the case. We consider the case of even k; the other case follows by reversing the signs of the inequalities.

Claim 1. $R_k \ncong CA_1$.

Proof. The outline of R_k does not contain a CA_1 for $k \geq 2$; thus, $R_k \ncong CA_1$ for $k \geq 2$. For $k \in \{0, 1\}$, the case $R_k \cong CA_1$ has already been excluded from our considerations. Therefore, R_k has at least one nonempty branch. ■

We denote the branches of R_k by $T_1, \ldots, T_d$, where some of them are allowed to be empty. We observe that the outline graphs of $T_1, \ldots, T_d$ are the branches of the outline graph of R_k unless $R_k \cong CA_\ell$ for some ℓ.

Claim 2. The outlines of T_i, $1 \leq i \leq d$, do not contain any CA_ℓ with $\ell < k$.

Proof. By the above observation and the assumptions of the lemma, this could only occur if $T_1 \cong \cdots \cong T_d \cong CA_{k-1}$ and $R_k \cong CA_k$, and this has already been ruled out. ■

Claim 3. If the outline of T_i contains CA_k for some $i \in \{1, 2, \ldots, d\}$, then $T_i \cong CA_k$.

Proof. Consider first the case $L_k \cong CA_k$. In that case, all CA_k in the outline graph of T are adjacent to the same vertex v by Lemma 7.8, that is, they are branches of R_k. Thus, the outline graph of T_i can only contain a CA_k if $T_i \cong CA_k$. So we may assume that $L_k \ncong CA_k$ and that the outline of T_d , say, contains a CA_k with $T_d \ncong CA_k$. We can decompose the outline of T_d such that we get a decomposition

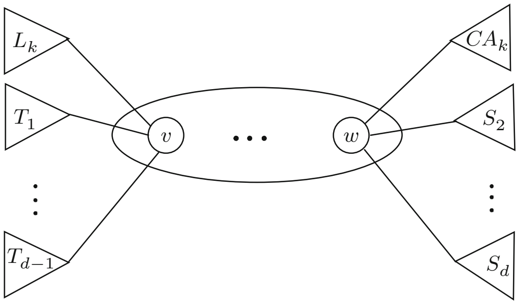


Fig. 7.7 The outline graph of T in the proof of Claim 3

of T as Fig. 7.7 for suitable (possibly empty) rooted trees $S_2, \ldots, S_d$. The outline of S_i is a subtree of the outline of T_d; therefore, it does not contain a CA_ℓ for $\ell < k$. We have $\tau(CA_k, x) < \tau(L_k, x)$ by Ineq. (7.12), and therefore, by Lemma 7.7, $\tau(S_i, x) \le \tau(L_k, x) < \tau(CA_{k+2}, x)$ for $2 \le i \le d$. From Lemma 7.6, we conclude that $S_2 \cong \cdots \cong S_d \cong CA_k$ (the other possibility cannot occur due to the strict inequality). But this means that the d copies of CA_k would have been merged to a CA_{k+1} in the outline of T_d, a contradiction, proving the claim. ■

Claim 4. If $T_1, \ldots, T_{d-1} \in \{CA_k, CA_{k+2}\}$, then we are done.

Proof. If $T_1 \cong \cdots \cong T_{d-1} \cong T_d$, then $R_k \in \{CA_{k+1}, CA_{k+3}\}$, which has been excluded. Otherwise, the outline of R_k decomposes into the outlines of $T_1, \ldots, T_d$. If $T_d \cong CA_k$, we exchange T_d and some $T_i \ncong CA_k$ (which exists since $R_k \ncong CA_{k+1}$). Thus, we may assume that $T_d \ncong CA_k$. In particular, T_d is not empty, since the outline of R_k is known not to contain any CA_ℓ for $\ell < k$. We set $B_{k,i} \cong T_i$ for $1 \le i \le d-1$ and $R_{k+1} \cong T_d$. By our above claim, we know that the outline of R_{k+1} does not contain a CA_ℓ for $\ell \le k$. The inequality

$$\tau(CA_{k+3}, x) = \frac{1}{1 + x\, d\tau(CA_{k+2}, x)} < \tau(L_{k+1}, x)$$
$$= \frac{1}{1 + x\,\tau(L_k, x) + x \sum_{i=1}^{d-1} \tau(B_{k,i}, x)}$$
$$\le \frac{1}{1 + x\, d\tau(CA_k, x)} = \tau(CA_{k+1}, x)$$

holds by Ineq. (7.12) and since $\tau(CA_k, x) \le \tau(B_{k,i}, x) \le \tau(CA_{k+2}, x)$ for all $1 \le i \le d-1$. To show that the right-hand inequality is strict, we note that $\tau(L_k, x) = \tau(B_{k,1}, x) = \tau(B_{k,d-1}, x) = \tau(CA_k, x)$ implies $L_k \cong B_{k,1} \cong \cdots \cong B_{k,d-1} \cong CA_k$, but then we have d copies of CA_k adjacent to the same vertex, which could therefore be merged to a CA_{k+1}. This is a contradiction to our assumption that the original decomposition of T into L_k and R_k is a decomposition of its outline graph. Thus, we arrive at Ineq. (7.14), and the claim is proved. ■

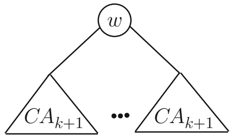


Fig. 7.8 The graph used in the proof of Lemma 7.9

Claim 5. If one of the T_i's, say T_d, contains a CA_{k+2} as a proper subtree, then we are done. For clarity, we emphasize that CA_{k+2} is assumed to be a subtree of T_d. We neither require it to be contained in the outline of T_d nor to be a branch of T_d.

Proof. We can decompose T as in Fig. 7.7 by replacing CA_k by CA_{k+2}, for suitable (possibly empty) rooted trees $S_2, \ldots, S_d$. By Ineq. (7.12), we have $\tau(L_k, x) < \tau(CA_{k+2}, x)$, and we apply Lemma 7.7 to deduce $\tau(T_i, x) \leq \tau(CA_{k+2}, x)$ for $1 \leq i \leq d-1$. Since the outline of T_i is known to contain no CA_ℓ for $\ell < k$, we obtain $T_i \in \{CA_k, CA_{k+2}\}$ from Lemma 7.6 for $1 \leq i \leq d-1$. We are done by the previous claim. ∎

We may now assume that none of the T_i's contains a CA_{k+2} as a proper subtree and claim that this implies that $T_i \in \{CA_k, CA_{k+1}, CA_{k+2}\}$ for all $1 \leq i \leq d$. Assume that $T_i \notin \{CA_k, CA_{k+1}, CA_{k+2}\}$. A leaf of the outline of T_i is of the form CA_ℓ for some ℓ by the definition of an outline graph. However, the range for ℓ is already very restricted: We have $\ell \geq k+1$ since the outline graph of T_i has been proven to contain no smaller CA_ℓ. On the other hand, we have $\ell \leq k+1$, since T_i does not contain CA_{k+2} as a proper subtree. In short, all leaves of T_i are equal to CA_{k+1}. Consider a leaf CA_{k+1} of maximum height (distance from the root). This leaf CA_{k+1} has a parent w, and all the children of w have to be leaves since our original leaf was assumed to be of maximum height, see Fig. 7.8. Thus, if we would found the subgraph of the outline graph of T_i, this would have to be contracted to a CA_{k+2}, a contradiction.

We are now in the situation that all $T_i \in \{CA_k, CA_{k+1}, CA_{k+2}\}$. If there are at least two copies of CA_{k+1} among the T_i's, we are in the second case. Otherwise, we have $T_1, \ldots, T_{d-1} \in \{CA_k, CA_{k+2}\}$ (after renumbering the branches), and we are done by the above Claim 4. ∎

Repeated application of Lemma 7.9 yields now Theorem 7.1 and thus also our main theorem.

Proof of Theorem 7.1. Let T be a minimal tree of order n with respect to x, and let j be the least integer such that the outline graph of T contains CA_j. We apply Lemma 7.9 inductively, starting with $k = j$ and $L_j \cong CA_j$, until we reach a point where either assertion (1) or assertion (2) holds in Lemma 7.9. Now, we expand L_j artificially: For $j \geq r \geq 1$, we further decompose $L_r \cong CA_r$ into its branches $L_{r-1} \cong CA_{r-1}$ and $B_{r-1,1} \cong \cdots \cong B_{r-1,d-1} \cong CA_{r-1}$. At the end, $L_0 \cong CA_0$ is discarded, but the $B_{0,i}$'s are retained even if they equal CA_0. Finally,

- If $R_k \cong CA_k$, we set $\ell = k$, $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_{\ell-1}$.
- If $R_k \cong CA_{k+1}$, we set $\ell = k$, $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_\ell$.

- If $R_k \cong CA_{k+3}$, we set $\ell = k + 1$, $B_{\ell-1,1} \cong \cdots \cong B_{\ell-1,d-1} \cong CA_{\ell+1}$, and $B_{\ell,1} \cong \cdots \cong B_{\ell,d} \cong CA_{\ell}$.
- If assertion (2) holds in Lemma 7.9, then we set $\ell = k$ and use the branches of R_k as our $B_{\ell,1}, \ldots, B_{\ell,d}$.

It is now seen that T has exactly the form that is described in the statement of the theorem. We only have to check that T is uniquely determined by this description. For this purpose, we count the number of vertices in the representation given in the theorem. Let r_k be the number of $B_{k,i}$'s which are equal to CA_{k+2}. Then the number of vertices in all $B_{k,i}$'s, together with the vertex they are all attached to, equals

$$(d - 1 - r_k) \cdot \frac{d^k - 1}{d - 1} + r_k \cdot \frac{d^{k+2} - 1}{d - 1} + 1 = d^k\,[1 + (d + 1)r_k]$$

for $1 \le k < \ell$. Furthermore, let q_ℓ, r_ℓ be the number of branches $B_{\ell,i}$ which are equal to $CA_{\ell+1}$ and $CA_{\ell+2}$, respectively. Then the number of vertices in all $B_{\ell,i}$'s, together with the vertex they are all attached to, equals either $(d^\ell - 1)/(d - 1)$ (if all $B_{\ell,i} \cong CA_{\ell-1}$) or $(d^{\ell+1} - 1)/(d - 1)$ (if all $B_{\ell,i} \cong CA_\ell$) or

$$\begin{aligned}(d - q_\ell - r_\ell) \cdot \frac{d^\ell - 1}{d - 1} &+ q_\ell \cdot \frac{d^{\ell+1} - 1}{d - 1} + r_\ell \cdot \frac{d^{\ell+2} - 1}{d - 1} \\ &= \frac{d^{\ell+1} - 1}{d - 1} + q_\ell\, d^\ell + r_\ell\,(d + 1)d^\ell.\end{aligned}$$

It follows that

$$(d - 1)n + 1 = \sum_{k=0}^{\ell} a_k\, d^k \tag{7.16}$$

where $a_k = (d - 1)[1 + (d + 1)r_k]$ with $0 \le r_k \le d - 1$ for $k < \ell$ and $a_\ell = 1$ or $a_\ell = d$ or $a_\ell = d + (d - 1)q_\ell + (d^2 - 1)r_\ell$ with $q_\ell \ge 2$ and $q_\ell + r_\ell \le d$.

Assume that there is another expansion

$$(d - 1)n + 1 = \sum_{k=0}^{\ell'} a'_k\, d^k \tag{7.17}$$

that satisfies the same conditions; in particular, r'_k and q'_ℓ are given analogously. Let h be the least integer such that $a_h \ne a'_h$. Then Eqs. (7.16) and (7.17) yield

$$\sum_{k=h}^{\ell} a_k\, d^{k-h} = \sum_{k=h}^{\ell'} a'_k\, d^{k-h}. \tag{7.18}$$

If $h < \min\{\ell, \ell'\}$, we consider Eq. (7.18) modulo d and see that $a_h \equiv a'_h \pmod d$ or $r_h \equiv r'_h \pmod d$, which is impossible, since $0 \le r_h, r'_h < d$ and $r_h \ne r'_h$, a contradiction. Hence, without loss of generality, we may assume that $h = \ell'$.

If $\ell = \ell' = h$, it follows that $a_\ell = a'_\ell$, yielding a contradiction once again. Thus, $\ell > \ell' = h$. Now, using Eq. (7.18) modulo d once again, we see that

$$a_h = (d-1)[1 + (d+1)r_h] \equiv d + (d-1)q'_h + (d^2-1)r'_h \equiv a'_h \pmod{d}$$

if $a'_h \notin \{1, d\}$, which simplifies to $r_h + 1 \equiv q'_h + r'_h \pmod{d}$. Since $1 \le r_h + 1 \le d$ and $1 \le q_h{}' + r_h{}' \le d$, it follows that $r_h = q'_h + r'_h - 1$. Now, using the condition $q'_h \ge 2$, we obtain the inequality

$$\begin{aligned} a'_h &= d + (d-1)q'_h + (d^2-1)r'_h \le d + 2(d-1) + (d^2-1)(q'_h + r'_h - 2) \\ &= 3d - 2 + (d^2-1)(r_h - 1) = -d^2 + 3d - 1 + (d^2-1)r_h \\ &\le d - 1 + (d^2-1)r_h = a_h. \end{aligned}$$

This estimate also holds if $a'_h = 1$ (trivially) and if $a'_h = d$. In the latter case, $a'_h \equiv a_h \pmod{d}$ implies $r_h = d-1$ and $a_h = (d-1)d^2 > a'_h$. But now it follows that the right-hand side of Eq. (7.18) is smaller than its left-hand side, contradiction. Thus, the uniqueness of the representation Eq. (7.16) is shown, which means that the minimal tree T is uniquely characterized up to isomorphism. ■

In the following, we will determine the value of the minimal energy and prove Theorem 7.3. Since the extremal trees are described in terms of complete d-ary trees, we have to study the energy of these trees first. Note that, in view of Eq. (7.7) and the definition of $\tau(M, x)$, we have $M(CA_h, x) = \frac{1}{\tau(CA_h, x)} \cdot M(CA_{h-1}, x)^d$. Iterating this equation yields $M(CA_h, x) = \prod_{j=1}^{h} \tau(CA_j, x)^{-d^{h-j}}$, and in view of Lemma 7.3, this gives us the explicit formula

$$M(CA_h, x) = \prod_{j=1}^{h} \left(\frac{Q_{j+1}(x)}{Q_j(x)} \right)^{d^{h-j}}$$

where

$$Q_j(x) := \frac{u(x)^j - v(x)^j}{u(x) - v(x)}; \quad u(x) := \frac{1 + \sqrt{1 + 4\mathrm{d}x}}{2}; \quad v(x) := \frac{1 - \sqrt{1 + 4\mathrm{d}x}}{2}.$$

The denominator $u(x) - v(x)$ has been introduced such that $Q_j(x)$ is always a polynomial: Indeed, the recursion $Q_1(x) \equiv 1,\ Q_2(x) \equiv 1,\ Q_j(x) = Q_{j-1}(x) + \mathrm{d}x\, Q_{j-2}(x)$ holds, and it follows by induction that Q_j is a polynomial of degree $\lfloor (j-1)/2 \rfloor$. It should be noted that Q_j is closely related to the so-called Fibonacci polynomials (see [263]). Now we have

$$\begin{aligned} M(CA_h, x) &= Q_{h+1}(x)\, Q_1(x)^{-d^{h-1}} \prod_{j=2}^{h} Q_j(x)^{d^{h+1-j}} \prod_{j=2}^{h} Q_j(x)^{-d^{h-j}} \\ &= Q_{h+1}(x) \prod_{j=1}^{h} Q_j(x)^{(d-1)d^{h-j}} \qquad (7.19) \end{aligned}$$

where the fact that $Q_1(x) \equiv 1$ has been used. It turns out that the zeros of Q_j can be explicitly computed. If $Q_j(x) \equiv 0$, then $u(x)^j = v(x)^j$, and so

$$\frac{u(x)}{v(x)} = \frac{1+\sqrt{1+4\mathrm{d}x}}{1-\sqrt{1+4\mathrm{d}x}}$$

has to be a j-th root of unity ζ. Then,

$$x = -\frac{\zeta}{d(1+\zeta)^2} = -\frac{1}{2d(1+\mathrm{Re}(\zeta))}.$$

Thus, x has to be of the form $x = -\frac{1}{2d\left(1+\cos\frac{2k\pi}{j}\right)}$ for some $0 \le k < j/2$. However, note that $x = -1/(4d)$ is also a zero of the denominator $u(x) - v(x) = \sqrt{1+4\mathrm{d}x}$ and that there are no double zeros, since the derivative is given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[u(x)^j - v(x)^j\right] = \frac{jd}{\sqrt{1+4\mathrm{d}x}}\left[u(x)^{j-1} + v(x)^{j-1}\right]$$

which cannot be 0 if $u(x) = \zeta v(x)$ for a j-th root of unity $\zeta \neq -1$. Hence, the zeros of Q_j are precisely the numbers $-\left[2d\left(1+\cos\frac{2k\pi}{j}\right)\right]^{-1}$, $k = 1, 2, \ldots, \lfloor (j-1)/2 \rfloor$, and it follows that the characteristic polynomial $\phi(CA_h, x)$ can be written as

$$\phi(CA_h, x) = x^n\, M(CA_h, -x^{-2}) = x^n\, Q_{h+1}(-x^{-2}) \prod_{j=1}^{h} Q_j(-x^{-2})^{(d-1)d^{h-j}}.$$

Hence, the nonzero eigenvalues of CA_h are

$$\pm\sqrt{2d\left(1+\cos\frac{2k\pi}{j}\right)} = \pm 2\sqrt{d}\,\cos\frac{k\pi}{j}, \quad k = 1, 2, \ldots, \lfloor (j-1)/2 \rfloor$$

with multiplicity $(d-1)d^{h-j}$ for $j = 1, 2, \ldots, h$ and multiplicity 1 for $j = h+1$. It follows that the energy of CA_h is given by

$$\mathscr{E}(CA_h) = \left(\sum_{j=1}^{h}(d-1)d^{h-j} \sum_{k=1}^{\lfloor (j-1)/2 \rfloor} 4\sqrt{d}\,\cos\frac{k\pi}{j}\right) + \sum_{k=1}^{\lfloor h/2 \rfloor} 4\sqrt{d}\,\cos\frac{k\pi}{h+1}.$$

Noting that

$$\sum_{k=1}^{\lfloor (j-1)/2 \rfloor} \cos\frac{k\pi}{j} = \begin{cases} \frac{1}{2}\left(\cot\frac{\pi}{2j} - 1\right) & \text{if } j \equiv 0 \pmod 2 \\ \frac{1}{2}\left(\csc\frac{\pi}{2j} - 1\right) & \text{if } j \equiv 1 \pmod 2, \end{cases}$$

this reduces to

$$\mathcal{E}(CA_h) = 2\sqrt{d}(d-1)\left(\sum_{\substack{j=1 \\ j\equiv 0 (\mathrm{mod}\ 2)}}^{h} d^{h-j}\left(\cot\frac{\pi}{2j}-1\right) + \sum_{\substack{j=1 \\ j\equiv 1 (\mathrm{mod}\ 2)}}^{h} d^{h-j}\left(\csc\frac{\pi}{2j}-1\right)\right) + \begin{cases} 2\sqrt{d}\left(\csc\dfrac{\pi}{2(h+1)}-1\right) & \text{if } h\equiv 0 \ (\mathrm{mod}\ 2) \\ 2\sqrt{d}\left(\cot\dfrac{\pi}{2(h+1)}-1\right) & \text{if } h\ \equiv 1 (\mathrm{mod}\ 2). \end{cases}$$

Next, we determine the asymptotic behavior of the energy of CA_h :

Lemma 7.10. *The energy of a complete d-ary tree CA_h satisfies $\mathcal{E}(CA_h) = \alpha_d|CA_h| + O(1)$, where $|CA_h|$ denotes the number of vertices of CA_h and α_d is given by Eq. (7.4).*

Proof. Note that

$$|CA_h| = \frac{d^h-1}{d-1} = \frac{d^h}{d-1} + O(1)$$

and

$$\cot\frac{\pi}{2j} = \frac{2j}{\pi} + O(1), \qquad \csc\frac{\pi}{2j} = \frac{2j}{\pi} + O(1)$$

so that

$$\begin{aligned}\mathcal{E}(CA_h) &= 2\sqrt{d}(d-1)d^h\left[\sum_{\substack{j=1 \\ j\equiv 0 (\mathrm{mod}\ 2)}}^{h} d^{-j}\left(\cot\frac{\pi}{2j}-1\right) + \sum_{\substack{j=1 \\ j\equiv 1 (\mathrm{mod}\ 2)}}^{h} d^{-j}\left(\csc\frac{\pi}{2j}-1\right)\right] + \frac{4\sqrt{d}\,h}{\pi} + O(1) \\ &= \alpha_d|CA_h| - 2\sqrt{d}(d-1)d^h\left[\sum_{\substack{j>h \\ j\equiv 0 (\mathrm{mod}\ 2)}} d^{-j}\left(\cot\frac{\pi}{2j}-1\right) + \sum_{\substack{j>h \\ j\equiv 1 (\mathrm{mod}\ 2)}} d^{-j}\left(\csc\frac{\pi}{2j}-1\right)\right] + \frac{4\sqrt{d}\,h}{\pi} + O(1)\end{aligned}$$

$$= \alpha_d |CA_h| - 2\sqrt{d}(d-1)d^h \sum_{j>h} d^{-j}\left(\frac{2j}{\pi} + O(1)\right) + \frac{4\sqrt{d}\,h}{\pi} + O(1)$$

$$= \alpha_d |CA_h| - 2\sqrt{d}(d-1)d^h \left(\frac{2hd^{-h}}{(d-1)\pi} + O(d^{-h})\right) + \frac{4\sqrt{d}\,h}{\pi} + O(1)$$

$$= \alpha_d |CA_h| + O(1)$$

as claimed. ■

Now, we are able to prove our main asymptotic result:

Proof of Theorem 7.3. Using the decomposition of $T^*_{n,d}$, we note that

$$\left(\prod_{k=0}^{\ell-1}\prod_{j=1}^{d-1} M(B_{k,j},x)\right)\left(\prod_{j=1}^{d} M(B_{\ell,j},x)\right)$$
$$\leq M(T^*_{n,d},x) \leq \left(\prod_{k=0}^{\ell-1}\prod_{j=1}^{d-1} M(B_{k,j},x)\right)\left(\prod_{j=1}^{d} M(B_{\ell,j},x)\right)(1+x)^{d(\ell+1)}$$

for arbitrary $x > 0$, since every matching in the union $\bigcup_k \bigcup_j B_{k,j}$ is also a matching in $T^*_{n,d}$, whereas every matching of $T^*_{n,d}$ consists of a matching in $\bigcup_k \bigcup_j B_{k,j}$ and a subset of the remaining $\leq d(\ell+1)$ edges. This implies

$$\sum_{k=0}^{\ell-1}\sum_{j=1}^{d-1} \mathscr{E}(B_{k,j}) + \sum_{j=1}^{d} \mathscr{E}(B_{\ell,j}) \leq \mathscr{E}(T^*_{n,d})$$
$$\leq \sum_{k=0}^{\ell-1}\sum_{j=1}^{d-1} \mathscr{E}(B_{k,j}) + \sum_{j=1}^{d} \mathscr{E}(B_{\ell,j}) + \frac{2}{\pi} d(\ell+1) \int_0^\infty x^{-2}\ln(1+x^2)\,\mathrm{d}x.$$

Since $\int_0^\infty x^{-2}\ln(1+x^2)\,\mathrm{d}x = \pi$,

$$\mathscr{E}(T^*_{n,d}) = \sum_{k=0}^{\ell-1}\sum_{j=1}^{d-1} \mathscr{E}(B_{k,j}) + \sum_{j=1}^{d} \mathscr{E}(B_{\ell,j}) + O(\ell)$$
$$= \sum_{k=0}^{\ell-1}\sum_{j=1}^{d-1} \big(\alpha_d |B_{k,j}| + O(1)\big) + \sum_{j=1}^{d} \big(\alpha_d |B_{k,j}| + O(1)\big) + O(\ell)$$
$$= \alpha_d \left(\sum_{k=0}^{\ell-1}\sum_{j=1}^{d-1} |B_{k,j}| + \sum_{j=1}^{d} |B_{k,j}|\right) + O(\ell)$$
$$= \alpha_d (|T^*_{n,d}| - O(\ell)) + O(\ell) = \alpha_d\, n + O(\ell).$$

Table 7.1 Numerical values of α_d

d	α_d
2	1.102947505597
3	0.970541979946
4	0.874794345784
5	0.802215758706
6	0.744941364903
7	0.698315075830
8	0.659425329682
9	0.626356806404
10	0.597794680849
20	0.434553264777
50	0.279574397741
100	0.198836515295

It is not difficult to see that $\ell = O(\log n)$ (this follows from Eq. (7.3), see [258] for a detailed analysis), and so we finally have $\mathscr{E}(T^*_{n,d}) = \alpha_d\, n + O(\log n)$, which completes the proof. ■

Table 7.1 shows some numerical values of the constants α_d. In fact, from Theorems 7.2 and 7.3, we obtain the following corollary:

Corollary 7.1. *For any tree* $T \in \mathscr{T}_{n,d}$, $\mathscr{E}(T) \geq \mathscr{E}(T^*_{n,d}) = \alpha_d\, n + O(\log n)$, *with equality if and only if* $T \cong T^*_{n,d}$. ■

Let BT_n denote the tree constructed by taking three disjoint copies of the complete 2-ary tree of height n and joining an additional vertex to their roots. At the end of [385], Nikiforov formulated two conjectures as follows:

Conjecture 7.1. The limit

$$c = \lim_{n\to\infty} \frac{\mathscr{E}(BT_n)}{3 \cdot 2^{n+1} - 2}$$

exists, and $c > 1$. ■

Conjecture 7.2. Let $\varepsilon > 0$. If T is a sufficiently large tree with $\Delta(T) \leq 3$, then $\mathscr{E}(T) \geq (c - \varepsilon)|T|$. ■

Li and Liu [334] confirmed both conjectures, by using Theorems 7.2 and 7.3.

Theorem 7.4. *Conjecture 7.1 is true.*

Proof. We only need to notice that BT_n is exactly the tree $T^*_{3\cdot 2^{n+1}-2,2}$ with $\ell = n + 1$, $B_{k,1} \cong CA_k$ for $0 \leq k < \ell$, $B_{\ell,1} \cong B_{\ell,2} \cong CA_{n+1}$. Therefore, by Theorem 7.3 and Table 7.1, we have

$$\lim_{n\to\infty} \left(\frac{\mathscr{E}(BT_n)}{3 \cdot 2^{n+1} - 2} \right) = \lim_{n\to\infty} \left(\alpha_2 + \frac{O(\log(3 \cdot 2^{n+1} - 2))}{3 \cdot 2^{n+1} - 2} \right) = \alpha_2 > 1. \quad ■$$

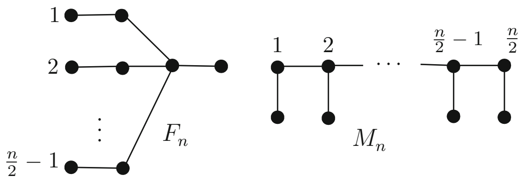


Fig. 7.9 F_n and M_n

In fact, from Theorems 7.2 and 7.3, we have that for any $T \in \mathscr{T}_{n,d}$, $\mathscr{E}(T) \geq \mathscr{E}(T^*_{n,d}) = \alpha_d \cdot n + O(\log n)$. Therefore, we obtain:

Theorem 7.5. *Let $\varepsilon > 0$. If T is a sufficiently large tree with $\Delta(T) = d + 1$, then $\mathscr{E}(T) \geq (\alpha_d - \varepsilon)|T|$, where α_d is given by Eq. (7.4).* ■

Corollary 7.2. *Let $\varepsilon > 0$. If T is a sufficiently large tree with $\Delta(T) = 3$, then $\mathscr{E}(T) \geq (\alpha_2 - \varepsilon)|T|$, where α_2 is given by Eq. (7.4).* ■

Remark 7.1. From Theorem 7.3 and Table 7.1, one can see that there does not exist either strongly hypoenergetic trees or hypoenergetic trees (see Chap. 9 for definition) of order n and maximum degree Δ for $\Delta \leq 3$ and any sufficiently large n.

Remark 7.2. From Theorem 7.3 and Table 7.1, one can also see that there exist both hypoenergetic trees and strongly hypoenergetic trees of order n and maximum degree Δ for $\Delta \geq 4$ and any sufficiently large n.

7.1.2 Minimal Energy of Acyclic Conjugated Graphs

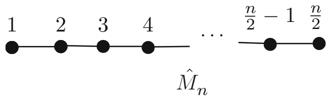
From a chemical point of view, a more interesting problem seems to be to determine extremal-energy acyclic conjugated hydrocarbons (in the language of graph theory, trees with a perfect matching). In this case, the path has also the maximal energy, see Sect. 4.3. As for the case of minimal energy, one of the present authors put forward two conjectures [155] and checked all the trees with a perfect matching with up to 16 vertices. Let F_n be a graph obtained by adding a pendent edge to each vertex of the star $K_{1,(n/2-1)}$, and M_n the comb obtained by adding a pendent edge to each vertex of the path $P_{n/2}$ (see Fig. 7.9). Given two positive integers n and d, denote by Φ_n the class of trees with n vertices which have perfect matchings and by $\Omega_{n,d}$ the subclass of Φ_n whose vertex degrees do not exceed $d + 1$.

Conjecture 7.3. Among trees with n vertices which have a perfect matching, the energy is minimal for the tree F_n. ■

Conjecture 7.4. Among trees with n vertices which have a perfect matching and whose vertex degrees do not exceed 3, the energy is minimal for the comb M_n. ■

Zhang and Li [517] confirmed that both conjectures are true. Li and Lian [333] obtained a much stronger result than Conjecture 7.4.

Fig. 7.10 The graph $\hat{M}_n$



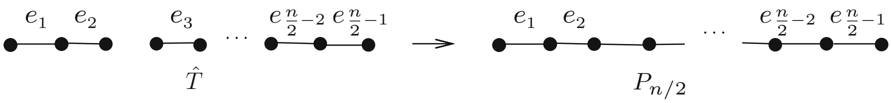


Fig. 7.11 Concatenation of $\hat{T}$ into $P_{n/2}$

We denote by $M(T)$ the perfect matching of the tree $T = (V(T), E(T))$ and $Q(T) = E(T) - M(T)$. Let $m = |M(T)|$. Denote by $\hat{T}$ the graph induced by $Q(T)$. We call $\hat{T}$ the *capped graph* of T and T the *original graph* of $\hat{T}$. For example, Fig. 7.10 shows the capped graphs of B_n and M_n. For each k-matching Ω of T, it is partitioned into two parts: $\Omega = R \cup S$, where $S \subset M(T)$ and R is a matching in $\hat{T}$. On the other hand, for any i-matching R of $\hat{T}$, any $k-i$ edges S of $M(T)$ not incident with R form a k-matching Ω of T with partition $\Omega = R \cup S$. From now on, when we say a k-matching of T including a certain i-matching R of $\hat{T}$, it is in such sense. This is our fundamental principle of counting the k-matchings of T.

Theorem 7.6. *For any tree $T \in \Phi_n$, $\mathscr{E}(T) \geq \mathscr{E}(F_n)$, with equality if and only if $T \cong F_n$.*

Proof. In order to prove the first part, it suffices to show that $F_n \preceq T$ for any tree T in Φ_n or, equivalently, to show that for each $k \leq n/2$, $m(F_n, k) \leq m(T, k)$.

Since F_n and T are of the same size, there is a bijection h from $Q(F_n)$ to $Q(T)$ such that the image $h(R)$ of a matching R in $\hat{F}_n$ is a matching in $\hat{T}$, aware of the fact that $\hat{F}_n$ is a star and has only 1-matchings. That is to say, h induces an injection from the matchings of $\hat{F}_n$ to those of $\hat{T}$. For $0 \leq i \leq 1$, the number of k-matchings in F_n including a certain i-matching R in $\hat{F}_n$ is $\binom{m-2i}{k-i}$, since no two independent edges in $Q(F_n)$ are incident with a common edge in $M(F_n)$. Hence, R is incident with exactly $2i$ edges in $M(F_n)$, and these cover all the k-matchings in F_n as R goes over all matchings in $\hat{F}_n$. Similarly, $h(R)$ determines at least $\binom{m-2i}{k-i}$ k-matchings in T, since $h(R)$ is incident with at most $2i$ edges in $M(T)$. Thus,

$$m(F_n, k) = \sum_{i=0}^{k} m(\hat{F}_n, i) \binom{m-2i}{k-i} \leq \sum_{i=0}^{k} m(\hat{T}, i) \binom{m-2i}{k-i} \leq m(T, k).$$

In order to prove the uniqueness, we simply mention that if $\hat{T}$ is disconnected, it has a 2-matching which cannot be the image of a 2-matching in $\hat{F}_n$ under h. Then T has sharply more 2-matchings than F_n. Thus, for a minimal T in $\Phi(n)$, $\hat{T}$ must be connected and have only 1-matchings; hence, it must be a star. This implies $T \cong F_n$ (Fig. 7.11). ∎

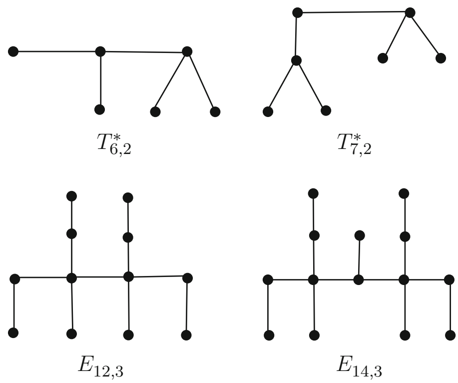


Fig. 7.12 Some small examples of $T^*_{n,d}$ and $E_{n,d}$

We now need to introduce some more notation. Recall that $\mathscr{T}_{n,d}$ denote the set of trees of order n with maximum degree $\Delta \leq d+1$ and $T^*_{n,d}$ is the tree defined in Definition 7.1. Let $E_{n,d}$ be a graph obtained by adding a pendent edge to each vertex of $T^*_{n/2,d-1}$. For given n and d, $T^*_{n,d}$ is uniquely determined. Figure 7.12 depicts the structures of $T^*_{6,2}$ and $T^*_{7,2}$. At the same time, $E_{12,3}$ and $E_{14,3}$ are also shown, which are obtained by adding a pendent edge to each vertex of $T^*_{6,2}$ and $T^*_{7,2}$, respectively.

Lemma 7.11. *Let $T \in \Omega_{n,d}$. If the number of connected components $\omega(\hat{T}) \geq 2$, then there is a tree $T' \in \Omega_{n,d}$ with a connected $\hat{T}'$ such that $T' \prec T$.*

Proof. In this case, $\hat{T}$ is the union of disjoint trees $\hat{T}_1, \hat{T}_2, \ldots, \hat{T}_\ell$ with $\Delta(\hat{T}_i) \leq d$, $1 \leq i \leq \ell$, since $\Delta(T) \leq d+1$. Each $\hat{T}_i$ contains at least two leaves. Concatenating one leaf of $\hat{T}_i$ with one of $\hat{T}_{i-1}$ and another with one of $\hat{T}_{i+1}$, we get a new graph $\hat{T}'$ with $\Delta(\hat{T}') \leq d$ and $E(\hat{T}') = E(\hat{T}) = n/2-1$. Let T' be a graph obtained by adding a pendent edge to each vertex of $\hat{T}'$; thus, $T' \in \Omega_{n,d}$. There is also a natural bijection h from $Q(T')$ to $Q(T)$, such that $h(R)$ is a matching in $\hat{T}$ for any matching R in $\hat{T}'$. In addition, an i-matching R is incident with exactly $2i$ edges in $M(T')$, while $h(R)$ is incident with at most $2i$ edges in $M(T)$. For any $i \geq 0$, the number of k-matchings in T' that contain a certain i-matching R in $\hat{T}'$ is $\binom{m-2i}{k-i}$, since no two independent edges in $Q(T')$ are incident with a common edge in $M(T')$, and hence, R is incident with exactly $2i$ edges in $M(T')$. These edges cover all the k-matchings in T' as R goes over all matchings in $\hat{T}'$. In the same way, $h(R)$ determines at least $\binom{m-2i}{k-i}$ k-matchings in T, since $h(R)$ is incident with at most $2i$ edges in $M(T)$. Therefore,

$$m(T',k) = \sum_{i=0}^{k} m(\hat{T}',i)\binom{m-2i}{k-i} \leq \sum_{i=0}^{k} m(\hat{T},i)\binom{m-2i}{k-i} \leq m(T,k).$$

In addition, since $\hat{T}$ is disconnected, it has a 2-matching that cannot be the image of any 2-matching in $\hat{T}'$. Then T has sharply more 2-matchings than T'. This implies $T' \prec T$. ■

From Theorems 7.1 and 7.2, we obtain the following result:

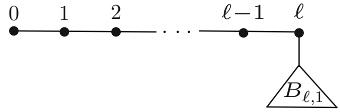


Fig. 7.13 The tree $T^*_{n/2,1}$

Lemma 7.12. *Let n and d be positive integers. For any tree $T \in \mathscr{T}_{n,d}$, $T \succeq T^*_{n,d}$. Equality holds if and only if $T \cong T^*_{n,d}$.* ∎

The main result is the following:

Theorem 7.7. *For any tree $T \in \Omega_{n,d}$, $\mathscr{E}(T) \geq \mathscr{E}(E_{n,d})$. Equality holds if and only if $T \cong E_{n,d}$.*

Proof. From the definition of $E_{n,d}$, we get $\hat{E}_{n,d} \cong T^*_{n/2,d-1}$, and any i-matching of $\hat{E}_{n,d}$ is incident to exactly $2i$ edges of $M(E_{n,d})$. Thus, the number of k-matchings in $E_{n,d}$, containing a certain i-matching R of $\hat{E}_{n,d}$, is $\binom{m-2i}{k-i}$. Thus,

$$m(E_{n,d}, k) = \sum_{i=0}^{k} m(\hat{E}_{n,d}, i) \binom{m-2i}{k-i}.$$

On the other hand, for any tree $T \in \Omega_{n,d}$, from Lemma 7.11, suppose $\hat{T}$ is connected. Otherwise, there is a tree $T' \in \Omega_{n,d}$, such that $T' \prec T$. Therefore, $\hat{T}$ is a tree with $n/2$ vertices and the maximum degree $\Delta(\hat{T}) \leq d$ since $T \in \Omega_{n,d}$, i.e., $\hat{T} \in \mathscr{T}_{n/2,d-1}$. From Lemma 7.12, for any nonnegative integer i, $m(\hat{T}, i) \geq m(\hat{E}_{n,d}, i)$. Moreover, any i-matching of $\hat{T}$ is also incident to exactly $2i$ edges of $M(T)$. Thus, the number of k-matchings in T, containing a certain i-matching of $\hat{T}$, is equal to $\binom{m-2i}{k-i}$. Again,

$$m(T, k) = \sum_{i=0}^{k} m(\hat{T}, i) \binom{m-2i}{k-i}.$$

Since for any $i \geq 0$, $m(\hat{T}, i) \geq m(\hat{E}_{n,d}, i)$, and if $T \ncong E_{n,d}$, there exists an integer i_0 such that $m(\hat{T}, i_0) > m(\hat{E}_{n,d}, i_0)$. Consequently,

$$m(T, k) \geq m(E_{n,d}, k) \qquad \text{for } k = 1, 2, \ldots, n/2$$

and there exists an integer k_0 such that $m(T, k_0) > m(E_{n,d}, k_0)$. Therefore, if $T \ncong E_{n,d}$, then $T \succ E_{n,d}$. ∎

From the above theorem, we easily obtain that Conjecture 7.4 is true.

Corollary 7.3. *For any tree $T \in \Omega_{n,2}$, $\mathscr{E}(T) \geq \mathscr{E}(M_n)$, with equality holding if and only if $T \cong M_n$.*

Proof. From Theorem 7.7, the unique minimal-energy tree in $\Omega_{n,2}$ is $E_{n,2}$, which is a tree obtained by adding a pendent edge to each vertex of $T^*_{n/2,1}$. $T^*_{n/2,1}$ is depicted in Fig. 7.13.

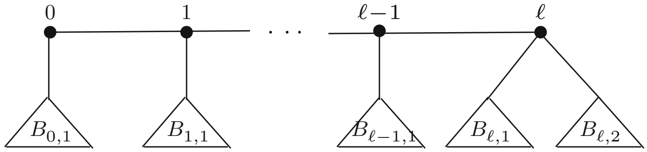


Fig. 7.14 The tree $T^*_{n,2}$

By the definition of $T^*_{n,d}$, for even n, $\ell = n/2$, $B_{\ell,1} \cong CA_{\ell-1} \cong P_{\ell-1}$, whereas for odd n, $\ell = (n-1)/2$, $B_{\ell,1} \cong CA_\ell \cong P_\ell$. Therefore, $T^*_{n/2,1} \cong P_{n/2}$ and $E_{n,2} \cong M_n$. ■

For minimal-energy trees of maximum degree 4, things become not so easy as in the above corollary. Nevertheless, we still can get some structural descriptions.

Corollary 7.4. *For conjugated trees of maximum degree* 4*,* $E_{n,3}$ *is the unique tree with minimal energy, the structure of which is completely determined by* $T^*_{n/2,2}$*.* ■

In the following, we design an algorithm for constructing $T^*_{n,2}$ for different n, which is shown in Fig. 7.14, where $B_{k,1} \in \{CA_k, CA_{k+2}\}$ for $0 \le k < \ell$ and either $B_{\ell,1} \cong B_{\ell,2} \cong CA_{\ell-1}$ or $B_{\ell,1} \cong B_{\ell,2} \cong CA_\ell$ or $B_{\ell,1} \cong B_{\ell,2} \cong CA_{\ell+1}$, while CA_k is the complete 2-ary tree of height $k-1$. This representation is unique, and now its "digital expansion" can be written as $n+1 = \sum_{k=0}^{\ell} a_k\, 2^k$, where $a_k = 1+3r_k$ and $r_k = 1$ if $B_{k,1} \cong CA_{k+2}$; otherwise, $r_k = 0$ (i.e., if $B_{k,1} \cong CA_k$) for $k < \ell$, and

- $a_\ell = 1$ if $B_{\ell,1} \cong B_{\ell,2} \cong CA_{\ell-1}$.
- $a_\ell = 2$ if $B_{\ell,1} \cong B_{\ell,2} \cong CA_\ell$.
- $a_\ell = 4$ if $B_{\ell,1} \cong B_{\ell,2} \cong CA_{\ell+1}$.

For any given $n \ge 4$, we determine the structure of $T^*_{n,2}$ by the following steps:

(1) If $n \equiv 0 \pmod 2$, then $a_0 = 1$, $B_{0,1} \cong CA_0$. Let $n_0 = n+1-a_0 = n+1-1 = n$.
    If $n \not\equiv 0 \pmod 2$, then $a_0 = 4$, $B_{0,1} \cong CA_2$. Let $n_0 = n+1-a_0 = n+1-4 = n-3$.
(2) If $n_0 = 2$, then $\ell = 1$ and $a_\ell = 1$. Now $B_{1,1} \cong B_{1,2} \cong CA_0$.
    If $n_0 = 2^2$, then $\ell = 1$ and $a_\ell = 2$. Now $B_{1,1} \cong B_{1,2} \cong CA_1$.
    If $n_0 = 2^3$, then $\ell = 1$ and $a_\ell = 4$. Now $B_{1,1} \cong B_{1,2} \cong CA_2$.
    Otherwise, if $n_0 \not\equiv 0 \pmod{2^2}$, then $a_1 = 1$ and $B_{1,1} \cong CA_1$. Let $n_1 = n_0 - 2^1$.
    If $n_0 \equiv 0 \pmod{2^2}$, then $a_1 = 4$ and $B_{1,1} \cong CA_3$. Let $n_1 = n_0 - 2^3$.
(3) If $n_1 = 2^2$, then $\ell = 2$ and $a_2 = 1$. Now $B_{2,1} \cong B_{2,2} \cong CA_1$.
    If $n_1 = 2^3$, then $\ell = 2$ and $a_2 = 2$. Now $B_{2,1} \cong B_{2,2} \cong CA_2$.
    If $n_1 = 2^4$, then $\ell = 2$ and $a_2 = 4$. Now $B_{2,1} \cong B_{2,2} \cong CA_3$.
    Otherwise, if $n_1 \not\equiv 0 \pmod{2^3}$, then $a_2 = 1$ and $B_{2,1} \cong CA_2$. Let $n_2 = n_1 - 2^2$.
    If $n_1 \equiv 0 \pmod{2^3}$, then $a_2 = 4$ and $B_{2,1} \cong CA_4$. Let $n_2 = n_1 - 2^4$.

    ⋮

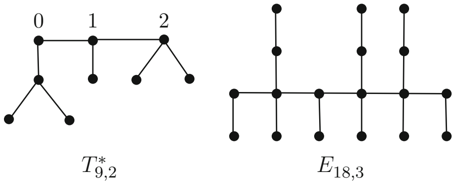


Fig. 7.15 The trees $T^*_{9,2}$ and $E_{18,3}$

(k+1) If $n_{k-1} = 2^k$, then $\ell = k$ and $a_k = 1$. Now $B_{k,1} \cong B_{k,2} \cong CA_{k-1}$.
If $n_{k-1} = 2^{k+1}$, then $\ell = k$ and $a_k = 2$. Now $B_{k,1} \cong B_{k,2} \cong CA_k$.
If $n_{k-1} = 2^{k+2}$, then $\ell = k$ and $a_k = 4$. Now $B_{k,1} \cong B_{k,2} \cong CA_{k+1}$.
Otherwise, if $n_{k-1} \not\equiv 0 \pmod{2^{k+1}}$, then $a_k = 1$ and $B_{k,1} \cong CA_k$.
Let $n_k = n_{k-1} - 2^k$ and $k - 1 := k$.
If $n_{k-1} \equiv 0 \pmod{2^{k+1}}$, then $a_k = 4$ and $B_{k,1} \cong CA_{k+2}$. Let $n_k = n_{k-1}$ -2^{k+2}
and $k - 1 := k$.

- Continue step $(k + 1)$ until we obtain the final structure of the tree $T^*_{n,2}$.

An example for $n = 9$, i.e., $T^*_{9,2}$, is depicted in Fig. 7.15.

(1) Since $n \not\equiv 0 \pmod 2$, it is $a_0 = 4$, $B_{0,1} \cong CA_2$, and $n_0 = n - 3 = 6$.
(2) Since $n_0 \not\equiv 0 \pmod{2^2}$, it is $a_1 = 1$, $B_{1,1} \cong CA_1$, and $n_1 = n_0 - 2 = 4$.
(3) Since $n_1 = 2^2$, it is $\ell = 2$, $a_2 = 1$, and $B_{2,1} \cong B_{2,1} \cong CA_1$.

Now for any even n, $T^*_{n/2,2}$ can be determined by the procedure above. Thus, we can get $E_{n,3}$ by adding a pendent edge to each vertex of $T^*_{n/2,2}$. Figure 7.15 depicts the trees $T^*_{9,2}$ and $E_{18,3}$.

From the above proof, we get the following:

Theorem 7.8. *Let T be a tree from Φ_n. If for any i-matching R in $\hat{T}$, R is incident with $2i$ edges of $M(T)$, or equivalently, $\hat{T}$ is connected, or $M(T)$ consists of pendent edges of T, and there is a bijection h from $Q(T)$ to $Q(T')$ for any tree T' in the same class, such that $h(R)$ is a matching in $\hat{T}'$ whenever R is a matching in $\hat{T}$, then T is minimal among this class.* ■

Zhang and Li [517] also determined the graphs that attain the second-minimal energy in classes Φ_n and $\Omega_{n,2}$, respectively. There are also some results on the ordering of the trees with a perfect matching by minimal energies. For these results, we refer readers to [141, 279, 324, 483, 487].

Remark 7.3. The minimal-energy problem was studied also for other classes of trees. For example, the trees with a given bipartition, having minimal and second-minimal energies, are characterized in [505]. In [497], it is shown that the tree with minimal-energy tree with given diameter is the comet (or broom) $P_{n,n-d+1}$:

Theorem 7.9. *Let $d \geq 2$ be a positive integer, and let T be a tree with n vertices having diameter at least d. Then $\mathscr{E}(T) \geq \mathscr{E}(P_{n,n-d+1})$, with equality if and only if $T \cong P_{n,n-d+1}$.*

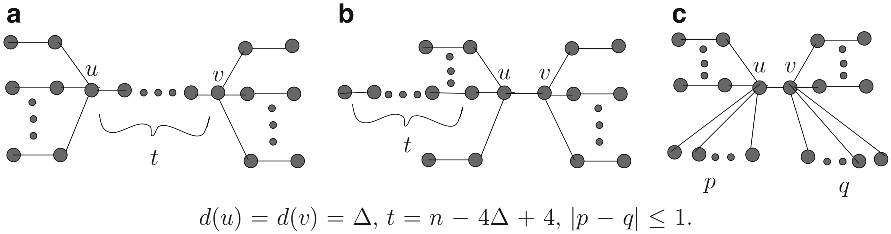


Fig. 7.16 The maximum-energy trees of order n with two vertices u and v of maximum degree Δ

7.1.3 Maximal Energy of Trees with Given Maximum Degree

A vertex of a tree whose degree is three or greater will be called a *branching vertex*. A pendent vertex attached to a vertex of degree two will be called a *2-branch*. The tree with maximal energy is said to be the *maximum-energy tree*.

Lin et al. [344] determined the trees with maximal energy among all trees with a fixed number n of vertices and fixed maximum vertex degree $\Delta(T)$ (see Theorem 7.10). Li et al. [339] offered a simplified proof of this result and also showed that a closely analogous result holds for trees with two maximum degree vertices. However, for the case of $n > 4\Delta - 2$, they could only show that the maximum-energy tree is one of the two trees but could not decide which one is exactly the maximum-energy tree. This is because the quasi-order method is invalid for comparing their energies. Eventually, Li et al. [316] succeeded to completely resolve the problem.

First of all, we list the results of [339]:

Theorem 7.10. *Among trees of order n with maximum degree Δ, the maximum-energy tree has exactly one branching vertex (of degree Δ) and as many as possible 2-branches.* ■

Theorem 7.11. *Among trees of order n with two vertices of maximum degree Δ, the maximum-energy tree has as many 2-branches as possible. (1) If $n \geq 4\Delta - 1$, then the tree with the maximal energy is either the graph (a) or the graph (b), depicted in Fig. 7.16. (2) If $n \leq 4\Delta - 2$, then the tree with the maximal energy is the graph (c) depicted in Fig. 7.16, in which the numbers of pendent vertices attached to the two branching vertices u and v differ by at most 1.* ■

We need the following lemmas to prove the above theorems. The proofs of them employ the method of quasi-orders, similar as in Sect. 4.3.

Gutman and Zhang [249] proved the following result:

Lemma 7.13. *Let $X_{n,i}$ be the graph whose structure is depicted in Fig. 7.17. For the fragment X being an arbitrary tree other than P_1 (or more generally, an arbitrary bipartite graph), $X_{n,1} \succ X_{n,3} \succ X_{n,5} \succ \cdots \succ X_{n,4} \succ X_{n,2}$.* ■

Fig. 7.17 The tree considered in Lemma 7.13

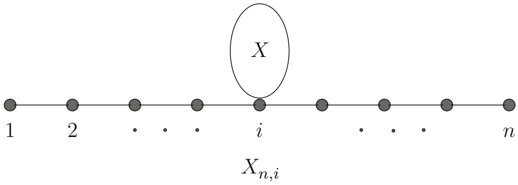
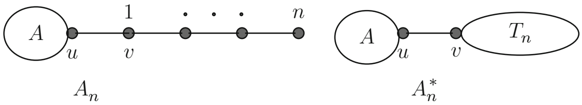


Fig. 7.18 The trees considered in Lemma 7.14



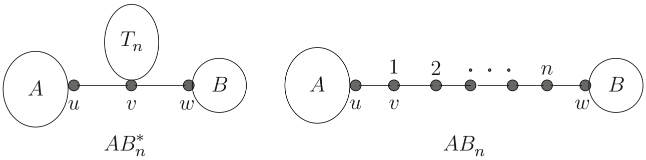


Fig. 7.19 The trees considered in Lemma 7.15

Let A_n and A_n^* be trees whose structures are depicted in Fig. 7.18. Let A be an arbitrary tree. In A_n the fragment A is attached via the vertex u to a leaf vertex v of the path P_n. In A_n^* the fragment A is attached to some n-vertex tree other than P_n.

Lemma 7.14. $A_n \succ A_n^*$.

Proof. Apply Lemma 4.4 to the edges of A_n and A_n^*, connecting the vertices u and v (as shown in Fig. 7.18). Then $m(A_n, k) = m(A \cup P_n, k) + m(A - u \cup P_{n-1}, k-1)$ and $m(A_n^*, k) = m(A \cup T_n, k) + m(A - u \cup T_n - v, k-1)$. Since $P_n \succ T_n$ and $P_{n-1} \succeq T_n - v$, we have that $m(A \cup P_n, k) \geq m(A \cup T_n, k)$, $m(A - u \cup P_{n-1}, k-1) \geq m(A - u \cup T_n - v, k-1)$, and therefore $m(A_n, k) \geq m(A_n^*, k)$, there exists k_0 such that $m(A_n, k_0) \geq m(A_n^*, k_0)$, and then the lemma follows. ■

Let AB_n and AB_n^* be trees whose structures are depicted in Fig. 7.19. Denote by A and B arbitrary tree fragments and by T_n an n-vertex tree.

Lemma 7.15. $AB_n \succ AB_n^*$.

Proof. Apply Lemma 4.4 to the edge connecting the vertices v and w of AB_n^*. Using the same notation as in Lemma 7.14, we get $m(AB_n^*, k) = m(A_n^* \cup B, k) + m(A \cup B - w \cup T_n - v, k-1)$ and, in an analogous manner, $m(AB_n, k) = m(A_n \cup B, k) + m(A_{n-1} \cup B - w, k-1)$. By a repeated application of Lemma 4.4 and in view of $P_{n-1} \succeq T_n - v$, we get

$$\begin{aligned} & m(A_{n-1} \cup B - w, k-1) \\ & \quad = m(A \cup B - w \cup P_{n-1}, k-1) + m(A - u \cup B - w \cup P_{n-2}, k-2) \\ & \quad \geq m(A \cup B - w \cup T_n - v, k-1) + m(A - u \cup B - w \cup P_{n-2}, k-2). \end{aligned}$$

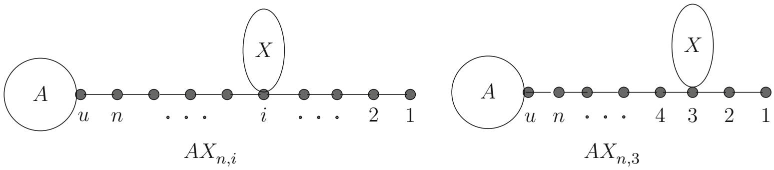


Fig. 7.20 The tree considered in Lemma 7.16

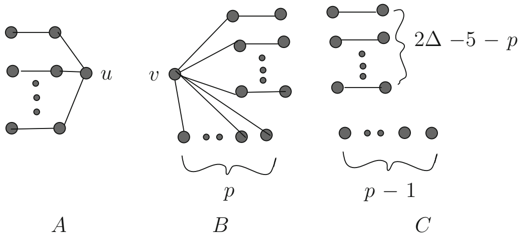


Fig. 7.21 The trees considered in Lemma 7.17

On the other hand, by Lemma 7.14, $A_n \succeq A_n^*$. Then $m(A_n \cup B, k) \geq m(A_n^* \cup B, k)$, which combined with the above relations yields $m(AB_n, k) \geq m(AB_n^*, k) + m(A - u \cup B - w \cup P_{n-2}, k-2)$, evidently implying $m(AB_n, k) \geq m(AB_n^*, k)$, which is strict for $k = 2$. The lemma follows. ∎

One easily obtains the following:

Lemma 7.16. *Let $AX_{n,i}$ be the graph whose structure is depicted in Fig. 7.20. For the fragments X and A being arbitrary trees other than P_1, we have $AX_{n,3} \succ AX_{n,i}$ for $2 \leq i \leq n-1$, and $i \neq 3$.* ∎

Lemma 7.17. *Let A and B be the graphs depicted in Fig. 7.21 such that $d(u) = d(v) = \Delta - 2,\ \Delta \geq 3,\ 0 < p \leq \Delta - 2$. Then $(A-u) \cup B \succ A \cup (B-v)$.*

Proof. Let $T_1 \cong (A-u) \cup B$ and $T_2 \cong A \cup (B-v)$. We show that $T_1 \succ T_2$. The orders of T_1 and T_2 are equal, i.e., $|V(T_1)| = |V(T_2)| = 4\Delta - p - 7$. For $0 < p \leq \Delta - 2$, direct calculation yields $\phi(T_1) = x^{p-1}(x^2-1)^{2\Delta-5-p}[x^4 - (\Delta-1)x^2 + p]$ and $\phi(T_2) = x^{p-1}(x^2-1)^{2\Delta-5-p}[x^4 - (\Delta-1)x^2]$. Then $\phi(T_1) - \phi(T_2) = p\,x^{p-1}(x^2-1)^{2\Delta-5-p}$. Also by direct calculation, the characteristic polynomial of the graph C depicted in Fig. 7.21 is $\phi(C) = x^{p-1}\,(x^2-1)^{2\Delta-5-p}$. Therefore, $\phi(T_1) - \phi(T_2) = p\,\phi(C)$.

On the other hand, for $i = 1, 2$, we have $\phi(T_i) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, m(T_i, k)\, x^{n-2k}$, where $n = 4\Delta - p - 7$ is the order of T_1 and T_2. The order of the graph C is $p - 1 + 2(2\Delta - 5 - p) = n - 4$. Then we have $\phi(C) = \sum_{k=0}^{\lfloor (n-4)/2 \rfloor} (-1)^k\, m(C, k)\, x^{n-4-2k}$. Since $\phi(T_1) - \phi(T_2) = p\,\phi(C)$, we have $m(T_1, k) - m(T_2, k) = p \cdot m(C, k-2) \geq 0$ for $2 \leq k \leq \lfloor n/2 \rfloor$ and $m(T_1, 0) = m(T_2, 0) = 1,\ m(T_1, 1) = m(T_2, 1) =$

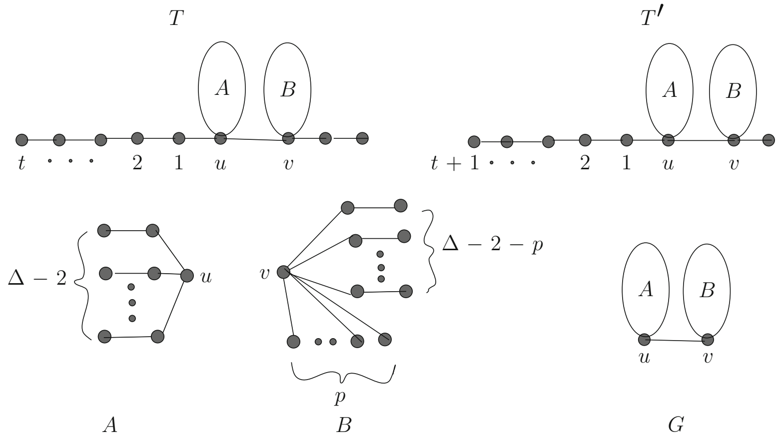


Fig. 7.22 The trees considered in Lemma 7.19

$3\Delta - p - 6$. Therefore, $m(T_1, k) \geq m(T_2, k)$ when $0 < p \leq \Delta - 2$, which is strict for $k = 2$, and thus, $T_1 \succ T_2$. The lemma follows. ■

Two vertices u and v of a graph G are said to be *equivalent* if the subgraphs $G - u$ and $G - v$ are isomorphic. The graph $G(u, v)(P_a, P_b)$ is obtained by joining the leaves of P_a and P_b to u and v, respectively. The following lemma was first stated in [249] and can be proved by Lemma 4.6:

Lemma 7.18. *If the vertices u and v of a graph G are adjacent and equivalent, then for* $n = 4k + i,\ i \in \{0, 1, 2, 3\},\ k \geq 1,$

$$\begin{aligned} G(u,v)(P_0,\ P_n) &\succ G(u,v)(P_2,\ P_{n-2}) \succ \cdots \succ G(u,v)(P_{2k},\ P_{n-2k}) \\ &\succ G(u,v)(P_{2k+1},\ P_{n-2k-1}) \succ G(u,v)(P_{2k-1},\ P_{n-2k+1}) \\ &\succ \cdots \succ G(u,v)(P_1,\ P_{n-1}). \end{aligned}$$ ■

Lemma 7.19. *Let T and T' be trees shown in Fig. 7.22. If* $d_T(u) = d_T(v) = d_{T'}(u) = d_{T'}(v) = \Delta,\ \Delta \geq 3,\ 0 \leq p \leq \Delta - 2,\ t \geq 2$, *then* $T \succ T'$.

Proof. T and T' can be denoted by $G(u, v)(P_t, P_2)$ and $G(u, v)(P_{t+1}, P_1)$, respectively, where G is shown in Fig. 7.22. If $p = 0$, then $A \cong B$. The vertices u and v are equivalent in G, and therefore, by Lemma 7.18, $T \succ T'$. In view of this, in what follows we assume that $0 < p \leq \Delta - 2$.

Applying Lemma 4.4 to T and T' and using the same notation as in Lemmas 7.14 and 7.16, we get

$$\begin{aligned} m(T,k) &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_t,P_0),k-1) \\ &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_0),k-1) \\ &\quad + m(G(u,v)(P_{t-2},P_0),k-2) \end{aligned}$$

$$\begin{aligned} m(T',k) &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_1),k-1) \\ &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_0),k-1) \\ &\quad + m(A_{t-1} \cup (B-v),k-2). \end{aligned}$$

Then $m(T,k) - m(T',k) = m(G(u,v)(P_{t-2},P_0),k-2) - m(A_{t-1} \cup B - v, k-2)$.

If $t = 2$, then the graph $A_{t-1} \cup (B-v)$ is a proper subgraph of $G(u,v)(P_{t-2},P_0)$, and then $m(T,k) \geq m(T',k)$ by Lemma 4.5.

When $t \geq 3$, a repeated application of Lemma 4.4 gives

$$\begin{aligned} &m(T,k) - m(T',k) \\ &= m(G(u,v)(P_{t-2},P_0),k-2) - m(A_{t-1} \cup (B-v),k-2) \\ &= m(A_{t-2} \cup B, k-2) + m((A-u) \cup (B-v) \cup P_{t-2}, k-3) \\ &\quad - m(A \cup (B-v) \cup P_{t-1}, k-2) - m((A-u) \cup (B-v) \cup P_{t-2}, k-3) \\ &= m(A_{t-2} \cup B, k-2) - m(A \cup (B-v) \cup P_{t-1}, k-2) \\ &= m(A \cup B \cup P_{t-2}, k-2) + m((A-u) \cup B \cup P_{t-3}, k-3) \\ &\quad - m(A \cup (B-v) \cup P_{t-2}, k-2) - m(A \cup (B-v) \cup P_{t-3}, k-3). \end{aligned}$$

Since $A \cup (B-v)$ is a proper subgraph of $A \cup B$, we have $A \cup B \succ A \cup (B-v)$ and $m(A \cup B \cup P_{t-2}, k-2) \geq m(A \cup (B-v) \cup P_{t-2}, k-2)$. On the other hand, $(A-u) \cup B \succ A \cup (B-v)$ follows by Lemma 7.17. Then $m((A-u) \cup B \cup P_{t-3}, k-3) \geq m(A \cup (B-v) \cup P_{t-3}, k-3)$. Consequently, $m(T,k) \geq m(T',k)$, which is strict for $k = 3$. The lemma follows. ■

Proof of Theorem 7.10. Let T be a tree of order n and maximum degree Δ with maximal energy. Let u be a vertex of maximum degree Δ in T. By Lemma 7.14, T must contain Δ pendent paths at u, i.e., T is a starlike tree with a unique branching vertex of degree Δ. By Lemma 7.13, T has as many as possible 2-branches. This completes the proof. ■

Proof of Theorem 7.11. Suppose that T is a tree of order n having exactly two vertices of maximum degree, with maximal energy. Let u and v be the vertices of maximum degree. Let P_t be the unique path connecting u and v. We first claim that there are no branching vertices in P_t. Otherwise, suppose that there is a branching vertex w in P_t and T_{n_1} is the tree attached to the path P_t at w. Assume that ww_1 and ww_2 are two edges in the path P_t. Then we obtain a new tree T' from T by deleting T_{n_1} and adding a path P_{n_1} whose two terminal vertices are adjacent to w_1

and w_2, respectively. From Lemma 7.15, $T' \succ T$, a contradiction. By Lemma 7.14, we know that there are $\Delta - 1$ pendent paths at u and v, respectively.

Next we claim that there is not more than one pendent path with length ≥ 3 in T. Otherwise, assume that there are two or more such paths. By Lemma 7.13, there is at most one pendent path of length ≥ 3 at each vertex of u and v. So we assume that P_{t_1} and P_{t_2} $(t_1 \geq 4,\ t_2 \geq 4)$ are the unique pendent paths of length ≥ 3 with terminal vertex u and v in T, respectively. From Lemma 7.13, the other pendent paths in T are all of length 2. If the length of the unique path P_t connecting u and v is equal to 1, i.e., $t = 2$, then u and v are adjacent. Then we construct a new tree T' from T by changing the paths P_{t_1} and P_{t_2} to $P_{t_1+t_2-3}$ and P_3, respectively. $T' \succ T$ follows from Lemma 7.18, a contradiction. If $t \geq 3$, then we also obtain a new tree T' from T by changing P_{t_2} and P_t to P_3 and P_{t+t_2-3}, respectively. $T' \succ T$ follows from Lemma 7.16, a contradiction. So the claim follows. From this claim, we have that there is at most one pendent path of length ≥ 3 in T. In what follows, we consider two cases.

Case 1. T has one such path. Without loss of generality, we may assume that it is attached to vertex u. By Lemma 7.13, we know that the other pendent paths at u are all of length 2. By Lemma 7.16, the length of the path P_t connecting u and v must be 1, i.e., u and v are adjacent in T. Then from Lemma 7.19, we get that all the pendent paths at v are of length 2. Therefore, T has the structure (b) depicted in Fig. 7.16.

Case 2. T has no pendent path of length ≥ 3. Then all the pendent paths at u and v are of length 1 or 2.

If the length of the path P_t is greater than 1, then from Lemma 7.16 all the pendent paths in T are of length 2. Then T has the structure (a) depicted in Fig. 7.16.

If the length of the path P_t is equal to 1, i.e., u and v are adjacent, then since each pendent path is either P_3 or a pendent edge, then $n \leq 4\Delta - 2$. Assume that there are p pendent edges and $\Delta - p - 1$ pendent paths P_3 at u, q pendent edges and $\Delta - q - 1$ pendent paths P_3 at v. Then $p + q = 4\Delta - n - 2 = m$.

By direct calculation, the characteristic polynomial of T is

$$\phi(T) = x^{m-2}(x^2-1)^{2\Delta-m-4}[x^8-(2\Delta+1)\,x^6+(\Delta^2+m+2)\,x^4-(\Delta m+1)\,x^2+pq].$$

Thus, when p and q are almost equal, i.e., $|p-q| \leq 1$, then the $\mathscr{E}$-value of T reaches the maximal which is depicted in (c) of Fig. 7.16. This completes the proof. ■

It remains to determine, for $n > 4\Delta - 2$, which of the graphs (a) and (b) in Theorem 7.11 has greatest energy. It turns out that this problem is much more complicated, because the quasi-order method does not work anymore. Li et al. [316] used the Coulson integral formula to find a solution whose details are shown in the following. For convenience, we denote the graphs (a) and (b) in Theorem 7.11 by $T_a = T_a(\Delta, t)$ and $T_b = T_b(\Delta, t)$, respectively.

In order to avoid the signs of coefficients in the matching polynomial, we use the so-called *signless matching polynomial* (see [310]):

$$m^+(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G,k)\, x^{2k} .$$

Then, for trees and forests, the Coulson integral formula can be rewritten as [145, 147]

$$\mathscr{E}(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln m^+(T,x)\, \mathrm{d}x \; . \tag{7.20}$$

Although $m^+(G,x)$ is just a variant of the ordinary matching polynomial $m(G,x)$ [80, 111, 112, 124, 151], namely,

$$m^+(G,x) = (\mathrm{i}x)^n\, m\left(G, \frac{1}{\mathrm{i}x}\right)$$

where $m(G,x)$ is defined via Eq. (1.4), we shall see later that its usage brings us a lot of computational convenience.

Only some basic properties of $m^+(G,x)$ are stated, those used for the calculation of $m^+(T_a)$ and $m^+(T_b)$. The proofs are omitted, since these are the same as those for the ordinary matching polynomial [80].

Lemma 7.20. *Let K_n be a complete graph with n vertices and $\overline{K_n}$ be the complement of K_n. Then*

$$m^+(\overline{K_n}, x) \equiv 1$$

for any $n \geq 0$, defining $m^+(\overline{K_0}, x) \equiv 1$, where both K_0 and $\overline{K_0}$ are the null graph. ■

Lemma 7.21. *Let G_1 and G_2 be two vertex disjoint graphs. Then*

$$m^+(G_1 \cup G_2, x) = m^+(G_1, x) \cdot m^+(G_2, x). \quad ■$$

Lemma 7.22. *Let $e = uv$ be an edge of the graph G. Then,*

$$m^+(G,x) = m^+(G-e,x) + x^2\, m^+(G-u-v,x). \quad ■$$

Lemma 7.23. *Let v be a vertex of G and $N(v) = \{v_1, v_2, \ldots, v_r\}$ the set of all neighbors of v in G. Then,*

$$m^+(G,x) = m^+(G-v,x) + x^2 \sum_{v_i \in N(v)} m^+(G-v-v_i,x). \qquad \blacksquare$$

The following recursive expressions are immediately obtained from Lemma 7.22:

Lemma 7.24. *Let P_t denote the path on t vertices. Then*

(1) $m^+(P_t,x) = m^+(P_{t-1},x) + x^2\, m^+(P_{t-2},x)$, *for any* $t \geq 1$

(2) $m^+(P_t,x) = (1+x^2)\, m^+(P_{t-2},x) + x^2\, m^+(P_{t-3},x)$, *for* $t \geq 2$.

The initial conditions are $m^+(P_0,x) = m^+(P_1,x) = 1$, *and we define* $m^+(P_{-1},x) = 0$. ■

From Lemma 7.24, one easily obtains:

Corollary 7.5. *Let P_t be a path on t vertices. Then for any real number x,*

$$m^+(P_{t-1},x) \leq m^+(P_t,x) \leq (1+x^2)\, m^+(P_{t-1},x), \text{ for any } t \geq 1. \qquad \blacksquare$$

We are now ready to compare the energies of T_a and T_b or, more precisely, of $T_a(\Delta,t)$ and $T_b(\Delta,t)$, which means to compare the values of two functions with the parameters Δ and t, denoted by $\mathscr{E}(T_a(\Delta,t))$ and $\mathscr{E}(T_b(\Delta,t))$, respectively. Since $\mathscr{E}(T_a(2,t)) = \mathscr{E}(T_b(2,t))$ for any $t \geq 2$ and $\mathscr{E}(T_a(\Delta,2)) = \mathscr{E}(T_b(\Delta,2))$ for any $\Delta \geq 2$, we always assume that $\Delta \geq 3$ and $t \geq 3$.

For convenience, we introduce the following notation:

$$\begin{aligned}
A_1 &= (1+x^2)(1+\Delta x^2)(2x^4 + (\Delta+2)x^2 + 1) \\
A_2 &= x^2(1+x^2)(x^6 + (\Delta^2+2)x^4 + (2\Delta+1)x^2 + 1) \\
B_1 &= (\Delta+2)x^8 + (2\Delta^2+6)x^6 + (\Delta^2+4\Delta+4)x^4 + (2\Delta+3)x^2 + 1 \\
B_2 &= x^2(1+x^2)(x^6 + (\Delta^2+2)x^4 + (2\Delta+1)x^2 + 1).
\end{aligned}$$

Using Lemmas 7.23 and 7.24 repeatedly, we easily get the following two recursive formulas:

$$m^+(T_a,x) = (1+x^2)^{2\Delta-5}\,[A_1\, m^+(P_{t-3},x) + A_2\, m^+(P_{t-4},x)] \qquad (7.21)$$

and

$$m^+(T_b,x) = (1+x^2)^{2\Delta-5}\,[B_1\, m^+(P_{t-3},x) + B_2\, m^+(P_{t-4},x)]. \qquad (7.22)$$

From Eqs. (7.21) and (7.22), by elementary calculations we obtain

$$m^+(T_a,x) - m^+(T_b,x) = (1+x^2)^{2\Delta-5}\,(\Delta-2)x^6\,[x^2-(\Delta-2)]\,m^+(P_{t-3},x). \tag{7.23}$$

Now we deal with the problem by distinguishing some cases for Δ. The first case is for $\Delta \geq 8$.

Theorem 7.12. *Among trees with n vertices and two vertices of maximum degree Δ, the maximal-energy tree has as many as possible 2-branches. If $\Delta \geq 8$ and $t \geq 3$, then the maximal-energy tree is the graph T_b, where $t = n+4-4\Delta$.*

Proof. From Eq. (7.20), we have

$$\begin{aligned}\mathscr{E}(T_a) - \mathscr{E}(T_b) &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\ln\frac{m^+(T_a,x)}{m^+(T_b,x)}\,\mathrm{d}x \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\ln\left[1+\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\right]\mathrm{d}x. \end{aligned}\tag{7.24}$$

We use $g(\Delta,t,x)$ to express

$$g(\Delta,t,x) = \frac{1}{x^2}\ln\left[1+\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\right].$$

Since $m^+(T_a,x) > 0$ and $m^+(T_b,x) > 0$, it follows that

$$\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)} = \frac{m^+(T_a,x)}{m^+(T_b,x)} - 1 > -1.$$

Therefore, by Lemma 4.8,

$$\frac{1}{x^2}\cdot\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_a,x)} \leq g(\Delta,t,x) \leq \frac{1}{x^2}\cdot\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}, \tag{7.25}$$

and thus,

$$\begin{aligned}\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\cdot\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_a,x)}\,\mathrm{d}x &\leq \mathscr{E}(T_a)-\mathscr{E}(T_b) \\ &\leq \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\cdot\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\,\mathrm{d}x.\end{aligned}$$

By Corollary 7.5, $m^+(P_{t-4},x) \le m^+(P_{t-3},x)$ and $m^+(P_{t-4},x) \ge \dfrac{m^+(P_{t-3},x)}{1+x^2}$ for $\Delta \ge 3$ and $t \ge 4$. This implies

$$
\begin{aligned}
&\mathscr{E}(T_a) - \mathscr{E}(T_b)\\
&\le \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\cdot\frac{m^+(T_a,x)-m^+(T_b,x)}{m^+(T_b,x)}\,\mathrm{d}x\\
&= \frac{2}{\pi}\int_0^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]\,m^+(P_{t-3},x)}{B_1\,m^+(P_{t-3},x)+B_2\,m^+(P_{t-4},x)}\,\mathrm{d}x\\
&\le \frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]}{B_1+B_2/(1+x^2)}\,\mathrm{d}x - \frac{2}{\pi}\int_0^{\sqrt{\Delta-2}} \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{B_1+B_2}\,\mathrm{d}x.
\end{aligned}
$$

We examine the last two terms separately. The first term is

$$
\begin{aligned}
&\frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]}{B_1+B_2/(1+x^2)}\,\mathrm{d}x\\
&=\frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]}{(\Delta+3)x^8+(3\Delta^2+8)x^6+(\Delta^2+6\Delta+5)x^4+(2\Delta+4)x^2+1}\,\mathrm{d}x\\
&< \frac{2}{\pi}\int_{\sqrt{\Delta-2}}^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]}{(\Delta+3)\,x^8}\,\mathrm{d}x = \frac{2}{\pi}\cdot\frac{2\sqrt{\Delta-2}}{3(\Delta+3)}.
\end{aligned}
$$

The second term is

$$
\begin{aligned}
&\frac{2}{\pi}\int_0^{\sqrt{\Delta-2}} \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{B_1+B_2}\,\mathrm{d}x\\
&= \frac{2}{\pi}\int_0^{\sqrt{\Delta-2}} \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{h(\Delta,x)}\,\mathrm{d}x
\end{aligned}
$$

$$> \frac{2}{\pi} \int_0^1 \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{\frac{5\Delta^2+11\Delta+26}{2}(x^2+1)}\,\mathrm{d}x + \frac{2}{\pi} \int_1^{\sqrt{\Delta-2}} \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{(5\Delta^2+11\Delta+26)x^{10}}\,\mathrm{d}x$$

$$= \frac{2}{\pi}\left(\frac{-45\pi\Delta - 34\Delta^2 + 74\Delta + 30\pi - 12 + 15\pi\Delta^2 + \frac{4}{\sqrt{\Delta-2}}}{30(26+11\Delta+5\Delta^2)}\right)$$

where $h(\Delta, x) = x^{10} + (\Delta^2+\Delta+5)x^8 + (3\Delta^2+2\Delta+9)x^6 + (\Delta^2+6\Delta+6)x^4 + (2\Delta+4)x^2 + 1$. Now, when $\Delta \geq 65$ we get that

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi}\cdot\frac{2\sqrt{\Delta-2}}{3(\Delta+3)}$$

$$-\frac{2}{\pi}\left(\frac{-45\pi\Delta - 34\Delta^2 + 74\Delta + 30\pi - 12 + 15\pi\Delta^2 + \frac{4}{\sqrt{\Delta-2}}}{30(26+11\Delta+5\Delta^2)}\right) \leq 0.$$

For $t = 3$, we have $m^+(P_{t-4}, x) = m^+(P_{-1}, x) = 0$. By a similar method as above, we can get that $\mathscr{E}(T_a) - \mathscr{E}(T_b) < 0$ when $\Delta \geq 24$.

Therefore, for $\Delta \geq 65$ and $t \geq 3$, it is $\mathscr{E}(T_a) < \mathscr{E}(T_b)$.

For $8 \leq \Delta \leq 64$, by direct calculation, we get that

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) \leq \frac{2}{\pi}\cdot f(\Delta, x) < 0$$

where

$$f(\Delta, x) = \int_{\sqrt{\Delta-2}}^{+\infty} \frac{(\Delta-2)x^4\,[x^2-(\Delta-2)]}{B_1+\frac{B_2}{1+x^2}}\,\mathrm{d}x - \int_0^{\sqrt{\Delta-2}} \frac{(\Delta-2)x^4\,(\Delta-2-x^2)}{B_1+B_2}\,\mathrm{d}x.$$

The respective numerical details are shown in Table 7.2.

The proof is thus complete. ■

We are left with the cases $3 \leq \Delta \leq 7$. At first, we consider the case of $\Delta = 3$ and $t \geq 3$. In this case, we have $n = 4\Delta - 4 + t \geq 11$.

Theorem 7.13. *Among trees with n vertices and two vertices of maximum degree $\Delta = 3$, the maximal-energy tree has as many as possible 2-branches. If $n \geq 11$, then the maximal-energy tree is the graph T_a.*

Table 7.2 The values of $f(\Delta, x)$ for $8 \leq \Delta \leq 67$

Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$	Δ	$f(\Delta, x)$
8	−0.00377	23	−0.20792	38	−0.29961	53	−0.35353
9	−0.02418	24	−0.21611	39	−0.30403	54	−0.35638
10	−0.04352	25	−0.22390	40	−0.30830	55	−0.35917
11	−0.06168	26	−0.23132	41	−0.31244	56	−0.36188
12	−0.07866	27	−0.23841	42	−0.31644	57	−0.36454
13	−0.09452	28	−0.24518	43	−0.32032	58	−0.36713
14	−0.10933	29	−0.25165	44	−0.32409	59	−0.36965
15	−0.12317	30	−0.25786	45	−0.32774	60	−0.37213
16	−0.13613	31	−0.26381	46	−0.33129	61	−0.37454
17	−0.14829	32	−0.26953	47	−0.33473	62	−0.37691
18	−0.15972	33	−0.27502	48	−0.33808	63	−0.37922
19	−0.17048	34	−0.28031	49	−0.34134	64	−0.38148
20	−0.18063	35	−0.28540	50	−0.34451	65	−0.38369
21	−0.19022	36	−0.29031	51	−0.34759	66	−0.38586
22	−0.19931	37	−0.29504	52	−0.35060	67	−0.38798

Proof. For $\Delta = 3$ and $t \geq 4$, by Eqs. (7.20) and (7.25) and Corollary 7.5,

$$\begin{aligned}
\mathscr{E}(T_a) - \mathscr{E}(T_b) &\geq \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \cdot \frac{m^+(T_a, x) - m^+(T_b, x)}{m^+(T_a, x)}\, \mathrm{d}x \\
&= \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \cdot \frac{x^6\,(x^2-1)\, m^+(P_{t-3}, x)}{A_1\, m^+(P_{t-3}, x) + A_2\, m^+(P_{t-4}, x)}\, \mathrm{d}x \\
&\geq \frac{2}{\pi} \int_1^{+\infty} \frac{x^4(x^2-1)}{A_1 + A_2}\, \mathrm{d}x - \frac{2}{\pi} \int_0^{1} \frac{x^4\,(1-x^2)}{A_1 + \frac{A_2}{1+x^2}}\, \mathrm{d}x \\
&= \frac{2}{\pi} \int_1^{+\infty} \frac{x^4\,(x^2-1)}{x^{10} + 18x^8 + 41x^6 + 33x^4 + 10x^2 + 1}\, \mathrm{d}x \\
&\quad - \frac{2}{\pi} \int_0^{1} \frac{x^4\,(1-x^2)}{7x^8 + 34x^6 + 32x^4 + 10x^2 + 1}\, \mathrm{d}x \\
&> \frac{2}{\pi} \cdot 0.00996 > 0.
\end{aligned}$$

For $\Delta = 3$ and $t = 3$, we can compute the energies of the two graphs directly and get that $\mathscr{E}(T_a) > \mathscr{E}(T_b)$.

Therefore, for $\Delta = 3$ and $t \geq 3$, we have $\mathscr{E}(T_a) > \mathscr{E}(T_b)$. ■

We now state two lemmas about the properties of $m^+(P_t, x)$ for our later use.

Lemma 7.25. *For $t \geq -1$, the polynomial $m^+(P_t, x)$ has the following form:*

$$m^+(P_t, x) = \frac{1}{\sqrt{1 + 4x^2}} \left(\lambda_1^{t+1} - \lambda_2^{t+1}\right)$$

where $\lambda_1 = \frac{1}{2}\left[1 + \sqrt{1 + 4x^2}\right]$ *and* $\lambda_2 = \frac{1}{2}\left[1 - \sqrt{1 + 4x^2}\right]$.

Proof. By Lemma 7.24, $m^+(P_t, x) = m^+(P_{t-1}, x) + x^2 m^+(P_{t-2}, x)$ for any $t \geq 1$. Thus, it satisfies the recursive formula $h(t, x) = h(t-1, x) + x^2 h(t-2, x)$, and the general solution of this linear homogeneous recurrence relation is $h(t, x) = P(x)\lambda_1^t + Q(x)\lambda_2^t$, where λ_1 and λ_2 are as given above. Considering the initial values $m^+(P_1, x) = 1$ and $m^+(P_2, x) = 1 + x^2$, by elementary calculation, we obtain

$$P(x) = \frac{1 + \sqrt{1 + 4x^2}}{2\sqrt{1 + 4x^2}}, \qquad Q(x) = \frac{-1 + \sqrt{1 + 4x^2}}{2\sqrt{1 + 4x^2}}.$$

Thus,

$$m^+(P_t, x) = P(x)\,\lambda_1^t + Q(x)\,\lambda_2^t = \frac{1}{\sqrt{1 + 4x^2}} \left(\lambda_1^{t+1} - \lambda_2^{t+1}\right).$$

As earlier defined, the initial conditions are $m^+(P_{-1}, x) = 0$ and $m^+(P_0, x) = 1$, from which we get the result for all $t \geq -1$. ■

Lemma 7.26. *Suppose that $t \geq 4$. If t is even, then*

$$\frac{2}{1 + \sqrt{1 + 4x^2}} < \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \leq 1.$$

If t is odd, then

$$\frac{1}{1 + x^2} \leq \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} < \frac{2}{1 + \sqrt{1 + 4x^2}}.$$

Proof. From Corollary 7.5, we know that

$$\frac{1}{1 + x^2} \leq \frac{m^+(P_{t-4}, x)}{m^+(P_{t-3}, x)} \leq 1.$$

By the definitions of λ_1 and λ_2, we conclude that $\lambda_1 > 0$ and $\lambda_2 < 0$ for any x. By Lemma 7.25, if t is even, then

$$\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} - \frac{2}{1+\sqrt{1+4x^2}} = \frac{\lambda_1^{t-3}-\lambda_2^{t-3}}{\lambda_1^{t-2}-\lambda_2^{t-2}} - \frac{1}{\lambda_1} = \frac{-\lambda_2^{t-3}(\lambda_1-\lambda_2)}{\lambda_1(\lambda_1^{t-2}-\lambda_2^{t-2})} > 0.$$

Thus,

$$\frac{2}{1+\sqrt{1+4x^2}} < \frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} \leq 1. \tag{7.26}$$

If t is odd, then obviously

$$\frac{1}{1+x^2} \leq \frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} < \frac{2}{1+\sqrt{1+4x^2}}. \tag{7.27}$$

■

Now we are ready to deal with the case $\Delta = 4$ and $t \geq 3$.

Theorem 7.14. *Among trees with n vertices and two vertices of maximum degree $\Delta = 4$, the maximum-energy tree has as many as possible 2-branches. The maximum-energy tree is the graph T_b if $t = 4$ and the graph T_a otherwise, where $t = n + 4 - 4\Delta$.*

Proof. By Eqs. (7.21)–(7.24),

$$\begin{aligned}\mathcal{E}(T_a) - \mathcal{E}(T_b) &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln\left[1 + \frac{m^+(T_a,x) - m^+(T_b,x)}{m^+(T_b,x)}\right] \mathrm{d}x \\ &= \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln\left[1 + \frac{(\Delta-2)x^6\,[x^2-(\Delta-2)]}{B_1 + B_2\,\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)}}\right] \mathrm{d}x.\end{aligned} \tag{7.28}$$

We first consider the case when t is odd and $t \geq 5$. By Eq. (7.28) and Lemma 7.26,

$$\begin{aligned}&\mathcal{E}(T_a) - \mathcal{E}(T_b) \\ &> \frac{2}{\pi}\int_{\sqrt{2}}^{+\infty} \frac{1}{x^2} \ln\left[1+\frac{2x^6\,(x^2-2)}{B_1+B_2\,\frac{2}{1+\sqrt{1+4x^2}}}\right] \mathrm{d}x + \frac{2}{\pi}\int_0^{\sqrt{2}} \frac{1}{x^2} \ln\left[1+\frac{2x^6\,(x^2-2)}{B_1+B_2\,\frac{1}{1+x^2}}\right] \mathrm{d}x \\ &> \frac{2}{\pi}\cdot 0.02088 > 0.\end{aligned}$$

If t is even, we want to find t and x satisfying

$$\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} < \frac{2}{-1+\sqrt{1+4x^2}}. \tag{7.29}$$

This is equivalent to solving

$$\frac{\lambda_1^{t-3}-\lambda_2^{t-3}}{\lambda_1^{t-2}-\lambda_2^{t-2}} < -\frac{1}{\lambda_2}$$

which means to solving

$$\left(\frac{\lambda_1}{-\lambda_2}\right)^{t-3} > -2\lambda_2, \qquad \text{i.e.,} \qquad \left(\frac{1+\sqrt{1+4x^2}}{2x}\right)^{2t-6} > \sqrt{1+4x^2}-1.$$

Thus,

$$2t-6 > \log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(\sqrt{1+4x^2}-1\right).$$

Since for $x \in (0,+\infty)$, $\frac{1+\sqrt{1+4x^2}}{2x}$ is decreasing and $\sqrt{1+4x^2}-1$ is increasing, we have that $\log_{\frac{1+\sqrt{1+4x^2}}{2x}}(\sqrt{1+4x^2}-1)$ is increasing. Thus, if $x \in [\sqrt{2},5]$, then

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}(\sqrt{1+4x^2}-1) \le \log_{\frac{1+\sqrt{101}}{10}}(\sqrt{101}-1) < 23.$$

Therefore, when $t \ge 15$, i.e., $2t-6 > 23$, then Ineq. (7.29) holds for $x \in [\sqrt{2},5]$.

We now calculate the difference of $\mathscr{E}(T_a)$ and $\mathscr{E}(T_b)$. When t is even and $t \ge 15$, from Eq. (7.28) it follows,

$$\begin{aligned}
&\mathscr{E}(T_a)-\mathscr{E}(T_b)\\
&> \frac{2}{\pi}\int_5^{+\infty}\frac{1}{x^2}\ln\left[1+\frac{2x^6\,(x^2-2)}{B_1+B_2}\right]\mathrm{d}x+\frac{2}{\pi}\int_{\sqrt{2}}^{5}\frac{1}{x^2}\ln\left[1+\frac{2x^6\,(x^2-2)}{B_1+B_2\,\frac{2}{-1+\sqrt{1+4x^2}}}\right]\mathrm{d}x\\
&\quad+\frac{2}{\pi}\int_0^{\sqrt{2}}\frac{1}{x^2}\ln\left[1+\frac{2x^6\,(x^2-2)}{B_1+B_2\,\frac{2}{1+\sqrt{1+4x^2}}}\right]\mathrm{d}x > \frac{2}{\pi}\cdot 0.003099 > 0.
\end{aligned}$$

For $t=3$ and any even t, such that $4 \le t \le 14$, by direct computation, we get that $\mathscr{E}(T_a) < \mathscr{E}(T_b)$ for $t=4$ and $\mathscr{E}(T_a) > \mathscr{E}(T_b)$ for the other cases.

By this proof is complete. ■

The following theorem gives settles the cases $\Delta = 5, 6, 7$.

Theorem 7.15. *For trees with n vertices and two vertices of maximum degree Δ, let $t = n - 4\Delta + 4 \geq 3$. Then*

(i) For $\Delta = 5$, the maximum-energy tree is the graph T_a if t is odd and $3 \leq t \leq 89$ and the graph T_b otherwise.
(ii) For $\Delta = 6$, the maximum-energy tree is the graph T_a if $t = 3, 5, 7$ and the graph T_b otherwise.
(iii) For $\Delta = 7$, the maximum-energy tree is the graph T_b for any $t \geq 3$.

Proof. Before considering the above three cases separately, we note that

$$\lim_{t\to\infty} \frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} = \frac{2}{1+\sqrt{1+4x^2}}.$$

Therefore, in view of Ineq. (7.26), if t is even and sufficiently large, then for some $\Theta' > 0$,

$$\frac{2+\Theta'}{1+\sqrt{1+4x^2}}$$

becomes an upper bound for $m^+(P_{t-4},x)/m^+(P_{t-3},x)$. Analogously, in view of Ineq. (7.27), if t is odd and sufficiently large, then for some $\Theta'' > 0$,

$$\frac{2-\Theta''}{1+\sqrt{1+4x^2}}$$

becomes a lower bound for $m^+(P_{t-4},x)/m^+(P_{t-3},x)$. By numerical testing, it was found that already $\Theta' = 0.1$ and $\Theta'' = 0.01$ suffice for our purposes, namely, for those values of the variable x that are encountered in the subsequent considerations. Thus, in what follows, the inequalities

$$\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} < \frac{2.1}{1+\sqrt{1+4x^2}} \tag{7.30}$$

and

$$\frac{m^+(P_{t-4},x)}{m^+(P_{t-3},x)} > \frac{1.99}{1+\sqrt{1+4x^2}} \tag{7.31}$$

will be used.

We now examine the cases $\Delta = 5, 6$, and 7 separately.

Case (i) $\Delta = 5$.

If t is even, we want to find t and x satisfying Ineq. (7.30). This is equivalent to solving

$$\frac{\lambda_1^{t-3}-\lambda_2^{t-3}}{\lambda_1^{t-2}-\lambda_2^{t-2}} < \frac{2.1}{2\lambda_1}$$

which is equivalent to

$$\left(\frac{\lambda_1}{-\lambda_2}\right)^{t-3} > \frac{-2.1\lambda_2 + 2\lambda_1}{0.1\lambda_1},$$

that is,

$$\left(\frac{1+\sqrt{1+4x^2}}{2x}\right)^{2t-6} > 41 - \frac{42}{\sqrt{1+4x^2}+1}.$$

Thus,

$$2t-6 > \log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(41 - \frac{42}{\sqrt{1+4x^2}+1}\right).$$

Since for $x \in (0, +\infty)$, $\frac{1+\sqrt{1+4x^2}}{2x}$ is a decreasing and $-\frac{42}{\sqrt{1+4x^2}+1}$ an increasing function of x, it follows that $\log_{\frac{1+\sqrt{1+4x^2}}{2x}}(41 - \frac{42}{\sqrt{1+4x^2}+1})$ is increasing. Thus, for $x \in (0, \sqrt{3}]$,

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(41 - \frac{42}{\sqrt{1+4x^2}+1}\right) \le \log_{\frac{1+\sqrt{13}}{2\sqrt{3}}}\left(41 - \frac{42}{1+\sqrt{13}}\right) < 13.$$

Therefore, when $t \ge 10$, i.e., $2t-6 > 13$, then Ineq. (7.30) holds for $x \in (0, \sqrt{3}]$. Thus, if t is even and $t \ge 10$, from Eq. (7.28) and Lemma 7.26, we obtain

$$\begin{aligned}\mathscr{E}(T_a) - \mathscr{E}(T_b) &< \frac{2}{\pi}\int_{\sqrt{3}}^{+\infty}\frac{1}{x^2}\ln\left[1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{2}{1+\sqrt{1+4x^2}}}\right]\mathrm{d}x \\ &\quad + \frac{2}{\pi}\int_0^{\sqrt{3}}\frac{1}{x^2}\ln\left[1 + \frac{3x^6(x^2-3)}{B_1 + B_2\frac{2.1}{1+\sqrt{1+4x^2}}}\right] \\ &< \frac{2}{\pi}\cdot(-4.43\times 10^{-4}) < 0.\end{aligned}$$

If t is odd, we want to find t and x satisfying the condition (7.31), that is,

$$2t-6 > \log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1+4x^2}+1}\right).$$

Since for $x \in (0, +\infty)$, $\log_{\frac{1+\sqrt{1+4x^2}}{2x}}(399 - \frac{398}{\sqrt{1+4x^2}+1})$ is an increasing function of x, we conclude that for $x \in [\sqrt{3}, 390]$,

$$\log_{\frac{1+\sqrt{1+4x^2}}{2x}}\left(399 - \frac{398}{\sqrt{1+4x^2}+1}\right) < 4671.$$

Therefore, for $t \geq 2339$, i.e., $2t-6 \geq 4671$, we have that Ineq. (7.31) holds for $x \in [\sqrt{3}, 390]$. Thus, if t is odd and $t \geq 2339$, from Eq. (7.28) and Lemma 7.26, it follows

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi} \int_{390}^{+\infty} \frac{1}{x^2} \ln\left[1 + \frac{3x^6(x^2-3)}{B_1 + B_2 \frac{1}{1+x^2}}\right] \mathrm{d}x$$

$$+ \frac{2}{\pi} \int_{\sqrt{3}}^{390} \frac{1}{x^2} \ln\left[1 + \frac{3x^6(x^2-3)}{B_1 + B_2 \frac{1.99}{1+\sqrt{1+4x^2}}}\right] \mathrm{d}x$$

$$+ \frac{2}{\pi} \int_{0}^{\sqrt{3}} \frac{1}{x^2} \ln\left[1 + \frac{3x^6(x^2-3)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}}\right] \mathrm{d}x < \frac{2}{\pi} \cdot (-6.66 \times 10^{-6}) < 0.$$

For any even t with $4 \leq t \leq 8$ and any odd t with $3 \leq t \leq 2337$, by directly computing the energies of the two graphs, we get that $\mathscr{E}(T_a) > \mathscr{E}(T_b)$ for any odd t with $3 \leq t \leq 89$, and $\mathscr{E}(T_a) < \mathscr{E}(T_b)$ for the other cases.

Case (ii) $\Delta = 6$.
If t is even and $t \geq 4$, from Eq. (7.28) and Lemma 7.26, we have

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi} \int_{2}^{+\infty} \frac{1}{x^2} \ln\left[1 + \frac{4x^6(x^2-4)}{B_1 + B_2 \frac{2}{1+\sqrt{1+4x^2}}}\right] \mathrm{d}x$$

$$+ \frac{2}{\pi} \int_{0}^{2} \frac{1}{x^2} \ln\left[1 + \frac{4x^6(x^2-4)}{B_1 + B_2}\right] \mathrm{d}x < \frac{2}{\pi} \cdot (-0.02027) < 0.$$

If t is odd, in a similar manner as in the proof of Case (i), we can show that when $t \geq 27$ and $x \in [2, 22]$, the following holds:

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi} \int_{22}^{+\infty} \frac{1}{x^2} \ln\left[1 + \frac{4x^6(x^2-4)}{B_1 + B_2 \frac{1}{1+x^2}}\right] \mathrm{d}x$$

$$+ \frac{2}{\pi} \int_{2}^{22} \frac{1}{x^2} \ln\left[1 + \frac{4x^6(x^2-4)}{B_1 + B_2 \frac{1}{1+\sqrt{1+4x^2}}}\right] \mathrm{d}x$$

$$+\frac{2}{\pi}\int_{0}^{2}\frac{1}{x^2}\ln\left[1+\frac{4x^6(x^2-4)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right]dx < \frac{2}{\pi}\cdot(-2.56\times 10^{-4}) < 0.$$

For any odd t such that $3 \leq t \leq 25$, by direct computation, we get $\mathscr{E}(T_a) > \mathscr{E}(T_b)$ for $t = 3, 5, 7$ and $\mathscr{E}(T_a) < \mathscr{E}(T_b)$ for the other cases.

(iii) $\Delta = 7$.

If t is even and $t \geq 4$, by the same method as used in the proof of Case (ii), we get

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi}\cdot(-0.04445) < 0.$$

If t is odd and $t \geq 5$, we have that

$$\mathscr{E}(T_a) - \mathscr{E}(T_b) < \frac{2}{\pi}\int_{\sqrt{5}}^{+\infty}\frac{1}{x^2}\ln\left[1+\frac{5x^6(x^2-5)}{B_1+B_2\frac{1}{1+x^2}}\right]dx$$

$$+\frac{2}{\pi}\int_{0}^{\sqrt{5}}\frac{1}{x^2}\ln\left[1+\frac{5x^6(x^2-5)}{B_1+B_2\frac{2}{1+\sqrt{1+4x^2}}}\right]dx < \frac{2}{\pi}\cdot(-0.01031) < 0.$$

For $t = 3$, we can compute the energies of the two graphs directly and verify that $\mathscr{E}(T_a) < \mathscr{E}(T_b)$.

The proof is now complete. ■

From the above theorems, one can observe the following noteworthy result:

Corollary 7.6. *For all chemical trees of order n with two vertices of maximum degree at least 3, the graph T_a has maximal energy, with only a single exception, namely, only if $\Delta = 4$ and $t = 4$, then $T_b(4,4)$ has energy greater than $T_a(4,4)$.* ■

Remark 7.4. Yao [502] employed the same technique as used in the proof of Theorem 7.11 to investigate the maximum-energy trees with one maximum and one second-maximum degree vertex. Only a result similar to Theorem 7.11 was reported there. Li and Li [317] used the same method as above and completely determined the maximum-energy trees, left unsolved by Yao. An interesting problem is to determine the maximal-energy trees with given number, say k, of maximum degree vertices.

Li and Lian [333] characterized the maximum-energy trees among conjugated trees with n vertices and maximum degree Δ.

7.2 Unicyclic Graphs with Extremal Energies

In the previous section, we have discussed the extremal problems on trees, and now we turn our attention to unicyclic graphs. In the following subsections, we use Method 3 "quasi-order," which is outlined in Sect. 4.3, to deal with the extremal problems. Recall that in Sect. 4.3, we defined $b_i(G) = |a_i(G)|$ for a given graph G, where $0 \leq i \leq n$, in connection with the Coulson integral formula (3.11).

Let $\mathscr{U}(n)$ be the class of graphs with n vertices whose components are all trees except at most one being a unicyclic graph. That is, any graph in $\mathscr{U}(n)$ is either acyclic or contains exactly one cycle.

Lemma 7.27. *Let G be a graph in $\mathscr{U}(n)$.*
(a) *If G contains exactly one cycle C_r and uv is an edge of this cycle, then*

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-r}(G - C_r) \qquad \text{if } r \equiv 0 \pmod 4$$
$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-r}(G - C_r) \qquad \text{if } r \not\equiv 0 \pmod 4.$$

(b) *If uv is a cut edge of G, then $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v)$.*
(c) *If G is connected and uv is a pendent edge of G with pendent vertex v, then $b_i(G) = b_i(G - v) + b_{i-2}(G - v - u)$.*

Proof. For the edge uv of G, from Theorem 1.3, if uv is a cut edge, then $\phi(G) = \phi(G - uv) - \phi(G - u - v)$. Now (a) and (b) follow by equating the coefficients of x^{n-i} on both sides of the above identities.

For (c), since v is a pendent vertex of G, we have $\phi(G) = x\,\phi(G - v) - \phi(G - v - u)$. Thus,

$$\begin{aligned} b_i(G) &= |a_i(G)| = |a_i(G - v) - a_{i-2}(G - v - u)| = |a_i(G - v)| + |a_{i-2}(G - v - u)| \\ &= b_i(G - v) + b_{i-2}(G - v - u). \end{aligned}$$

■

7.2.1 Minimal Energy of Unicyclic Graphs

Caporossi et al. [53] posed the following conjecture. They also confirmed the conjecture for $m = n - 1,\ 2(n - 2)$.

Conjecture 7.5. Among all connected graphs G with $n \geq 6$ vertices and $n - 1 \leq m \leq 2(n - 2)$ edges, the graphs with minimal energy are the following. If $m \leq n + \lfloor (n - 7)/2 \rfloor$, then this graph is the star S_n with $m - n + 1$ additional edges all connected to the same vertex. Otherwise, this is the bipartite graph with two vertices on one side, one of which is connected to all vertices on the other side. ■

In [266] it was proven that the conjecture is true for $m = n$, i.e., the minimal energy among all unicyclic graphs of order n ($n \geq 6$) was determined.

Let $G(n,\ell)$ be the set of all unicyclic graphs with n vertices and with a cycle C_ℓ. Then from the Sachs theorem, Theorem 1.1, we get the following lemma:

Lemma 7.28. *Let $G \in G(n,\ell)$. Then $(-1)^k a_{2k} \geq 0$ for all $k \geq 0$, and $(-1)^k a_{2k+1} \geq 0$ (respectively ≤ 0) for all $k \geq 0$ if $\ell = 2r+1$ and r is odd (respectively even).*

Proof. If ℓ is even, then G is bipartite, and $a_{2k} = (-1)^k b_{2k}$, $a_{2k+1} = 0$ for all $k \geq 0$. Hence, the result follows.

Suppose that ℓ is odd and $\ell = 2r+1$. If $i = 2k$, then every Sachs subgraph of G with i vertices must consist of only k-matchings and $a_{2k} = (-1)^k m(G;k)$. If $i = 2k+1$, then $a_{2k+1} = 0$ when $2k+1 < \ell$, and every Sachs subgraph of G with $2k+1$ vertices must contain the cycle C_ℓ when $2k+1 \geq \ell$, thus $a_{2k+1} = 2(-1)^{k-r+1} m(G - C_\ell, k-r)$. Hence, the result follows. ■

From the Coulson integral formula (3.11), we have that for a unicyclic graph G, $\mathscr{E}(G)$ is a monotonically increasing function of $b_i(G)$ ($i = 1,2,\ldots,n$). That is, let G_1 and G_2 be unicyclic graphs; if $b_i(G_1) \geq b_i(G_2)$ holds for all $i \geq 0$, then $\mathscr{E}(G_1) \geq \mathscr{E}(G_2)$. If $b_i(G_1) \geq b_i(G_2)$ holds for all $i \geq 0$, then in a similar manner we can define a quasi-order $G_1 \succeq G_2$ or $G_2 \preceq G_1$ and will write $G_1 \succ G_2$ if $G_1 \succeq G_2$ but not $G_2 \succeq G_1$.

Let A_n^ℓ denote the graph obtained from the cycle C_ℓ by adding $n-\ell$ pendent edges to a vertex of C_ℓ.

Lemma 7.29. *Let $G \in G(n,\ell)$ and $G \not\cong A_n^\ell$. Then $G \succ A_n^\ell$.*

Proof. We prove the theorem by induction on $n-\ell$.

If $n-\ell = 0$, then the theorem clearly follows. Let $p \geq 1$, and suppose that the result is true for $n-\ell < p$. Consider $n-\ell = p$. Since G is unicyclic and $n > \ell$, G is not a cycle. Hence, G must have a pendent vertex v which is adjacent to a unique vertex u. By Lemma 7.27 (*c*), $b_i(G) = b_i(G-v) + b_{i-2}(G-v-u)$ and $b_i(A_n^\ell) = b_i(A_{n-1}^\ell) + b_{i-2}(P_{\ell-1})$. By the induction hypothesis,

$$b_i(G-v) \geq b_i(A_{n-1}^\ell) \qquad \textit{for all } i \geq 0. \tag{7.32}$$

As

$$b_{i-2}(P_{\ell-1}) = \begin{cases} 0 & \text{if } i \text{ is odd} \\ m\left(P_{\ell-1}, \frac{i-2}{2}\right) & \text{if } i \text{ is even and } i \leq \ell+1 \\ 0 & \text{if } i \text{ is even and } i > \ell+1 \end{cases}$$

and $G-v-u$ contains the path $P_{\ell-1}$ as its subgraph, $b_{i-2}(G-v-u) \geq b_{i-2}(P_{\ell-1})$ if i is odd or if i is even and $i > \ell+1$. If i is even and $i \leq \ell+1$, then $b_{i-2}(G-v-u) = m(G-v-u,(i-2)/2) \geq m(P_{\ell-1},(i-2)/2)$. Therefore,

$$b_{i-2}(G-v-u) \geq b_{i-2}(P_{\ell-1}) \qquad \text{for all } i \geq 0. \tag{7.33}$$

From Ineqs. (7.32) and (7.33) follows $b_i(G) \geq b_i(A_n^\ell)$. It is easy to see that if $G \ncong A_n^\ell$, then $b_2(G-v-u) > \ell-2 = b_2(P_{\ell-1})$. Hence, $\mathscr{E}(A_n^\ell) < \mathscr{E}(G)$, and the theorem holds. ■

Theorem 7.16. *Let $n \geq \ell \geq 5$. Then $A_n^\ell \succ A_n^4$.*

Proof. We prove the theorem by induction on $n-\ell$. It is easy to obtain that $\phi(A_n^4) = x^{n-4}[x^4 - nx^2 + 2(n-4)]$. Thus, $b_4(A_n^4) = 2(n-4)$ and $b_i(G) = 0$ for all $i \neq 0, 2, 4$. If $n-\ell = 0$, then $G \cong C_n$ and $b_4(C_n) = n(n-3)/2$. Hence, $b_4(C_n) > b_4(A_n^4)$ for all $n \geq 5$, and the theorem holds. Let $p \geq 1$, and suppose that the result is true for $n-\ell < p$. Now we consider $n-\ell = p$. By Lemma 7.27 (c),

$$b_4(A_n^\ell) = b_4(A_{n-1}^\ell)+b_2(P_{\ell-1}) = b_4(A_{n-1}^\ell)+\ell-2 \geq 2(n-1-4)+\ell-2 > 2(n-4).$$

Thus, the theorem follows. ■

Theorem 7.17. *Let G be a unicyclic graph with $n \geq 6$ vertices and $G \ncong A_n^3$. Then $\mathscr{E}(A_n^3) < \mathscr{E}(G)$.*

Proof. From Lemmas 7.29 and 7.16, it is sufficient to prove that $\mathscr{E}(A_n^3) < \mathscr{E}(A_n^4)$ for $n \geq 6$. It is easy to obtain $\phi(A_n^3) = x^{n-4}[x^4 - nx^2 - 2x + (n-3)]$. Then from Eq. (3.11), it follows

$$\mathscr{E}(A_n^4) - \mathscr{E}(A_n^3) = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln \frac{[1+nx^2+2(n-4)x^4]^2}{[1+nx^2+(n-3)x^4]^2 + (2x^3)^2}\,\mathrm{d}x.$$

Set $f(x) = [1+nx^2+2(n-4)x^4]^2 - [1+nx^2+(n-3)x^4]^2 - 4x^6$. Then $f(x) = 2(n-5)x^4 + 2[n(n-5)-2]x^6 + (n-5)^2x^8 + 2(n-5)(n-3)x^8 > 0$ for $n \geq 6$. Therefore, $\mathscr{E}(A_n^3) < \mathscr{E}(A_n^4)$ for $n \geq 6$. ■

7.2.2 *Minimal Energy of Unicyclic Conjugated Graphs*

In Sect. 7.1.2, we discussed the minimal energy among all acyclic conjugated graphs. In this subsection, we discuss the minimal energies among all unicyclic conjugated graphs, i.e., unicyclic graphs with a perfect matching [342].

Let $U(k)$ be the set of all unicyclic graphs on $2k$ vertices with a perfect matching. Denote by ℓ the length of the unique cycle of the unicyclic graph $G = (V(G), E(G))$. Let C_ℓ be the unique cycle of G with length ℓ and $M(G)$ a perfect matching of G. Let $U^0(k)$ be the subset of $U(k)$ such that $\ell \equiv 0 \pmod 4$, there are $\frac{\ell}{2}$ independent edges of $M(G)$ in C_ℓ and there are some edges of $E(G) \setminus M(G)$ in $G \setminus C_\ell$ for any $G \in U^0(k)$. Let $S_3^1(k)$ be the graph on $2k$ vertices obtained from C_3 by attaching one pendent edge and $k-2$ paths of length 2 together to one of the three vertices of C_3 (see Fig. 7.23). Let $S_4^1(k)$ be the graph obtained from C_4

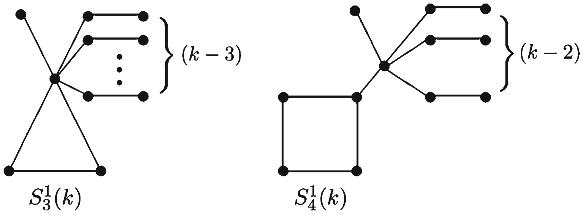


Fig. 7.23 The graphs $S_3^1(k)$ and $S_4^1(k)$

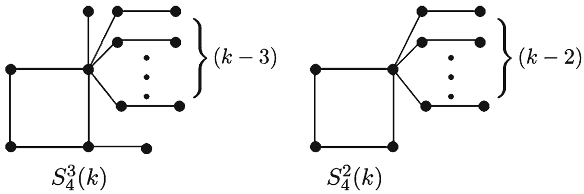


Fig. 7.24 The graphs $S_4^3(k)$ and $S_4^2(k)$

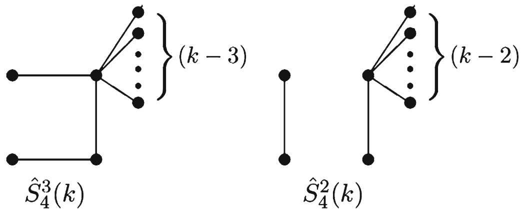


Fig. 7.25 The graphs $\hat{S}_4^3(k)$ and $\hat{S}_4^2(k)$

by attaching one path P of length 2 to one vertex of C_4 and then attaching $k-3$ paths of length 2 to the second vertex of the path P (see Fig. 7.23). Let $S_4^2(k)$ be the graph on $2k$ vertices obtained from C_4 by attaching $k-2$ paths of length 2 to one of the four vertices of C_4 (see Fig. 7.24). Let $S_4^3(k)$ be the graph on $2k$ vertices obtained from C_4 by attaching one pendent edge and $k-3$ paths of length 2 together to one of the four vertices of C_4 and one pendent edge to the adjacent vertex of C_4, respectively (see Fig. 7.24).

At first, we show that $S_3^1(k)$ and $S_4^3(k)$ ($k \geq 31$) are the graphs with the minimal and second-minimal energies in $U^*(k) = U(k) \setminus U^0(k)$, respectively, and $S_4^1(k)$ is the graph with minimal energy in $U^0(k)$.

We denote $G[E(G) \setminus M(G)]$ by $\hat{G}$. For example, $\hat{S}_4^2(k)$ and $\hat{S}_4^3(k)$ are shown in Fig. 7.25. Let $r_j^{(2i)}(G)$ be the number of ways to choose i independent edges in G such that j edges are in $\hat{G}$. Obviously, $r_0^{(2i)}(G) = \binom{k}{i}$, $r_1^{(2i)}(G) = k\binom{k-2}{i-1}$.

Lemma 7.30. *Let $G \in U^*(k)$, $\ell \equiv 1 \pmod 2$, and $\ell \geq 5$. Then $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.*

Proof. Combining Theorem 1.1 and the case $\ell \equiv 1 \pmod 2$, we obtain

$$b_{2i}(S_4^3(k)) = r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + r_2^{(2i)}(S_4^3(k)) - 2r_0^{(2i-4)}(S_4^3(k) \setminus C_4)$$

$$= r_0^{(2i)}(S_4^3(k)) + r_1^{(2i)}(S_4^3(k)) + \binom{k-3}{i-2} + (k-3)\binom{k-4}{i-2} - 2\binom{k-3}{i-2} \tag{7.34}$$

$$b_{2i}(G) = r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_{k-1}^{(2i)}(G).$$

It suffices to prove that

$$r_2^{(2i)}(G) \geq (k-3)\binom{k-4}{i-2} - \binom{k-3}{i-2}.$$

For $i = 1, 2, \ldots, \ell$, let v_i be the vertex of C_ℓ, T_i the tree planting at v_i $(v_i \in V(T_i))$, and n_i the number of edges of $\hat{G}$ in T_i. Obviously, $k - (\ell+1)/2 \geq n_1 + n_2 + \cdots + n_\ell \geq k - \ell$. Let β_2 be the number of ways of choosing two independent edges of $\hat{G}$.

If there exist at least two trees T_i, T_j such that $n_i \geq n_j > 0$, then $k - (\ell+1)/2 \geq 2n_j$ and $\beta_2 - (k-3) \geq n_j(k - n_j - 2) - k + 3 = n_j k - n_j^2 - 2n_j - k + 3 \geq 0$.

If there is exactly one tree T_i such that $n_i > 0$, then there exists an edge e of C_ℓ such that e belongs to $E(\hat{G})$ and is not adjacent to v_i. Thus, $\beta_2 \geq k - 1 - 2$. Then $r_2^{(2i)}(G) \geq (k-3)\binom{k-4}{i-2}$. ■

Lemma 7.31. *Let $G \in U^*(k)$. If $\ell = 3$ and $G \not\cong S_3^1(k)$, then $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.*

Proof. Similarly, it suffices to prove that $\beta_2 \geq k-3$, where $v_i, n_i,$ *and* β_2 are defined same as in the proof of Lemma 7.30.

Case 1. There is exactly one edge $e \in M(G)$ in C_3. Without loss of generality, let $e = v_1v_2$. Then $n_1 + n_2 + n_3 = k - 2$.

Subcase 1.1. There are at least two trees T_i, T_j such that $n_i, n_j > 0$. Then, in a similar manner as in the proof of Lemma 7.30, we obtain $\beta_2 \geq k - 3$.

Subcase 1.2. There is one tree T_i such that $n_i > 0$. Then i can only be 3. Let $P = v_3u_1 \ldots u_{t-2}u_{t-1}u_t$ be the longest path of T_3 from v_3. Then u_t is a pendent edge and $u_{t-2}u_{t-1} \in E(\hat{G})$. Since $G \not\cong S_3^1(k)$, we have $t \geq 3$ and so $t - 2 \geq 1$. Let x be the number of edges of $E(\hat{G})$ adjacent to u_{t-2}. Then $\beta_2 \geq k - 2$ when $x = 1$, and $\beta_2 \geq (x-1)(k-x) \geq k - 3$ when $x \geq 2$, since $k \geq x + 2$.

Case 2. There is no edge of $M(G)$ in C_3. Then $\beta_2 \geq n_1 + n_2 + n_3 = k - 3$.

The proof is complete. ■

Lemma 7.32. *Let $G \in U^*(k)$. If $\ell \equiv 2 \pmod 4$, then $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.*

Proof. By Theorem 1.1,

$$b_{2i}(G) = r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_i^{(2i)}(G) \\ +2\left[r_0^{(2i-\ell)}(G \setminus C_\ell) + r_1^{(2i-\ell)}(G \setminus C_\ell) + \cdots + r_{i-\ell/2}^{(2i-\ell)}(G \setminus C_\ell)\right].$$

It suffices to prove that $r_2^{(2i)}(G) \geq r_2^{(2i)}(S_4^3(k)) - 2\binom{k-3}{i-2}$. The inequality is obtained in a similar manner as in the proof of Lemma 7.30. ∎

Lemma 7.33. *Let $G \in U^*(k)$, $\ell \geq 8$, and $\ell \equiv 0 \pmod 4$.*

(i) *If there are at most $\ell/2-1$ edges of $M(G)$ in C_ℓ, then $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.*
(ii) *If there are exactly $\ell/2$ edges of $M(G)$ in C_ℓ, then $\mathscr{E}(G) > \mathscr{E}(S_4^2(k))$.*

Proof. In the case (i), by Theorem 1.1, we obtain

$$b_{2i}(G) = r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) + \cdots + r_i^{(2i)}(G)$$
$$-2\left[r_0^{(2i-\ell)}(G \setminus C_\ell) + r_1^{(2i-\ell)}(G \setminus C_\ell) + \cdots + r_{i-\ell/2}^{(2i-\ell)}(G \setminus C_\ell)\right]. \tag{7.35}$$

Case 1. There are $\ell/2-1$ edges of $M(G)$ in C_ℓ. Then there are $\ell/2+1$ edges of $E(\hat{G})$ in C_ℓ. Let M_1 *and* M_2 be two matchings in C_ℓ with cardinality $\ell/2$.

Subcase 1.1. If $M_1 \not\subset E(\hat{G})$ and $M_2 \not\subset E(\hat{G})$, then M_1 *and* M_2 contain at least two edges of $E(\hat{G})$ and one of those contains at least three edges of $E(\hat{G})$. Let M_0 be a matching in $G \setminus C_\ell$ with cardinality $i-\ell/2$ such that it contains at least one edge of $E(\hat{G})$. Then there are two matchings $M_1 \cup M_0$ *and* $M_2 \cup M_0$ with cardinality i corresponding to M_0. Thus, $b_{2i}(G) \geq r_0^{(2i)}(G) + r_1^{(2i)}(G) + \beta_2^0\binom{k-4}{i-2} - \binom{k-\ell/2-1}{i-\ell/2}$, where β_2^0 denotes the number of ways in which two independent edges are chosen in $E(\hat{G})$ such that at least one edge is in C_ℓ. Let $n_1, n_2, \ldots, n_\ell$ be defined same as in the proof of Lemma 7.30. Then,

$$\beta_2^0 \geq (\ell/2+1-2)(n_1+n_2+\cdots+n_\ell) + \binom{\ell/2-1}{2}$$
$$= (\ell/2-1)(k-\ell/2-1) + \binom{\ell/2-1}{2} \geq k-3.$$

Subcase 1.2. Without loss of generality, let $M_1 \subset E(\hat{G})$. Then M_2 contains exactly one edge of $E(\hat{G})$. Similarly, we have $b_{2i}(G) \geq r_0^{(2i)}(G) + r_1^{(2i)}(G) + \beta_2^*\binom{k-4}{i-2} - \binom{k-\ell/2-1}{i-\ell/2}$, where β_2^* denotes the number of choices two independent edges of $E(\hat{G})$ such that at least one edge is in M_1 and no edge is in M_2. Then

$$\beta_2^* \geq (\ell/2-1)(n_1+\cdots+n_\ell) + \binom{\ell/2}{2} = (\ell/2-1)(k-\ell/2-1) + \binom{\ell/2}{2} \geq k-3.$$

Since $\binom{k-3}{i-2} \geq \binom{k-\ell/2-1}{i-\ell/2}$, we obtain $b_{2i}(G) \geq b_{2i}(S_4^3(k))$ for $0 \leq i \leq \lfloor n/2 \rfloor$, and these equalities do not always hold.

Case 2. There are at most $\ell/2-2$ edges of $M(G)$ in C_ℓ. Then M_1 *and* M_2 contain at least two edges of $E(\hat{G})$. Similar as in Case 1, $b_{2i}(G) \geq b_{2i}(S_4^3(k))$ for $0 \leq i \leq \lfloor n/2 \rfloor$, and these equalities do not always hold. Thus, $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.

For (ii), there are exactly $\ell/2$ edges of $M(G)$ in C_ℓ. By Theorem 1.1 and $G \in U^*(k)$, similar to Eqs. (7.34) and (7.35), we have

$$b_{2i}(S_4^2(k)) = r_0^{(2i)}(S_4^2(k)) + r_1^{(2i)}(S_4^2(k)) + \binom{k-2}{i-2} + (k-2)\binom{k-3}{i-2} - 2\binom{k-2}{i-2}$$

$$b_{2i}(G) \geq r_0^{(2i)}(G) + r_1^{(2i)}(G) + \beta_2' \binom{k-3}{i-2} - \binom{k-\ell/2}{i-\ell/2}$$

where β_2' is the number of ways in which two independent edges of $E(\hat{G})$ are chosen, such that both are adjacent to one edge of $M(G)$. Without loss of generality, let $v_1v_2, v_3v_4, \ldots, v_{\ell-1}v_\ell \in E(\hat{G})$. Then $\beta_2' \geq n_1 + n_2 + \cdots + n_\ell + \ell/2 = k - \ell/2 + \ell/2 > k-2$. Combining this with

$$\binom{k-2}{i-2} \geq \binom{k-\ell/2}{i-\ell/2}$$

we obtain $\mathscr{E}(G) > \mathscr{E}(S_4^2(k))$. ■

Similarly, we have

Lemma 7.34. *Let $G \in U^*(k)$ and $\ell = 4$.*

(i) If there is exactly one edge of $M(G)$ in C_4, then $\mathscr{E}(G) > \mathscr{E}(S_4^3(k))$.
(ii) If there are exactly two edges of $M(G)$ in C_4, then $\mathscr{E}(G) > \mathscr{E}(S_4^2(k))$. ■

The following two lemmas, which come from [81] and [512], respectively, will be used later:

Lemma 7.35. *$\phi(S_4^3(k), x) < \phi(S_4^2(k), x)$ for all $x \geq \lambda_1(S_4^2(k))$. In particular, $\lambda_1(S_4^3(k)) > \lambda_1(S_4^2(k))$.* ■

Lemma 7.36. *$S_3^1(k)$ is the graph with maximal spectral radius in $U(k)$.* ■

From [81] and Theorem 1.3, we get:

Lemma 7.37. *Let G be a graph with characteristic polynomial $\phi(G, x)$. Then*

$$\phi(S_4^3(k)) = (x^2-1)^{k-4}\,[x^8 - (k+4)x^6 + (3k+2)x^4 - (k+3)x^2 + 1]$$
$$\phi(S_4^2(k)) = x^2(x^2-1)^{k-3}\,[x^4 - (k+3)x^2 + 2k]$$
$$\phi(S_3^1(k)) = (x^2-1)^{k-2}\,[x^4 - (k+2)x^2 - 2x + 1]$$
$$\phi(S_4^1(k)) = x^2(x^2-1)^{k-4}\,[x^6 - (k+4)x^4 + 4kx^2 - 6].$$ ■

For convenience, in Table 7.3 are given $\mathscr{E}(S_4^1(k))$, $\mathscr{E}(S_3^1(k))$, $\mathscr{E}(S_4^2(k))$, and $\mathscr{E}(S_4^3(k))$ for the first few values of k.

Lemma 7.38. *$\mathscr{E}(S_4^2(k)) > \mathscr{E}(S_4^3(k))$ for $k \geq 30$.*

Proof. Let x_1, x_2, x_3, x_4, $(x_1 > x_2 \geq x_3 \geq x_4)$ be the positive roots of

$$f(x) = x^8 - (k+4)\,x^6 + (3k+2)\,x^4 - (k+3)\,x^2 + 1 = 0.$$

Let y_1, y_2, $(y_1 > y_2)$ be the two positive roots of

$$g(y) = y^4 - (k+3)\,y^2 + 2k = 0.$$

It suffices to prove that $x_1 + x_2 + x_3 + x_4 < y_1 + y_2 + 1$ for $k \geq 50$.

When $k \geq 50$, $f(0) > 0$, $f(0.145) < 0$, $f(0.62)$, $f(\frac{\sqrt{5}+1}{2}) < 0$, $f(\sqrt{k+6/5}) > 0$; $g(1.4) < 0$, $g(\sqrt{k+1}) > 0$, $g(\sqrt{k+2}) < 0$. Then we obtain that $x_4 < 0.145$, $x_3 < 0.62$, $x_2 < 1.618$, $x_1 < \sqrt{k+6/5}$, $y_2 > 1.4$, $y_1 > \sqrt{k+1}$. Furthermore, by Lemma 7.35, we have $\sqrt{k+6/5} > x_1 > y_1 > \sqrt{k+1}$, $y_1 > x_1 - \left(\sqrt{k+6/5} - \sqrt{k+1}\right) > x_1 - 0.0143$. Thus, $x_1 + x_2 + x_3 + x_4 < 0.145 + 0.62 + 1.618 + x_1 = 2.383 + x_1 < 1 + 1.4 + x_1 - 0.0143 < 1 + y_1 + y_2$. ■

Lemma 7.39. *$\mathscr{E}(S_4^3(k)) > \mathscr{E}(S_3^1(k))$ for $k \geq 43$.*

Proof. Let t_1, t_2 $(t_1 > t_2)$ be the two positive roots of $h(t) = t^4 - (k+2)t^2 - 2t + 1 = 0$.
By Lemma 7.37, $\mathscr{E}(S_4^3(k)) = 2k - 8 + 2(x_1 + x_2 + x_3 + x_4)$ and $\mathscr{E}(S_3^1(k)) = 2k - 4 + 2(t_1 + t_2)$. It suffices to prove that $x_1 + x_2 + x_3 + x_4 > t_1 + t_2 + 2$ for $k \geq 51$. If $k \geq 51$, then $f(0) > 0$, $f(\frac{\sqrt{5}-1}{2}) < 0$, $f(1.597) > 0$, $f(\frac{\sqrt{5}+1}{2}) < 0$, $h(0) > 0$, and $h(0.12) < 0$. Then $x_2 + x_3 + x_4 - t_2 - 2 \geq 0.618 + 1.597 - 0.12 - 2 = 0.095 = \varepsilon$, i.e., $x_2 + x_3 + x_4 > 2 + t_2 + \varepsilon$.

We now prove that $t_1 < x_1 + \varepsilon$. It suffices to show that $h(x_1 + \varepsilon) > 0$. If $k \geq 51$, then $x_1 > \sqrt{k+1} > 7.1$. Then

$$\frac{h(t)}{t^2} = t^2 - (k+2) - \frac{2}{t} + \frac{1}{t^2} = t^2 - (k+2) + \left(\frac{1}{t} - 1\right)^2 - 1$$

and

$$\begin{aligned}\frac{h(x_1+\varepsilon)}{(x_1+\varepsilon)^2} &\geq (x_1+\varepsilon)^2 - (k+2) + 0.7381 - 1 \\ &= x_1^2 - (k+1) + 2\varepsilon x_1 + \varepsilon^2 - 1.2619 \geq 2\varepsilon x_1 - 1.2619 > 0.\end{aligned}$$

This implies $h(x_1 + \varepsilon) > 0$ and $x_1 + x_2 + x_3 + x_4 > t_1 + t_2 + 2$. ■

Combining Table 7.3, Theorem 1.3, and Lemmas 7.30, 7.38, and 7.39, we obtain:

Table 7.3 Energies of $S_4^1(k)$, $S_3^1(k)$, $S_4^2(k)$, $S_4^3(k)$ for $5 \leq k \leq 50$

k=5	11.4006	12.0355	11.5696	11.9997
k=6	13.7663	14.3551	13.9820	14.3547
k=7	16.1047	16.6598	16.3626	16.6890
k=8	18.4251	18.9516	18.7178	19.0058
k=9	20.7301	21.2319	21.0521	21.3076
k=10	23.0219	23.5020	23.3689	23.5965
k=11	25.3019	25.7628	25.6707	25.8739
k=12	27.5715	28.0153	27.9595	28.1411
k=13	29.8318	30.2602	30.2368	30.3992
k=14	32.0837	32.4982	32.5039	32.6839
k=15	34.3279	34.7297	34.7619	34.8913
k=16	36.5652	36.9553	37.0116	37.1268
k=17	38.7960	39.1754	39.2538	39.3559
k=18	41.0209	41.3904	41.4991	41.5793
k=19	43.2403	43.6006	43.7182	43.7972
k=20	45.4545	45.8064	45.9414	46.0101
k=21	47.6641	48.0079	48.1592	48.2183
k=22	49.8691	50.2055	50.3720	50.4221
k=23	52.0700	52.3994	52.5801	52.6218
k=24	54.2669	54.5897	54.7838	54.8176
k=25	56.4602	56.7767	56.9834	57.0098
k=26	58.6499	58.9605	59.1791	59.1985
k=27	60.8362	61.1413	61.3712	61.3839
k=28	63.0194	63.3192	63.5597	63.5661
k=29	65.1996	65.4944	65.7450	65.7454
k=30	67.3770	67.6669	67.9272	67.3922
k=31	69.5516	69.8370	70.1065	70.0957
k=32	71.7236	72.0046	72.2829	72.2669
k=33	73.8931	74.1699	74.4566	74.4357
k=34	76.0603	76.3331	76.6277	76.6020
k=35	78.2251	78.4941	78.7964	78.7662
k=36	80.3878	80.6530	80.9627	80.9281
k=37	82.5483	82.8100	83.1268	83.0880
k=38	84.7068	84.9651	85.2886	85.2458
k=39	86.8634	87.1184	87.4484	87.4017
k=40	89.0180	89.2699	89.6062	89.5558
k=41	91.1709	91.4197	91.7621	91.7080
k=42	93.3219	93.5678	93.9161	93.8585
k=43	95.4713	95.7144	96.0683	96.0074
k=44	97.6191	97.8594	98.2187	98.1546
k=45	99.7652	100.0029	100.3675	100.3002
k=46	101.9099	102.1449	102.5146	102.4443
k=47	104.0530	104.2856	104.6602	104.5869
k=48	106.1947	106.4249	106.8043	106.7281
k=49	108.3350	108.5628	108.9469	108.8679
k=50	110.4739	110.6994	111.0880	111.0064

Theorem 7.18. *(i) For $5 \le k \le 13$, $S_4^2(k)$ is the minimal-energy graph in $U^*(k)$. (ii) For $14 \le k \le 39$, $S_3^1(k)$ is the minimal-energy graph in $U^*(k)$. (iii) For $k = 30$, $S_4^3(k)$ is the minimal-energy graph in $U^*(k)$. (iv) For $k \ge 31$, $S_3^1(k)$ and $S_4^3(k)$ are, respectively, the graphs in $U^*(k)$ with minimal and second-minimal energy.* ∎

Lemma 7.40. *Let $G \in U^0(k)$, $G \not\cong S_4^1(k)$, and $\ell = 4$. Then $\mathscr{E}(G) > \mathscr{E}(S_4^1(k))$.*

Proof. Let x be the number of edges in $E(\hat{G})$ that are adjacent to the vertices of C_4 except for two edges in C_4. Since there are exactly two edges of $M(G)$, $G \setminus C_4$ contains some edges of $E(\hat{G})$. Then $1 \le x \le k-3$. By Theorem 1.1, similar to Eq. (7.35), we obtain

$$\begin{aligned}
b_{2i}(G) &\ge r_0^{(2i)}(G) + r_1^{(2i)}(G) + x\binom{k-3}{i-2} + 2(k-2-x)\binom{k-4}{i-2} \\
&\quad +(x-1)\binom{k-4}{i-2} - \binom{k-2}{i-2} - (k-2-x)\binom{k-4}{i-3} \\
&= r_0^{(2i)}(G) + r_1^{(2i)}(G) + x\left[\binom{k-3}{i-2} - \binom{k-4}{i-2} + \binom{k-4}{i-3}\right] \\
&\quad +2(k-2)\binom{k-4}{i-2} - \binom{k-4}{i-2} - (k-2)\binom{k-4}{i-3} - \binom{k-2}{i-2} \\
&\ge r_0^{(2i)}(G) + r_1^{(2i)}(G) + 1\cdot\left[\binom{k-3}{i-2} - \binom{k-4}{i-2} + \binom{k-4}{i-3}\right] \\
&\quad +2(k-2)\binom{k-4}{i-2} - \binom{k-4}{i-2} - (k-2)\binom{k-4}{i-3} - \binom{k-2}{i-2} = b_{2i}(S_4^1(k))
\end{aligned}$$

where the equality holds if and only if $G \cong S_4^1(k)$. So we have $G \succ S_4^1(k)$, and so $\mathscr{E}(G) > \mathscr{E}(S_4^1(k))$. ∎

Lemma 7.41. *Let $G \in U^0(k)$ and $\ell \ge 8$. Then $\mathscr{E}(G) > \mathscr{E}(S_4^1(k))$.*

Proof. By Theorem 1.1, similar to Eqs. (7.34) and (7.35), we obtain

$$\begin{aligned}
b_{2i}(S_4^1(k)) &= r_0^{(2i)}(S_4^1(k)) + r_1^{(2i)}(S_4^1(k)) + \binom{k-3}{i-2} + 2(k-3)\binom{k-4}{i-2} \\
&\quad -\binom{k-2}{i-2} - (k-3)\binom{k-4}{i-3}
\end{aligned}$$

$$b_{2i}(G) \geq r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) - r_0^{(2i-\ell)}(G \setminus C_\ell) - r_1^{(2i-\ell)}(G \setminus C_\ell)$$

$$\geq r_0^{(2i)}(G) + r_1^{(2i)}(G) + r_2^{(2i)}(G) - \binom{k-\ell/2}{i-\ell/2}$$

$$-(k-\ell/2-1)\binom{k-\ell/2-2}{i-\ell/2-1}.$$

Let v_i , $i = 1, 2, \ldots, \ell$, be the vertices of C_ℓ. Let T_i be the tree planting at v_i ($v_i \in V(T_i)$), n_i the number of edges in $\hat{G}$. Obviously, $n_1 + n_2 + \cdots + n_\ell = k - \ell/2$. Let β_2 be the number of ways in which two independent edges of $\hat{G}$ are chosen, such that at least one edge is in C_ℓ. Then

$$\beta_2 \geq \left(\frac{\ell}{2} - 1\right)(n_1 + \cdots + n_\ell) + \binom{\ell/2}{2} = (\ell/2 - 1)(k - \ell/2) + \binom{\ell/2}{2} \geq 3k - 9$$

and

$$r_2^{(2i)}(G) > \binom{k-3}{i-2} + 2(k-3)\binom{k-4}{i-2}.$$

Since $\binom{k-2}{i-2} > \binom{k-\ell/2}{i-\ell/2}$, it follows

$$(k-3)\binom{k-4}{i-3} > (k-\ell/2-1)\binom{k-\ell/2-2}{i-\ell/2-1}$$

which implies $G \succ S_4^1(k)$ and $\mathscr{E}(G) \geq \mathscr{E}(S_4^1(k))$. ∎

Using Lemmas 7.40 and 7.41, it is not difficult to obtain:

Theorem 7.19. *$S_4^1(k)$ is the minimal-energy graph in $U^0(k)$.* ∎

By Theorems 7.18 and 7.19, Lemmas 7.40 and 7.41, and Table 7.3, we conclude that either $S_3^1(k)$ or $S_4^1(k)$ is the graph with the minimal energy in $U(k)$. Li and Li [331] provided a complete solution of this problem:

Theorem 7.20. *$S_4^1(k)$ is the minimal-energy graph in $U(k)$.*

Proof. We proceed our proof by estimating the roots of the characteristic polynomials of $S_3^1(k)$ and $S_4^1(k)$. When $k < 100$, the result can be obtained similarly as that in Table 7.3. In the following, we only focus on the case of $k \geq 100$. Let x_1, x_2 ($x_1 > x_2$) be the two positive roots of $f(x) = x^4 - (k+2)\,x^2 - 2x + 1$ and y_1, y_2, y_3 ($y_1 > y_2 > y_3$) the three roots of $g(y) = y^3 - (k+4)\,y^2 + 4ky - 6$. Noticing that $g(1) > 0$ and $g(4) = g(0) = -6$, we have $y_i > 0$ ($i = 1, 2, 3$). Hence,

$$E(S_3^1) = 2(k-2) + 2(x_1 + x_2), \qquad E(S_4^1) = 2(k-4) + 2(\sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}).$$

It suffices to prove that $x_1 + x_2 + 2 > \sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}$ for $k \geq 100$. Consider the above function $f(x)$. Because $f(\sqrt{k+2}) < 0$, we have $x_1 > \sqrt{k+2}$. Moreover, since $f(\sqrt{0.7/k}) > 0$ for $k \geq 100$, it follows that $x_2 > \sqrt{0.7/k}$. Therefore, we only need to show that $\sqrt{k+2} + \sqrt{0.7/k} + 2 > \sqrt{y_1} + \sqrt{y_2} + \sqrt{y_3}$. Since $g(1) > 0$ and $g(4) = g(0) = -6$, we have $y_2 < 4$. Let $y = 2/k$. Note that $g(2/k) = (2/k)^3 - 4/k - 16/k^2 + 8 - 6 > 0$ for $k \geq 100$, which means that $y_3 < 2/k$. Hence, to complete the proof, it suffices to show that $\sqrt{y_1} < \sqrt{k+2} + \sqrt{0.7/k} - \sqrt{2/k}$.

If $y = k + 1/2$ and $k \geq 100$, then

$$g(k+1/2) = -7/2(k+1/2)^2 + 4k(k+1/2) - 6 = (k+1/2)(k/2 - 7/4) - 6 > 0$$

which implies $y_1 < k + 1/2$. Then we only need to prove that

$$\sqrt{\frac{k+1}{2}} < \sqrt{k+2} + \sqrt{\frac{0.7}{k}} - \sqrt{\frac{2}{k}}. \tag{7.36}$$

In fact, it is easy to check that $(\sqrt{2} - \sqrt{0.7})^2 + 2(\sqrt{2} - \sqrt{0.7})\sqrt{k(k+1/2)} < 1.5k$ for $k \geq 100$, from which we have that

$$k^2 + k/2 + (\sqrt{2} - \sqrt{0.7})^2 + 2(\sqrt{2} - \sqrt{0.7})\sqrt{k(k+1/2)} < k^2 + 2k.$$

Then we get that $\sqrt{k(k+1/2)} + (\sqrt{2} - \sqrt{0.7}) < \sqrt{k(k+2)}$, which implies the required Ineq. (7.36), and the proof is thus complete. ■

Remark 7.5. The minimal energies of some other classes of unicyclic graphs were studied. For instance, the minimal-energy unicyclic graph of order n with a given bipartition is determined in [312, 315], the minimal-energy unicyclic graph with given diameter is determined in [313], and so on.

7.2.3 Maximal Energy of Unicyclic Graphs

Concerning unicyclic graphs with maximal energy, Caporossi et al. [53] put forward the following conjecture.

Let P_n^ℓ be the unicyclic graph obtained by connecting a vertex of C_ℓ with a leaf of $P_{n-\ell}$. Denote by $G(n,\ell)$ the set of all connected unicyclic graphs on n vertices, containing the cycle C_ℓ as a subgraph, and by $C(n,\ell)$ the set of all unicyclic graphs obtained from C_ℓ by adding to it $n-\ell$ pendent vertices.

Conjecture 7.6. Among all unicyclic graphs on n vertices, the cycle C_n has maximal energy if $n \leq 7$ and $n = 9, 10, 11, 13$, and 15. For all other values of n, i.e., $n = 8, 12, 14$ and $n \geq 16$, the unicyclic graph with maximal energy is P_n^6.

In [270], a result was proven that is weaker than the above conjecture, namely, that $\mathscr{E}(P_n^6)$ is maximal within the class of connected unicyclic bipartite n-vertex graphs differing from C_n.

Lemma 7.42. *Let* $G \in G(n,\ell)$*, where* $\ell \not\equiv 0 \pmod 4$*. If* $G \ncong P_n^\ell$*, then* $G \prec P_n^\ell$*.*

Proof. We prove the lemma by induction on $n-\ell$.

Case 1. ℓ is odd. In a trivial manner, the lemma holds for $n-\ell=0$ and $n-\ell=1$, because then $G(n,\ell)$ has only a single element. If $n-\ell=2$, $G \ncong P_n^\ell$, then $G \in C(n,\ell)$. Since G is unicyclic and not a cycle, for $n=\ell+2$, G must have a pendent edge uv with pendent vertex v, clearly $G-v \cong P_{\ell+1}^\ell$. By Lemma 7.27, $b_i(G)=b_i(G-v)+b_{i-2}(G-v-u)$ and $b_i(P_{\ell+2}^\ell)=b_i(P_{\ell+1}^\ell)+b_{i-2}(C_\ell)$. If $G-u-v$ is acyclic with ℓ vertices, then $b_{i-2}(G-v-u)=0$ when i is odd, whereas for $i=2k$, $b_{2k-2}(G-v-u)=m(G-v-u,k-1) \le m(P_\ell,k-1) < m(C_\ell,k-1)=b_{2k-2}(C_\ell)$. Thus, the lemma holds for $n-\ell=2$.

Let $p \ge 3$ and suppose that the result is true for $n-\ell<p$. Consider first the case $n-\ell=p$. Since G is unicyclic and not a cycle, for $n>\ell$, G must have a pendent edge uv with pendent vertex v. As $G \ncong P_n^\ell$ and $n \ge \ell+3$, we may choose a pendent edge uv of G such that $G-v \ncong P_{n-1}^\ell$. By Lemma 7.27,

$$b_i(G)=b_i(G-v)+b_{i-2}(G-v-u) \tag{7.37}$$

$$b_i(P_n^\ell)=b_i(P_{n-1}^\ell)+b_{i-2}(P_{n-2}^\ell). \tag{7.38}$$

By the induction hypothesis, $G-v \prec P_{n-1}^\ell$.

If $G-v-u$ contains the cycle C_ℓ, then by the induction hypothesis, we have $G-v-u \preceq P_{n-2}^\ell$. (It is easy to show that this relation holds also if $G-v-u$ is not connected.) Thus, the lemma follows from Eqs. (7.37) and (7.38) and the induction hypothesis.

If $G-v-u$ does not contain the cycle C_ℓ, then it is acyclic. Then $b_{i-2}(G-v-u)=0$ when i is odd, whereas for $i=2k$,

$$\begin{aligned} b_{2k-2}(G-v-u) &= m(G-v-u,k-1) \le m(P_{n-2},k-1)) \\ &< m(P_{n-2}^\ell,k-1)=b_{2k-2}(P_{n-2}^\ell). \end{aligned} \tag{7.39}$$

Lemma 7.42 now follows from Eqs. (7.37) through (7.39) and the induction hypothesis.

Case 2. ℓ is even; hence, $\ell=4r+2$. In this case, all elements of $G(n,\ell)$ are bipartite graphs and $b_i(G)=0$ when i is odd. Evidently, the lemma holds when $n-\ell=0,1$. For $n-\ell=2$, $G \ncong P_n^\ell$, and therefore, $G \in C(n,\ell)$. Since G is unicyclic and not a cycle, for $n=\ell+2$, G must have a pendent edge uv with pendent vertex v. Then $G-v \cong P_{\ell+1}^\ell$. By Lemma 7.27,

$$b_{2k}(G)=b_{2k}(G-v)+b_{2k-2}(G-v-u)$$

$$b_{2k}(P_{\ell+2}^{\ell}) = b_{2k}(P_{\ell+1}^{\ell}) + b_{2k-2}(C_\ell).$$

In addition, $G - u - v$ is acyclic, possessing ℓ vertices. Then for odd values of i, $b_{i-2}(G - v - u) = 0$, whereas for $i = 2k$,

$$\begin{aligned} b_{2k-2}(G - v - u) &= m(G - v - u, k-1) \leq m(P_\ell, k-1) \\ &< m(C_\ell, k-1) \leq b_{2k-2}(C_\ell). \end{aligned}$$

Thus, the lemma holds for $n - \ell = 2$.

Let $p \geq 3$ and suppose that the result is true for $n - \ell < p$. Consider the case $n - \ell = p$. Since for $n > \ell$, G is unicyclic and not a cycle, G must have a pendent edge uv with pendent vertex v. As $G \ncong P_n^\ell$ and $n \geq \ell + 3$, we may choose a pendent edge uv of G such that $G - v \ncong P_{n-1}^\ell$. By Lemma 7.27,

$$b_{2k}(G) = b_{2k}(G - v) + b_{2k-2}(G - v - u) \tag{7.40}$$

$$b_{2k}(P_n^\ell) = b_{2k}(P_{n-1}^\ell) + b_{2k-2}(P_{n-2}^\ell). \tag{7.41}$$

By the induction hypothesis, we have $G - v \prec P_{n-1}^\ell$.

If $G - v - u$ contains the cycle C_ℓ, then by the induction hypothesis, $G - v - u \preceq P_{n-2}^\ell$. Thus, the lemma follows from Eqs. (7.40) and (7.41) and the induction hypothesis.

If $G - v - u$ does not contain the cycle C_ℓ, then it is acyclic. Thus, $b_{i-2}(G - v - u) = 0$ when i is odd and when $i = 2k$,

$$\begin{aligned} b_{2k-2}(G - v - u) &= m(G - v - u, k-1) \leq m(P_{n-2}, k-1) \\ &< m(P_{n-2}^\ell, k-1) \leq m(P_{n-2}^\ell, k-1) + 2m(P_{n-\ell-2}, k-1-\ell/2) \\ &= b_{2k-2}(P_{n-2}^\ell) \end{aligned} \tag{7.42}$$

where the last equality follows from the Sachs theorem. The lemma follows from Eqs. (7.40) through (7.42) and the induction hypothesis.

The proof of Lemma 7.42 is now complete. ■

Similar to Lemma 7.42, we have:

Lemma 7.43. *Let $\ell = 4r$ and $G \in G(n, \ell)$, but $G \notin C(n, \ell)$. If $G \ncong P_n^\ell$, then $G \prec P_n^\ell$.* ■

Remark 7.6. In Lemma 7.43, the condition $G \notin C(n, \ell)$ is necessary. For example, for the graph H depicted in Fig. 7.26 ($\ell = 4, n = 6$), $H \nprec P_6^4$, but $\mathscr{E}(H) > \mathscr{E}(P_6^4)$.

Combining Lemmas 7.27, 7.42 and 7.43, we arrive at:

Theorem 7.21. *Let $G \in G(n, \ell), n > \ell$. If G has the maximal energy in $G(n, \ell)$, then G is either P_n^ℓ or, when $\ell = 4r$, a graph from $C(n, \ell)$.* ■

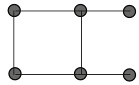
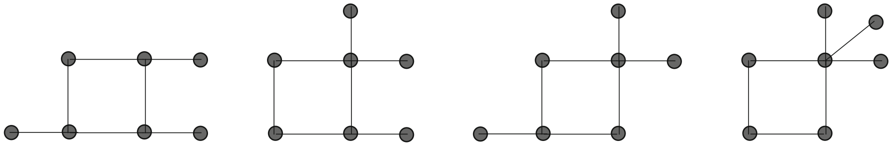


Fig. 7.26 The graph H mentioned in Remark 7.6



$x^7 - 7x^5 + 8x^3 - 4x$ $x^7 - 7x^5 + 8x^3 - 2x$ $x^7 - 7x^5 + 8x^3$ $x^7 - 7x^5 + 6x^3$

Fig. 7.27 All graphs from $C(7,4)$ and their characteristic polynomials

Follow a few easy lemmas.

Lemma 7.44. *Let $n \geq 6$. Then $P_n^4 \prec P_n^6$.*

Proof. We verify Lemma 7.44 by induction on n. By direct calculation, we check that the lemma holds for $n = 6$ and 7. Indeed, the respective characteristic polynomials are $\phi(P_6^4) = x^6 - 6x^4 + 6x^2$, $\phi(P_6^6) = x^6 - 6x^4 + 9x^2 - 4$, $\phi(P_7^4) = x^7 - 7x^5 + 11x^3 - 2x$, and $\phi(P_7^6) = x^7 - 7x^5 + 13x^3 - 7x$. We now suppose that $n \geq 8$ and that the statement of the lemma is true for graphs with $n-1$ and $n-2$ vertices, i.e., that $b_{2k}(P_{n-1}^4) \leq b_{2k}(P_{n-1}^6)$ and $b_{2k}(P_{n-2}^4) \leq b_{2k}(P_{n-2}^6)$. By Lemma 7.27, $b_{2k}(P_n^4) = b_{2k}(P_{n-1}^4) + b_{2k-2}(P_{n-2}^4)$ and $b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6)$, from which Lemma 7.44 follows straightforwardly. ∎

Lemma 7.45. *Let $n \geq 6$ and $G \in C(n,4)$. Then $G \prec P_n^6$.*

Proof. Again, we use induction on n. The lemma holds for $n = 6$ and 7, which can be checked by means of the table of graphs on six vertices [79] and the data given in Fig. 7.27.

Suppose that $n \geq 8$ and the statement of the lemma holds for $n-1$ and $n-2$. Let uv be a pendent edge of G with pendent vertex v. By Lemma 7.27, $b_{2k}(G) = b_{2k}(G-v) + b_{2k-2}(G-v-u)$ and $b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6)$. Since the subgraph $G-v-u$ is necessarily acyclic, $b_{2k-2}(G-v-u) = m(G-v-u, k-1) \leq m(P_{n-2}, k-1) < b_{2k-2}(P_{n-2}^6)$. ∎

It is easy to see that

$$b_{2k}(P_n^\ell) = \begin{cases} m(P_n^\ell, k) & \text{if } 2k < \ell \\ m(P_n^\ell, k) - 2m(P_{n-\ell}, k - \ell/2) & \text{if } 2k \geq \ell,\ \ell = 4r \\ m(P_n^\ell, k) + 2m(P_{n-\ell}, k - \ell/2) & \text{if } 2k \geq \ell,\ \ell = 4r + 2. \end{cases}$$

Thus, $b_{2k}(P_n^\ell) \leq m(P_n^\ell, k) + 2$ when $n = \ell + 1$ and $n = \ell + 2$.

Lemma 7.46. *Let ℓ be even and $\ell \geq 8$. Then $P_{\ell+1}^\ell \prec P_{\ell+1}^6$.*

Proof. For $k \geq 3$, by Lemma 4.6,

$$\begin{aligned} b_{2k}(P_{\ell+1}^6) &= m(P_{\ell+1}^6, k) + 2m(P_{\ell-5}, k-3) \\ &= m(P_{\ell+1}, k) + m(P_4 \cup P_{\ell-5}, k-1) + 2m(P_{\ell-5}, k-3) \\ &\geq m(P_{\ell+1}, k) + m(P_1 \cup P_{\ell-2}, k-1) + 2m(P_{\ell-5}, k-3) \\ &= m(P_{\ell+1}^\ell, k) + 2m(P_{\ell-5}, k-3) \\ &\geq m(P_{\ell+1}^\ell, k) \pm 2m(P_1, k-\ell/2) = b_{2k}(P_{\ell+1}^\ell) \end{aligned}$$

where one should note that $m(P_1, k - \ell/2)$ is equal to zero unless $k - \ell/2 = 0$, when it is unity. Similarly, we have $b_4(P_{\ell+1}^6) = b_4(P_{\ell+1}^\ell)$. ∎

The following two formulas [80, 216] are needed in the proof of Lemma 7.47:

$$m(G_1 \cup G_2, k) = \sum_{i=0}^{k} m(G_1, i)\, m(G_2, k-i) \tag{7.43}$$

$$m(P_n, k) = m(P_{n-1}, k) + m(P_{n-2}, k-1). \tag{7.44}$$

Lemma 7.47. *Let ℓ be even and $\ell \geq 8$. Then $P_{\ell+2}^\ell \prec P_{\ell+2}^6$.*

Proof. For $3 \leq k \leq \ell/2 + 1$, by a repeated use of Eqs. (7.43), (7.44) and Lemma 7.27, we get

$$\begin{aligned} b_{2k}(P_{\ell+2}^6) &= m(P_{\ell+2}^6, k) + 2m(P_{\ell-4}, k-3) \\ &= m(P_{\ell+2}, k) + m(P_4 \cup P_{\ell-4}, k-1) + 2m(P_{\ell-4}, k-3) \\ &= m(P_{\ell+2}, k) + m(P_{\ell-4}, k-1) + 3m(P_{\ell-4}, k-2) + 3m(P_{\ell-4}, k-3) \end{aligned}$$

$$\begin{aligned} b_{2k}(P_{\ell+2}^\ell) &\leq m(P_{\ell+2}^\ell, k) + 2 = m(P_{\ell+2}, k) + m(P_2 \cup P_{\ell-2}, k-1) + 2 \\ &= m(P_{\ell+2}, k) + m(P_{\ell-2}, k-1) + m(P_{\ell-2}, k-2) + 2 \\ &= m(P_{\ell+2}, k) + m(P_{\ell-4}, k-1) + m(P_{\ell-5}, k-2) \\ &\quad + 2m(P_{\ell-4}, k-2) + m(P_{\ell-4}, k-3) + m(P_{\ell-5}, k-3) + 2. \end{aligned}$$

As $3 \le k \le \ell/2+1$, we have $0 \le k-3 \le (\ell-4)/2$. If $k-3 < (\ell-4)/2$, then $k-4 < (\ell-6)/2$ and $m(P_{\ell-4}, k-3) = m(P_{\ell-5}, k-3) + m(P_{\ell-6}, k-4) > m(P_{\ell-5}, k-3)$. If $k-3 = (\ell-4)/2$, then $m(P_{\ell-4}, k-3) = 1 > 0 = m(P_{\ell-5}, k-3)$. Hence, for $3 \le k \le \ell/2+1$, $m(P_{\ell-4}, k-2) + 2m(P_{\ell-4}, k-3) \ge m(P_{\ell-5}, k-2) + m(P_{\ell-5}, k-3) + 2$. Therefore, $b_{2k}(P_{\ell+2}^6) \ge b_{2k}(P_{\ell+2}^\ell)$ for all $k \ge 3$, and $b_6(P_{\ell+2}^6) > b_6(P_{\ell+2}^\ell)$. Similarly, $b_4(P_{\ell+2}^6) = b_4(P_{\ell+2}^\ell)$. Thus, $P_{\ell+2}^\ell \prec P_{\ell+2}^6$. ∎

Lemma 7.48. *Let ℓ be even and $\ell \ge 8$. Then $P_n^\ell \prec P_n^6$.*

Proof. We prove the lemma by induction on n. By Lemmas 7.46 and 7.47, the statement is true for $n = \ell+1$ and $\ell+2$. Suppose that $n > \ell+2$ and Lemma 7.48 holds for $n-1$ and $n-2$. By Lemma 7.27, $b_{2k}(P_n^\ell) = b_{2k}(P_{n-1}^\ell) + b_{2k-2}(P_{n-2}^\ell)$ and $b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6)$. ∎

Lemma 7.49. *Let ℓ be even, $\ell \ge 8$, $n > \ell$, and $G \in C(n,\ell)$. Then $G \prec P_n^6$.*

Proof. We use induction on $n-\ell$. By Lemma 7.46, the statement is true for $n-\ell = 1$. Let $p \ge 2$ and suppose that the statement is true for $n-\ell < p$. Consider $n-\ell = p$. Let uv be a pendent edge of G with pendent vertex v. By Lemma 7.27, $b_{2k}(G) = b_{2k}(G-v) + b_{2k-2}(G-v-u)$ and $b_{2k}(P_n^6) = b_{2k}(P_{n-1}^6) + b_{2k-2}(P_{n-2}^6)$. Because $G-v-u$ is acyclic, $b_{2k-2}(G-v-u) = m(G-v-u, k-1) \le m(P_{n-2}, k-1) < b_{2k-2}(P_{n-2}^6)$. ∎

Summarizing Lemmas 7.44, 7.45, 7.48, and 7.49, we arrive at:

Theorem 7.22. *Let G be any connected, unicyclic, and bipartite graph on n vertices and $G \not\cong C_n$. Then $G \prec P_n^6$, and hence, $\mathcal{E}(G) < \mathcal{E}(P_n^6)$.* ∎

Computer-aided calculation shows that $\mathcal{E}(C_n) > \mathcal{E}(P_n^6)$ for $n \le 7$ and $n = 9, 10, 11, 13, 15$, while $\mathcal{E}(C_n) < \mathcal{E}(P_n^6)$ for $n = 8, 12, 14$. However, the proof of the seemingly very simple inequality $\mathcal{E}(C_n) < \mathcal{E}(P_n^6)$ has not been accomplished until quite recently. The reason for this lies in the fact that the graphs C_n and P_n^6 are not comparable by the relation $\prec$. Andriantiana [16, 18] and Huo et al. [281] independently proved that $\mathcal{E}(C_n) < \mathcal{E}(P_n^6)$ for $n \ge 16$. Huo et al. [282] completely resolved the Conjecture 7.6. In the following, we prove Theorem 7.23, using the method from [281], based on the application of the Coulson integral formula and some combinatorial techniques, similar to the method in Sect. 4.4.

Theorem 7.23. *For $n = 8, 12, 14$ and $n \ge 16$, $\mathcal{E}(P_n^6) > \mathcal{E}(C_n)$.* ∎

For convenience, we introduce the following notation:

$$Y_1(x) = \frac{x + \sqrt{x^2-4}}{2}, \qquad Y_2(x) = \frac{x - \sqrt{x^2-4}}{2}.$$

It is easy to verify that $Y_1(x) + Y_2(x) = x$, $Y_1(x)Y_2(x) = 1$, $Y_1(\mathrm{i}x) = \frac{x+\sqrt{x^2+4}}{2}\,\mathrm{i}$ and $Y_2(\mathrm{i}x) = \frac{x-\sqrt{x^2+4}}{2}\,\mathrm{i}$. We define

$$Z_1(x) = -\mathrm{i}\, Y_1(\mathrm{i}x) = \frac{x + \sqrt{x^2+4}}{2}, \qquad Z_2(x) = -\mathrm{i}\, Y_2(\mathrm{i}x) = \frac{x - \sqrt{x^2+4}}{2}.$$

Observe that $Z_1(x) + Z_2(x) = x$ and $Z_1(x)Z_2(x) = -1$. In addition, for $x > 0$, $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$. In addition, for $x < 0$, $0 < Z_1(x) < 1$ and $Z_2(x) < -1$. In the sequel, we write Z_j instead of $Z_j(x)$ for $j = 1, 2$.

Some more notation will be used frequently later.

$$A_1(x) = \frac{Y_1(x)\,\phi(P_8^6, x) - \phi(P_7^6, x)}{Y_1(x)^9 - Y_1(x)^7},\ A_2(x) = \frac{Y_2(x)\,\phi(P_8^6, x) - \phi(P_7^6, x)}{Y_2(x)^9 - Y_2(x)^7}\ ,$$

$$B_1(x) = \frac{Y_1(x)\,\phi(P_{t+2}^t, x) - \phi(P_{t+1}^t, x)}{Y_1(x)^{t+3} - Y_1(x)^{t+1}},\ B_2(x) = \frac{Y_2(x)\,\phi(P_{t+2}^t, x) - \phi(P_{t+1}^t, x)}{Y_2(x)^{t+3} - Y_2(x)^{t+1}},$$

$$C_1(x) = \frac{Y_1(x)\,(x^2-1) - x}{Y_1(x)^3 - Y_1(x)},\ C_2(x) = \frac{Y_2(x)\,(x^2-1) - x}{Y_2(x)^3 - Y_2(x)}.$$

By direct calculation, we get $\phi(P_8^6, x) = x^8 - 8x^6 + 19x^4 - 16x^2 + 4$ and $\phi(P_7^6, x) = x^7 - 7x^5 + 13x^3 - 7x$, from which

$$A_1(\mathrm{i}x) = -\frac{Z_1\, f_8 + f_7}{Z_1^2 + 1}\, Z_2^7, \qquad A_2(\mathrm{i}x) = -\frac{Z_2\, f_8 + f_7}{Z_2^2 + 1}\, Z_1^7$$

where $f_8 = \phi(P_8^6, \mathrm{i}x) = x^8 + 8x^6 + 19x^4 + 16x^2 + 4$ and $f_7 = \mathrm{i}\,\phi(P_7^6, \mathrm{i}x) = x^7 + 7x^5 + 13x^3 + 7x$.

From Theorem 1.3, we easily obtain:

Lemma 7.50. $\phi(P_n^6, x) = x\,\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x)$ *and* $\phi(C_n, x) = \phi(P_n, x) - \phi(P_{n-2}, x) - 2.$ ∎

Lemma 7.51. *For* $n \geq 10$ *and* $x \neq \pm 2$*, the characteristic polynomials of* P_n^6 *and* C_n *have the following form:*

$$\phi(P_n^6, x) = A_1(x)\,Y_1(x)^n + A_2(x)\,Y_2(x)^n$$
$$\phi(C_n, x) = Y_1(x)^n + Y_2(x)^n - 2.$$

Proof. By Lemma 7.50, we notice that $\phi(P_n^6, x)$ satisfies the recursive formula $f(n,x) = x\,f(n-1,x) - f(n-2,x)$. Therefore, the general solution of this linear homogeneous recurrence relation is $f(n,x) = D_1(x)\,Y_1(x)^n + D_2(x)\,Y_2(x)^n$. By elementary calculation and from the initial conditions $\phi(P_8^6, x)$, $\phi(P_7^6, x)$, we obtain that $D_i(x) = A_i(x)$, $i = 1, 2$, holds for $\phi(P_n^6, x)$.

By Lemma 7.50, $\phi(C_n, x) = \phi(P_n, x) - \phi(P_{n-2}, x) - 2$, whereas $\phi(P_n, x)$ satisfies the recursive formula $f(n,x) = x\,f(n-1,x) - f(n-2,x)$. Similarly, we can obtain the general solution of this linear nonhomogeneous recurrence relation from the initial conditions $\phi(P_1, x) = x$, $\phi(P_2, x) = x^2 - 1$. ∎

Proof of Theorem 7.23. For $n = 8, 12, 14$, it is easy to verify that $\mathscr{E}(P_n^6) > \mathscr{E}(C_n)$. In what follows, we always suppose that $n \geq 16$. From Eq. (3.9),

$$\mathscr{E}(C_n) - \mathscr{E}(P_n^6) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(C_n, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)} \right| \mathrm{d}x.$$

From Lemma 7.51,

$$\begin{aligned} \phi(C_n, \mathrm{i}x) &= Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2 = [Z_2^2(x^2+1) - Z_2^3\, x] Z_1^n \cdot i^n \\ &\quad + [Z_1^2(x^2+1) - Z_1^3 x]\, Z_2^n \cdot i^n - 2 \end{aligned}$$

$$\begin{aligned} \phi(P_n^6, \mathrm{i}x) &= A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n \\ &= \frac{Z_1\, f_8 + f_7}{Z_1^9 + Z_1^7}\, Z_1^n \cdot i^n + \frac{Z_2\, f_8 + f_7}{Z_2^9 + Z_2^7}\, Z_2^n \cdot i^n. \end{aligned}$$

We first show that $E(C_n) - E(P_n^6)$ is decreasing in n for $n = 4k + j$, $j = 1, 2, 3$, namely,

$$\begin{aligned} &\ln \left| \frac{Y_1(\mathrm{i}x)^{n+4} + Y_2(\mathrm{i}x)^{n+4} - 2}{A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^{n+4} + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^{n+4}} \right| \\ &- \ln \left| \frac{Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2}{A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n} \right| = \ln \left[1 + \frac{K_0(n,x)}{H_0(n,x)} \right] < 0. \end{aligned}$$

Case 1. $n = 4k + 2$.

In this case, $H_0(n,x) = \left| \phi(C_n, \mathrm{i}x) \cdot \phi(P_{n+4}^6, \mathrm{i}x) \right| > 0$ and

$$\begin{aligned} K_0(n,x) &= [A_1(\mathrm{i}x) - A_2(\mathrm{i}x)] \left[Y_2(\mathrm{i}x)^4 - Y_1(\mathrm{i}x)^4 \right] \\ &\quad - 2A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n \left[1 - Y_1(\mathrm{i}x)^4 \right] \\ &\quad - 2A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n \left[1 - Y_2(\mathrm{i}x)^4 \right]. \end{aligned}$$

Then, by elementary calculation, we have

$$\begin{aligned} K_0(n,x) &= x(x^2+1) \Big[x^9 + 9x^7 + 30x^5 + 46x^3 + 28x \\ &\quad + Z_2^n \left[x^5 + 5x^3 + 6x + \sqrt{x^2+4}\,(x^4 + 3x^2 + 4) \right] \\ &\quad + Z_1^n \left[x^5 + 5x^3 + 6x - \sqrt{x^2+4}\,(x^4 + 3x^2 + 4) \right] \Big]. \end{aligned}$$

If $x > 0$, then $Z_1 > 1$, $-1 < Z_2 < 0$, and we obtain

$$K_0(n,x) = x(x^2+1)\, Z_1^n\, q(n,x) < x(x^2+1)\, Z_1^n\, q(10,x)$$

where

$$\begin{aligned} q(n,x) = {} & Z_2^n\,(x^9+9x^7+30x^5+46x^3+28x) \\ & + Z_2^{2n}\left[x^5+5x^3+6x+\sqrt{x^2+4}\,(x^4+3x^2+4)\right] \\ & + x^5+5x^3+6x-\sqrt{x^2+4}\,(x^4+3x^2+4). \end{aligned}$$

After some simplification, we get

$$\begin{aligned} q(10,x) = {} & -\frac{1}{2}\,x(x^2+4)(2x^8+17x^6+47x^4+46x^2+10)\cdot \\ & \Big[x^{10}+10x^8+35x^6+50x^4+25x^2+2 \\ & \quad -\sqrt{x^2+4}(x^9+8x^7+21x^5+20x^3+5x)\Big]. \end{aligned}$$

Since

$$\begin{aligned} & (x^{10}+10x^8+35x^6+50x^4+25x^2+2)^2 \\ & -\left[\sqrt{x^2+4}\,(x^9+8x^7+21x^5+20x^3+5x)\right]^2 = 4, \end{aligned}$$

we have $q(10,x) < 0$, and hence, $K_0(n,x)/H_0(n,x) < 0$. Similarly, we prove that $K_0(n,x)/H_0(n,x) < 0$ for $x < 0$.

Therefore, we have shown that $\mathscr{E}(C_n) - \mathscr{E}(P_n^6)$ is decreasing in n for $n = 4k+2$.

Case 2. $n = 4k + j$, $j = 1, 3$.

In this case, $H_0(n,x) = \left|\phi(C_n, \mathrm{i}x)\cdot\phi(P_{n+4}^6, \mathrm{i}x)\right| > 0$ and

$$\begin{aligned} K_0(n,x) = {} & \left|\left[Y_1(\mathrm{i}x)^{n+4} + Y_2(\mathrm{i}x)^{n+4} - 2\right][A_1(\mathrm{i}x)\,Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\,Y_2(\mathrm{i}x)^n]\right| \\ & - \left|\left[A_1(\mathrm{i}x)\,Y_1(\mathrm{i}x)^{n+4} + A_2(\mathrm{i}x)\,Y_2(\mathrm{i}x)^{n+4}\right][Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2]\right| \\ = {} & \sqrt{p(n,x)} - \sqrt{w(n,x)} \end{aligned}$$

where

$$\begin{aligned} p(n,x) = {} & \left[A_2(\mathrm{i}x)\,Z_1^4 + A_1(\mathrm{i}x)\,Z_2^4 - A_1(\mathrm{i}x)\,Z_1^{2n+4} - A_2(\mathrm{i}x)\,Z_2^{2n+4}\right]^2 \\ & + \left[-2A_1(\mathrm{i}x)\,Z_1^n - 2A_2(\mathrm{i}x)\,Z_2^n\right]^2 \end{aligned}$$

$$w(n,x) = \left[A_1(\mathrm{i}x)\,Z_1^4 + A_2(\mathrm{i}x)\,Z_2^4 - A_1(\mathrm{i}x)\,Z_1^{2n+4} - A_2(\mathrm{i}x)\,Z_2^{2n+4}\right]^2 + \left[-2A_1(\mathrm{i}x)\,Z_1^{n+4} - 2A_2(\mathrm{i}x)\,Z_2^{n+4}\right]^2.$$

We now only need to check if $p(n,x) - w(n,x) < 0$ for all x and n. First, suppose that $n = 4k+1$. If $x > 0$, then $Z_1^{2n} > Z_1^{10}$, $Z_2^{2n} < Z_2^{10}$, and we have

$$\begin{aligned} &p(n,x) - w(n,x) \\ &\quad = x(x^2+2)^3\,(x^2+1)^3\Big[x^{11} + 11x^9 + 46x^7 + 92x^5 + 88x^3 + 28x \\ &\qquad -2Z_1^{2n}\left(\sqrt{x^2+4}\,(x^2+2) + x\right) + 2Z_2^{2n}\left(\sqrt{x^2+4}\,(x^2+2) - x\right)\Big] \\ &\quad < p(5,x) - w(5,x) \\ &\quad = -x^2(x^2+4)(x^2+1)^4(x^2+2)^3(2x^8 + 19x^6 + 60x^4 + 68x^2 + 14) < 0. \end{aligned}$$

If $x < 0$, then $Z_1^{2n} < Z_1^{10}$, $Z_2^{2n} > Z_2^{10}$. Similarly, $p(n,x) - w(n,x) < p(5,x) - w(5,x) < 0$. By an analogous argument as used in the case of $n = 4k+1$, for $n = 4k+3$ and $x > 0$ or $x < 0$, we deduce that

$$\begin{aligned} p(n,x) - w(n,x) &< p(7,x) - w(7,x) \\ &= -x^2(x^2+4)(x^2+2)^3(x^2+1)^3\,(2x^{14} + 30x^{12} + 178x^{10} \\ &\quad + 533x^8 + 849x^6 + 690x^4 + 242x^2 + 22) < 0. \end{aligned}$$

Thus, we are done for $n = 4k+j$, $j = 1, 3$.

So far, we have shown that $\mathscr{E}(C_n) - \mathscr{E}(P_n^6)$ is decreasing in n for $n = 4k+j$, $j = 1, 2, 3$. So, when $n = 4k+2$, $\mathscr{E}(C_n) - \mathscr{E}(P_n^6) < \mathscr{E}(C_{18}) - \mathscr{E}(P_{18}^6) \doteq -0.03752 < 0$. For $n = 4k+1$, $\mathscr{E}(C_n) - \mathscr{E}(P_n^6) < \mathscr{E}(C_{17}) - \mathscr{E}(P_{17}^6) \doteq -0.00961 < 0$. For $n = 4k+3$, $\mathscr{E}(C_n) - \mathscr{E}(P_n^6) < \mathscr{E}(C_{19}) - \mathscr{E}(P_{19}^6) \doteq -0.02290 < 0$.

Finally, we will deal with the case of $n = 4k$. Notice that in this case both $\phi(C_n, \mathrm{i}x)$ and $\phi(P_n^6, \mathrm{i}x)$ are polynomials in the variable x with all real coefficients. For $n \to \infty$,

$$\frac{Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2}{A_1(\mathrm{i}x)\,Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\,Y_2(\mathrm{i}x)^n} \to \begin{cases} \dfrac{1}{A_1(\mathrm{i}x)} & \text{if } x > 0 \\[2ex] \dfrac{1}{A_2(\mathrm{i}x)} & \text{if } x < 0. \end{cases}$$

In this case, we will show

$$\ln \frac{Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2}{A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n} < \ln \frac{1}{A_1(\mathrm{i}x)}$$

for $x > 0$ and

$$\ln \frac{Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2}{A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n} < \ln \frac{1}{A_2(\mathrm{i}x)}$$

for $x < 0$. In the following, we only check the case of $x > 0$ as the case of $x < 0$ is analogous. Assume that

$$\ln \frac{Y_1(\mathrm{i}x)^n + Y_2(\mathrm{i}x)^n - 2}{A_1(\mathrm{i}x)\, Y_1(\mathrm{i}x)^n + A_2(\mathrm{i}x)\, Y_2(\mathrm{i}x)^n} - \ln \frac{1}{A_1(\mathrm{i}x)} = \ln \left(1 + \frac{K_1(n,x)}{H_1(n,x)}\right).$$

By elementary calculation, we obtain that $H_1(n,x) > 0$ and

$$\begin{aligned} K_1(n,x) &= -\frac{x^2+1}{x^2+4}\Big[x^8 + 9x^6 + 28x^4 + 36x^2 + 16 \\ &\qquad + (Z_2(x)^n - 1)\sqrt{x^2+4}\,(x^7 + 7x^5 + 16x^3 + 14x)\Big] \\ &< -\frac{x^2+1}{x^2+4}\Big[x^8 + 9x^6 + 28x^4 + 36x^2 + 16 \\ &\qquad - \sqrt{x^2+4}\,(x^7 + 7x^5 + 16x^3 + 14x)\Big] < 0 \end{aligned}$$

since

$$\begin{aligned} &\left(x^8 + 9x^6 + 28x^4 + 36x^2 + 16\right)^2 - \left(\sqrt{x^2+4}\,(x^7 + 7x^5 + 16x^3 + 14x\right)^2 \\ &\quad = 4x^8 + 48x^6 + 204x^4 + 368x^2 + 256 > 0. \end{aligned}$$

Notice that if $x > 0$, then

$$A_1(\mathrm{i}x) = \frac{Z_1 f_8 + f_7}{Z_1^9 + Z_1^7} > 0,$$

whereas if $x < 0$, then

$$A_2(\mathrm{i}x) = \frac{Z_2 f_8 + f_7}{Z_2^9 + Z_2^7} = \frac{Z_1\ (Z_2 f_8 + f_7)}{Z_1\ \left(Z_2^9 + Z_2^7\right)} = \frac{f_8 - Z_1 f_7}{Z_2^8 + Z_2^6} > 0.$$

Thus, by Lemma 4.8,

$$\frac{1}{\pi}\int_0^{+\infty} \ln \frac{1}{A_1(\mathrm{i}x)}\,\mathrm{d}x < \frac{1}{\pi}\int_0^{+\infty}\left(\frac{1}{A_1(\mathrm{i}x)}-1\right)\mathrm{d}x \doteq -0.047643$$

$$\frac{1}{\pi}\int_{-\infty}^{0} \ln \frac{1}{A_2(\mathrm{i}x)}\,\mathrm{d}x < \frac{1}{\pi}\int_0^{+\infty}\left(\frac{1}{A_2(\mathrm{i}x)}-1\right)\mathrm{d}x \doteq -0.047643.$$

Therefore,

$$\mathscr{E}(C_n) - \mathscr{E}(P_n^6) < \frac{1}{\pi}\int_0^{+\infty} \ln \frac{1}{A_1(\mathrm{i}x)}\,\mathrm{d}x + \int_{-\infty}^{0} \ln \frac{1}{A_2(\mathrm{i}x)}\,\mathrm{d}x$$

$$< -0.047643 - 0.047643 < 0.$$

The proof is now complete. ■

In the following, we resolve Conjecture 7.6 by proving the following theorem and its corollary. However, we find that for $n = 4$ the conjecture is not true and P_4^3 should be the unicyclic graph with maximal energy.

Theorem 7.24. *Among all unicyclic graphs of order* $n \geq 16$, *the unicyclic graph with maximal energy is* P_n^6. ■

Corollary 7.7. *Among all unicyclic graphs on n vertices, the cycle* C_n *has maximal energy if* $n \leq 7$ *but* $n \neq 4$, *and* $n = 9, 10, 11, 13$ *and* 15; P_4^3 *has maximal energy if* $n = 4$. *For all other values of n, the unicyclic graph with maximal energy is* P_n^6. ■

From Lemmas 7.44, 7.45, 7.48, and 7.49, we arrive at the following two lemmas:

Lemma 7.52. *Let* $G \in C(n, \ell)$ *and* $n > \ell$. *If* ℓ *is even with* $\ell \geq 8$ *or* $\ell = 4$, *then* $\mathscr{E}(G) < \mathscr{E}(P_n^6)$. ■

Lemma 7.53. *Let* ℓ *be even and* $\ell \geq 8$ *or* $\ell = 4$. *Then* $\mathscr{E}(P_n^\ell) < \mathscr{E}(P_n^6)$. ■

From Lemmas 7.52 and 7.53 and Theorems 7.21 and 7.23, we conclude that for any n-vertex unicyclic graph G, when the length of the unique cycle of G is even, and $n = 8, 12, 14$ and $n \geq 16$, $\mathscr{E}(G) < \mathscr{E}(P_n^6)$. When the length of the unique cycle of G is odd, if $G \in G(n, \ell)$, then $\mathscr{E}(G) < \mathscr{E}(P_n^\ell)$. For proving Theorem 7.24, we only need to show that $\mathscr{E}(P_n^\ell) < \mathscr{E}(P_n^6)$ for every odd ℓ and $n \geq 16$.

From Theorem 1.3, we can easily obtain that for any positive integer $t \leq n-2$, $\phi(P_n^t, x) = x\,\phi(P_{n-1}^t, x) - \phi(P_{n-2}^t, x)$. In a similar manner as in the proof of Lemma 7.51, we obtain:

Lemma 7.54. *For* $n \geq 7$ *and odd integer* $3 \leq t \leq n$, *the characteristic polynomial of* P_n^t *has the following form:*

$$\phi(P_n^t, x) = B_1(x)\,Y_1(x)^n + B_2(x)\,Y_2(x)^n$$

where $x \neq \pm 2$. ■

Lemma 7.55. *For positive integer $t \geq 3$, we have*

$$\phi(P^t_{t+2}, x) = \big(C_1(x)\, Y_1(x)^{t-2}(Y_1(x)^4 - x^2 + 1)\big) + \big(C_2(x)\, Y_2(x)^{t-2}(Y_2(x)^4 - x^2 + 1)\big) - 2(x^2 - 1)$$

$$\phi(P^t_{t+1}, x) = \big(C_1(x)\, Y_1(x)^{t-2}(Y_1(x)^3 - x)\big) + \big(C_2(x)\, Y_2(x)^{t-2}\,(Y_2(x)^3 - x)\big) - 2x.$$

Proof. By Theorem 1.3, we notice that $\phi(P_n, x)$ satisfies the recursive formula $f(n, x) = x\, f(n-1, x) - f(n-2, x)$. Therefore, the general solution of this linear homogeneous recurrence relation is $f(n, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n$. From the initial values $\phi(P_2, x)$ and $\phi(P_1, x)$, by elementary calculation, we obtain that $D_i(x) = C_i(x)$ for $\phi(P_n, x)$, $i = 1, 2$. According to Theorem 1.3,

$$\phi(P^t_{t+2}, x) = \phi(P_{t+2}, x) - \phi(P_{t-2}, x)\, \phi(P_2, x) - 2\phi(P_2, x)$$
$$\phi(P^t_{t+1}, x) = \phi(P_{t+1}, x) - \phi(P_{t-2}, x)\, \phi(P_1, x) - 2\phi(P_1, x).$$

Therefore, we obtain the required expression for $\phi(P^t_{t+2}, x)$ and $\phi(P^t_{t+1}, x)$. ■

Notice that $(x^2 + 1)Z_1 + x = Z_1^3$ and $(x^2 + 1)Z_2 + x = Z_2^3$. Bearing this in mind, we get the following corollary of Lemma 7.55:

Corollary 7.8. $B_1(\mathrm{i}x) = B_{11}(t, x) + B_{12}(t, x)\, i^t$ *and* $B_2(\mathrm{i}x) = B_{21}(t, x) + B_{22}(t, x)\, i^t$, *where*

$$B_{11}(t, x) = \frac{Z_1^2\,(Z_1^2 + 2)}{(Z_1^2 + 1)^2} - \frac{Z_2^{2t-2}}{x^2 + 4}\,, \qquad B_{12}(t, x) = \frac{-2Z_2^{\,t-2}}{Z_1^2 + 1},$$

$$B_{21}(t, x) = \frac{Z_2^2\,(Z_2^2 + 2)}{(Z_2^2 + 1)^2} - \frac{Z_1^{2t-2}}{x^2 + 4}\,, \qquad B_{12}(t, x) = \frac{-2Z_1^{\,t-2}}{Z_2^2 + 1}.$$

■

For the brevity of the exposition, we denote

$$g_1 = \frac{Z_1^2(Z_1^2 + 2)}{(Z_1^2 + 1)^2},\quad g_2 = \frac{Z_2^2(Z_2^2 + 2)}{(Z_2^2 + 1)^2},\quad m_1 = \frac{-2}{Z_1^2 + 1},\quad m_2 = \frac{-2}{Z_2^2 + 1},\quad h = \frac{1}{x^2 + 4}.$$

Observe that each of g_i, m_i, and h is a real function only in x, $i = 1, 2$.

From now on, we use A_j and B_{jk} instead of $A_j(\mathrm{i}x)$ and $B_{jk}(t, x)$ for $j, k = 1, 2$, respectively. According to Lemma 7.54 and Corollary 7.8, it is not hard to get

$$\big|\phi(P^6_n, \mathrm{i}x)\big|^2 = A_1^2\, Z_1^{2n} + A_2^2\, Z_2^{2n} + (-1)^n\, 2A_1\, A_2 \tag{7.45}$$

$$\left|\phi(P_n^t, \mathrm{i}x)\right|^2 = (B_{11}^2 + B_{12}^2)\, Z_1^{2n} + (B_{21}^2 + B_{22}^2) Z_2^{2n} \\ +(-1)^n\, 2(B_{11}\, B_{21} + B_{12}\, B_{22}). \tag{7.46}$$

Proof of Theorem 7.24. In view of the above analysis, we only need to show that $\mathscr{E}(P_n^t) < \mathscr{E}(P_n^6)$ for every odd $t \le n$ and $n \ge 16$. From Eq. (3.9),

$$\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)} \right| \mathrm{d}x.$$

We distinguish between two cases with regard to the parity of n.

Case 1. n is odd and $n \ge 17$.

We now prove that the integrand $\ln \left| \frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)} \right|$ is monotonically decreasing in n.

$$\ln \left| \frac{\phi(P_{n+2}^t, \mathrm{i}x)}{\phi(P_{n+2}^6, \mathrm{i}x)} \right| - \ln \left| \frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)} \right| = \frac{1}{2} \ln \frac{\left|\phi(P_{n+2}^t, \mathrm{i}x) \cdot \phi(P_n^6, \mathrm{i}x)\right|^2}{\left|\phi(P_{n+2}^6, \mathrm{i}x) \cdot \phi(P_n^t, \mathrm{i}x)\right|^2} \\ = \frac{1}{2} \ln \left[1 + \frac{K(n,t,x)}{H(n,t,x)} \right]$$

where $H(n,t,x) = \left|\phi(P_{n+2}^6, \mathrm{i}x) \cdot \phi(P_n^t, \mathrm{i}x)\right|^2 > 0$ and

$$K(n,t,x) = \left|\phi(P_{n+2}^t, \mathrm{i}x) \cdot \phi(P_n^6, \mathrm{i}x)\right|^2 - \left|\phi(P_n^6, \mathrm{i}x) \cdot \phi(P_n^t, \mathrm{i}x)\right|^2.$$

Bearing in mind Lemma 4.8, we only need to prove $K(n,t,x) < 0$. By elementary calculation, we obtain

$$K(n,t,x) = \alpha(t,x)(Z_1^4 - Z_2^4) + \beta(t,x)\, Z_1^{2n}\, (Z_1^4 - 1) + \gamma(t,x)\, Z_2^{2n}\, (1 - Z_2^4)$$

where

$$\alpha(t,x) = A_2^2\, (B_{11}^2 + B_{12}^2) - A_1^2\, (B_{21}^2 + B_{22}^2)$$
$$\beta(t,x) = 2A_1^2\, (B_{11}\, B_{21} + B_{12}\, B_{22}) - 2A_1\, A_2\, (B_{11}^2 + B_{12}^2)$$
$$\gamma(t,x) = 2A_1\, A_2\, (B_{21}^2 + B_{22}^2) - 2A_2^2\, (B_{11}\, B_{21} + B_{12}\, B_{22}).$$

In the following, we examine the sign of $\alpha(t,x)$, $\beta(t,x)$, and $\gamma(t,x)$.

$$\alpha(t,x) = \alpha_0 + \alpha_1\, Z_1^{2t-4} + \alpha_2\, Z_2^{2t-4} + \alpha_3\, Z_1^{4t-4} + \alpha_4\, Z_2^{4t-4}$$
$$\beta(t,x) = \beta_0 + \beta_1\, Z_1^{2t-2} + \beta_2\, Z_2^{2t-2} + \beta_4\, Z_2^{4t-4}$$
$$\gamma(t,x) = \gamma_0 + \gamma_1\, Z_1^{2t-2} + \gamma_2\, Z_2^{2t-2} + \gamma_3\, Z_1^{4t-4}$$

where

$$\alpha_0 = A_2^2\, g_1^2 - A_1^2\, g_2^2, \alpha_1 = 2A_1^2\, g_2\, h\, Z_1^2 - A_1^2\, m_2^2,$$

$$\alpha_2 = A_2^2\, m_1^2 - 2A_2^2\, g_1\, h\, Z_2^2, \alpha_3 = -A_1^2\, h^2, \alpha_4 = A_2^2\, h^2,$$

$$\beta_0 = -2A_1 \left(\frac{2(x^2+3)}{(x^2+4)^2}\, A_1 + A_2\, g_1^2 \right), \beta_1 = -2A_1^2\, g_1\, h,$$

$$\beta_2 = 2A_1\,(2A_2\, g_1\, h - A_1\, g_2\, h - A_2\, m_1^2\, Z_1^2), \beta_4 = -2A_1\, A_2\, h^2,$$

$$\gamma_0 = 2A_2 \left(A_1\, g_2^2 + \frac{2(x^2+3)}{(x^2+4)^2}\, A_2 \right),$$

$$\gamma_1 = 2A_2\,(A_1\, m_2^2\, Z_2^2 + A_2\, g_1\, h - 2A_1\, g_2\, h), \quad \gamma_2 = 2A_2^2\, g_2\, h, \quad \gamma_3 = 2A_1\, A_2\, h^2.$$

Claim 1. For any real x and positive integer t, $\beta(t, x) < 0$.

Notice that

$$Z_1\, f_8 + f_7 = \left(\frac{x}{2}\, f_8 + f_7\right) + \frac{\sqrt{x^2+4}}{2}\, f_8$$

$$Z_2\, f_8 + f_7 = \left(\frac{x}{2}\, f_8 + f_7\right) - \frac{\sqrt{x^2+4}}{2}\, f_8$$

and

$$\left(\frac{x}{2}\, f_8 + f_7\right)^2 - \left(\frac{\sqrt{x^2+4}}{2}\, f_8\right)^2 = -\left(x^{10} + 10x^8 + 36x^6 + 62x^4 + 51x^2 + 16\right) < 0.$$

Then

$$A_1 = -\frac{Z_1\, f_8 + f_7}{Z_1^2 + 1}\, Z_2^7 > 0 \quad \text{and} \quad A_2 = -\frac{Z_2\, f_8 + f_7}{Z_2^2 + 1}\, Z_1^7 > 0$$

since $Z_1 > 0$ and $Z_2 < 0$. Therefore, $\beta_0 < 0$.

$$\beta_2 = -\frac{A_1(x^2+1)}{(x^2+4)^{5/2}}\big[x^9 + 11x^7 + 47x^5 + 93x^3 + 74x$$
$$+\sqrt{x^2+4}(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)\big] < 0$$

since

$$(x^9 + 11x^7 + 47x^5 + 93x^3 + 74x)^2 \\ -(x^2 + 4)(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)^2 < 0. \tag{7.47}$$

It is easy to check that $\beta_1 < 0$ and $\beta_4 < 0$. Hence, the claim follows.

Claim 2. For any real x and positive integer t, $\gamma(t, x) > 0$.

In an analogous manner, we get $\gamma_0 > 0$, $\gamma_2 > 0$, and $\gamma_3 > 0$. From Eq. (7.47), we have

$$\gamma_1 = \frac{A_2(x^2 + 1)}{(x^2 + 4)^{5/2}}\Big[- (x^9 + 11x^7 + 47x^5 + 93x^3 + 74x) \\ + \sqrt{x^2 + 4}(3x^8 + 27x^6 + 85x^4 + 111x^2 + 52)\Big] > 0.$$

Therefore, $\gamma(t, x) > 0$.

Claim 3. For any real x and odd $n \geq t$,

$$K(n, t, x) \leq \alpha(t, x)\,(Z_1^4 - Z_2^4) + \beta(t, x)\,Z_1^{2t}\,(Z_1^4 - 1) + \gamma(t, x)\,Z_2^{2t}\,(1 - Z_2^4).$$

Since $Z_1(x) > 1$ and $-1 < Z_2(x) < 0$ for $x > 0$, we have $Z_1^{2n} \geq Z_1^{2t}$ and $Z_2^{2n} \leq Z_2^{2t}$ when $n \geq t$. Since $0 < Z_1(x) < 1$ and $Z_2(x) < -1$ for $x < 0$, we have $Z_1^{2n} \leq Z_1^{2t}$ and $Z_2^{2n} \geq Z_2^{2t}$ when $n \geq t$. Claims 1 and 2 imply $\beta(t, x) < 0$ and $\gamma(t, x) > 0$ for any real x. Thus, Claim 3 follows.

Claim 4.

$$f(t, x) = \alpha(t, x)\,(Z_1^4 - Z_2^4) + \beta(t, x)\,Z_1^{2t}\,(Z_1^4 - 1) + \gamma(t, x)\,Z_2^{2t}\,(1 - Z_2^4)$$

is a monotonically decreasing function in the variable t.

It is not difficult to get

$$f(t, x) = d_0 + d_1\,Z_1^{2t} + d_2\,Z_2^{2t} + d_3\,Z_1^{4t} + d_4\,Z_2^{4t} \\ = d_0 + d_1\,(Z_1^2)^t + d_2\,(Z_1^2)^{-t} + d_3\,(Z_1^2)^{2t} + d_4\,(Z_1^2)^{-2t}$$

where

$$d_0 = \alpha_0\,(Z_1^4 - Z_2^4) + \beta_2\,(Z_1^4 - 1)\,Z_1^2 + \gamma_1\,(1 - Z_2^4)\,Z_2^2$$
$$d_1 = \alpha_1\,(1 - Z_2^8) + \beta_0\,(Z_1^4 - 1) + \gamma_3\,(Z_2^4 - Z_2^8)$$
$$d_2 = \alpha_2\,(Z_1^8 - 1) + \gamma_0\,(1 - Z_2^4) + \beta_4\,(Z_1^8 - Z_1^4)$$
$$d_3 = \alpha_3\,(1 - Z_2^8) + \beta_1\,(Z_1^2 - Z_2^2)$$
$$d_4 = \alpha_4\,(Z_1^8 - 1) + \gamma_2\,(Z_1^2 - Z_2^2).$$

We define

$$p_1(x) := x^3 + 6x$$
$$q_1(x) := \left(3x^2 + 4\right)\sqrt{x^2+4}$$
$$p_2(x) := x^7 + 9x^5 + 24x^3 + 18x$$
$$q_2(x) := \left(x^6 + 7x^4 + 12x^2 + 4\right)\sqrt{x^2+4}$$
$$p_3(x) := x^{13} + 15x^{11} + 89x^9 + 264x^7 + 405x^5 + 288x^3 + 56x$$
$$q_3(x) := \left(x^{12} + 15x^{10} + 85x^8 + 234x^6 + 331x^4 + 220x^2 + 48\right)\sqrt{x^2+4}.$$

Then by direct calculation,

$$d_1 = \frac{x(x^2+4)(x^2+1)^2\left(x-\sqrt{x^2+4}\right)^7 [p_2(x)+q_2(x)][p_3(x)+q_3(x)]}{4(x^2+4-x\sqrt{x^2+4})^2\left(x^2+4+x\sqrt{x^2+4}\right)^4}$$

$$d_2 = \frac{x(x^2+4)(x^2+1)^2\left(x+\sqrt{x^2+4}\right)^7 [p_2(x)-q_2(x)][p_3(x)-q_3(x)]}{4(x^2+4+x\sqrt{x^2+4})^2\left(x^2+4-x\sqrt{x^2+4}\right)^4}$$

$$d_3 = -\frac{x(x^2+1)^2\left(x-\sqrt{x^2+4}\right)^{14} [p_1(x)+q_1(x)][p_2(x)+q_2(x)]^2}{8192\left(x^2+4+x\sqrt{x^2+4}\right)^4}$$

$$d_4 = -\frac{x(x^2+1)^2(x+\sqrt{x^2+4})^{14} [p_1(x)-q_1(x)][p_2(x)-q_2(x)]^2}{8192\left(x^2+4-x\sqrt{x^2+4}\right)^4}.$$

Since $p_1(x)^2 - q_1(x)^2 < 0$, $p_2(x)^2 - q_2(x)^2 < 0$ and $p_3(x)^2 - q_3(x)^2 < 0$, we deduce that $d_1, d_3 < 0$ and $d_2, d_4 > 0$ for $x > 0$. In addition, $d_1, d_3 > 0$ and $d_2, d_4 < 0$ for $x < 0$. Therefore, for both $x > 0$ and $x < 0$,

$$\frac{\partial f(t,x)}{\partial t} = \left[d_1\,(Z_1^2)^t - d_2\,(Z_1^2)^{-t} + 2d_3\,(Z_1^2)^{2t} - 2d_4\,(Z_1^2)^{-2t}\right]\ln Z_1^2 < 0.$$

The proof of Claim 4 is thus complete.

From Claim 4, it follows that for $t \geq 5$,

$$K(n,t,x) \leq f(5,x) = -x^2(x^2+1)^2(x^4+3x^2+1)(2x^{12}+31x^{10} +189x^8+574x^6+899x^4+661x^2+160) < 0.$$

Table 7.4 Values of $\mathscr{E}(P_{17}^t) - \mathscr{E}(P_{17}^6)$ for $t \leq 15$

t	$\mathscr{E}(P_{17}^t) - \mathscr{E}(P_{17}^6)$	t	$\mathscr{E}(P_{17}^t) - \mathscr{E}(P_{17}^6)$
3	−0.05339	11	−0.12030
5	−0.09835	13	−0.11425
7	−0.11405	15	−0.09493
9	−0.12006		

If $t = 3$, then $n > t + 2$, and therefore,

$$\begin{aligned} K(n,3,x) &< \alpha(3,x)\,(Z_1^4 - Z_2^4) + \beta(3,x)\,Z_1^{2\times3+4}\,(Z_1^4 - 1) \\ &\quad + \gamma(3,x)\,Z_2^{2\times3+4}\,(1 - Z_2^4) \\ &= -x^2\,(x^2+1)^3\,(x^2+5)(2x^{12} + 23x^{10} + 104x^8 + 238x^6 + 290x^4 \\ &\quad + 171x^2 + 32) < 0. \end{aligned}$$

We conclude that the integrand $\ln\left|\dfrac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|$ is monotonically decreasing in n. Therefore, by Theorem 7.23, for $n \geq 17$ and $t \geq 17$, $\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6) < \mathscr{E}(P_t^t) - \mathscr{E}(P_t^6) < 0$. For $n \geq 17$ and $t \leq 15$, the data given in Table 7.4 show that $\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6) < \mathscr{E}(P_{17}^t) - \mathscr{E}(P_{17}^6) < 0$.

Case 2. n is even and $n \geq 8$.

From Eqs. (7.45) and (7.46) follows

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 = \ln\frac{(B_{11}^2 + B_{12}^2)Z_1^{2n} + (B_{21}^2 + B_{22}^2)\,Z_2^{2n} + 2(B_{11}\,B_{21} + B_{12}\,B_{22})}{A_1^2\,Z_1^{2n} + A_2^2\,Z_2^{2n} + 2A_1\,A_2}.$$

Therefore, when $n \to \infty$,

$$\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 \to \begin{cases} \dfrac{B_{11}^2 + B_{12}^2}{A_1^2} & \text{if } x > 0 \\[2ex] \dfrac{B_{21}^2 + B_{22}^2}{A_2^2} & \text{if } x < 0. \end{cases}$$

In this case, we prove that

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 < \ln\frac{B_{11}^2 + B_{12}^2}{A_1^2}$$

for $x > 0$ and

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 < \ln\frac{B_{21}^2 + B_{22}^2}{A_2^2}$$

for $x < 0$. We simplify the expressions of α_i for $i = 0, 1, 2$ as

$$\alpha_0 = \frac{x(x^2+1)^2(x^8+11x^6+43x^4+73x^2+50)(x^8+9x^6+27x^4+33x^2+12)}{(x^2+4)^{5/2}}$$

$$\alpha_1 = -\frac{(p_2(x)+q_2(x))^2(3x^2+10+x\sqrt{x^2+4})(x-\sqrt{x^2+4})^{14}(x^2+1)^2}{4096(x^2-x\sqrt{x^2+4}+4)^2(x^2+x\sqrt{x^2+4}+4)^2(x^2+4)}$$

$$\alpha_2 = \frac{(p_2(x)-q_2(x))^2(3x^2+10-x\sqrt{x^2+4})(x+\sqrt{x^2+4})^{14}(x^2+1)^2}{4096(x^2-x\sqrt{x^2+4}+4)^2(x^2+x\sqrt{x^2+4}+4)^2(x^2+4)}.$$

Subcase 2.1. $x > 0$.

By direct calculation, we obtain

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 - \ln\frac{B_{11}^2+B_{12}^2}{A_1^2} = \ln\left(1+\frac{K_1(n,t,x)}{H_1(n,t,x)}\right)$$

where $H_1(n,t,x) = \left|\phi(P_n^6, \mathrm{i}x)\right|^2 (B_{11}^2 + B_{12}^2) > 0$ and $K_1(n,t,x) = -\alpha(t,x)Z_2^{2n} + \beta(t,x)$. Suppose that $\alpha(t,x) < 0$. Otherwise, $K_1(n,t,x) < 0$ since $\beta(t,x) < 0$ by Claim 1, and then we are done. Since $-1 < Z_2 < 0$,

$$K_1(n,t,x) \le -\alpha(t,x)\,Z_2^{2t} + \beta(t,x) = \overline{d}_0 + \overline{d}_1\,Z_1^{2t-2} + \overline{d}_2\,Z_2^{2t-2} + \overline{d}_3\,Z_2^{4t-4} + \overline{d}_4\,Z_2^{6t-4}$$

where $\overline{d}_0 = \beta_0 - \alpha_1 Z_2^4$, $\overline{d}_1 = \beta_1 - \alpha_3 Z_2^2$, $\overline{d}_2 = \beta_2 - \alpha_0 Z_2^2$, $\overline{d}_3 = \beta_4 - \alpha_2$, $\overline{d}_4 = -\alpha_4$. Since $\beta_i < 0$ for $i = 0, 1, 2, 4$, α_0, α_2, $\alpha_4 > 0$ and α_1, $\alpha_3 < 0$, we have $\overline{d}_i < 0$ for $i = 2, 3, 4$ and

$$\overline{d}_1 = -2A_1^2 g_1 h + A_1^2 h^2 Z_2^2 = A_1^2 h\,(hZ_2^2 - 2g_1) = -\frac{A_1^2 h(2Z_1^2 - Z_2^2 + 4)}{x^2+4} < 0.$$

Denote

$$p_0(x) := x^{14} + 19x^{12} + 146x^{10} + 584x^8 + 1300x^6 + 1582x^4 + 928x^2 + 160$$
$$q_0(x) := \left(x^{13} + 17x^{11} + 116x^9 + 404x^7 + 756x^5 + 722x^3 + 272x\right)\sqrt{x^2+4}.$$

Then

$$\overline{d}_0 = -\frac{A_1(x^2+1)}{(Z_1^2+1)^4\,(Z_2^2+1)^2}\,[p_0(x) + q_0(x)] < 0.$$

Thus, for $x > 0$, $K_1(n,t,x) < 0$, and then

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 < \ln\frac{B_{11}^2+B_{12}^2}{A_1^2}.$$

Subcase 2.2. $x < 0$.

In a similar manner as before,

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 - \ln\frac{B_{21}^2 + B_{22}^2}{A_2^2} = \ln\left(1 + \frac{K_2(n,t,x)}{H_2(n,t,x)}\right)$$

where $H_2(n,t,x) = \left|\phi(P_n^6, \mathrm{i}x)\right|^2 (B_{21}^2 + B_{22}^2) > 0$ and $K_2(n,t,x) = \alpha(t,x)Z_1^{2n} - \gamma(t,x)$. Now we suppose that $\alpha(t,x) > 0$. Otherwise, $K_2(n,t,x) < 0$ since $\gamma(t,x) > 0$ by Claim 2, and then we are done. Since $0 < Z_1 < 1$,

$$K_2(n,t,x) \le \alpha(t,x)\, Z_1^{2t} - \gamma(t,x) = \widetilde{d}_0 + \widetilde{d}_1\, Z_1^{2t-2} + \widetilde{d}_2\, Z_2^{2t-2} + \widetilde{d}_3\, Z_1^{4t-4} + \widetilde{d}_4\, Z_1^{6t-4}$$

where $\widetilde{d}_0 = \alpha_2 Z_1^4 - \gamma_0$, $\widetilde{d}_1 = \alpha_0 Z_1^2 - \gamma_1$, $\widetilde{d}_2 = \alpha_4 Z_1^2 - \gamma_2$, $\widetilde{d}_3 = \alpha_1 - \gamma_3$, $\widetilde{d}_4 = \alpha_3$. Since $\gamma_i > 0$ for $i = 0, 1, 2, 3$, $\alpha_0, \alpha_1, \alpha_3 < 0$ and $\alpha_2, \alpha_4 > 0$, we have $\widetilde{d}_i < 0$ for $i = 1, 3, 4$ and

$$\widetilde{d}_0 = -\frac{A_2(x^2+1)}{(Z_2^2+1)^4(Z_1^2+1)^2}\,[p_0(x) - q_0(x)] < 0$$

$$\widetilde{d}_2 = A_2^2 h^2 Z_1^2 - 2A_2^2 g_2 h = A_2^2 h(h\, Z_1^2 - 2g_2) = -\frac{A_2^2 h(2Z_2^2 - Z_1^2 + 4)}{x^2+4} < 0.$$

Thus, for $x < 0$, $K_2(n,t,x) < 0$, and then

$$\ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 < \ln\frac{B_{21}^2 + B_{22}^2}{A_2^2}.$$

From the two subcases, we conclude that

$$E(P_n^t) - E(P_n^6) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right| \mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \ln\left|\frac{\phi(P_n^t, \mathrm{i}x)}{\phi(P_n^6, \mathrm{i}x)}\right|^2 \mathrm{d}x$$

$$< \frac{1}{2\pi}\int_{0}^{+\infty} \ln\frac{B_{11}^2 + B_{12}^2}{A_1^2}\,\mathrm{d}x + \frac{1}{2\pi}\int_{-\infty}^{0} \ln\frac{B_{21}^2 + B_{22}^2}{A_2^2}\,\mathrm{d}x.$$

Denote

$$p_4(x) := x^{16} + 14x^{14} + 83x^{12} + 274x^{10} + 551x^8 + 686x^6 + 507x^4 + 190x^2 + 22$$

$$q_4(x) := \left(x^{15} + 12x^{13} + 61x^{11} + 172x^9 + 291x^7 + 296x^5 + 167x^3 + 40x\right)\sqrt{x^2+4}.$$

Notice that $Z_1^2/(Z_1^2+1)^2 = Z_2^2/(Z_2^2+1)^2 = 1/(x^2+4)$ and $p_4(x)^2 - q_4(x)^2 = 4(x^2+1)^2\,(2x^{10} + 24x^8 + 104x^6 + 225x^4 + 248x^2 + 121) > 0$ whenever $x > 0$ or $x < 0$. If $x > 0$, then $Z_2^2 < 1$ and we have

$$\begin{aligned}
B_{11}^2 + B_{12}^2 - A_1^2 &= \left(\frac{Z_1^2+2}{x^2+4} - \frac{Z_2^{2t-2}}{x^2+4}\right)^2 + \left(-\frac{2(Z_1^2+1)Z_2^t}{x^2+4}\right)^2 - A_1^2 \\
&= \frac{1}{(x^2+4)^2}\left[(Z_1^2+2)^2 + (2Z_1^2+4Z_2^2+4)Z_2^{2t-2} + Z_2^{4t-4}\right] - A_1^2 \\
&< \frac{1}{(x^2+4)^2}\left[(Z_1^2+2)^2 + (2Z_1^2+4Z_2^2+4)Z_2^4 + Z_2^8\right] - A_1^2 \\
&= -\frac{p_4(x) - q_4(x)}{(x^2+4)(x^2+2+x\sqrt{x^2+4})} < 0.
\end{aligned}$$

When $x < 0$, $Z_1^2 < 1$, we have

$$\begin{aligned}
B_{21}^2 + B_{22}^2 - A_2^2 &= \left(\frac{Z_2^2+2}{x^2+4} - \frac{Z_1^{2t-2}}{x^2+4}\right)^2 + \left(-\frac{2(Z_2^2+1)Z_1^t}{x^2+4}\right)^2 - A_2^2 \\
&= \frac{1}{(x^2+4)^2}\left((Z_2^2+2)^2 + (2Z_2^2+4Z_1^2+4)Z_1^{2t-2} + Z_1^{4t-4}\right) - A_2^2 \\
&< \frac{1}{(x^2+4)^2}\left((Z_2^2+2)^2 + (2Z_2^2+4Z_1^2+4)Z_1^4 + Z_1^8\right) - A_2^2 \\
&= -\frac{p_4(x) + q_4(x)}{(x^2+4)(x^2+2-x\sqrt{x^2+4})} < 0.
\end{aligned}$$

Therefore,

$$\int_0^{+\infty} \ln \frac{B_{11}^2 + B_{12}^2}{A_1^2}\,\mathrm{d}x < 0 \qquad \text{and} \qquad \int_{-\infty}^{0} \ln \frac{B_{21}^2 + B_{22}^2}{A_2^2}\,\mathrm{d}x < 0.$$

We thus arrive at the conclusion that $\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6) < 0$ if n is even. ■

Proof of Corollary 7.7. There are only two unicyclic graphs of order 4, which are shown in Fig. 7.28. Observe that P_4^3 has maximal energy for $n = 4$. In view of Lemmas 7.52 and 7.53 and Theorems 7.21, 7.23, and 7.24, we only need to show that for $n \le 16$ ($n \ne 4$) and any odd t with $3 \le t \le n$, $\mathscr{E}(P_n^t) < \mathscr{E}(P_n^6)$ or $\mathscr{E}(P_n^t) < \mathscr{E}(C_n)$. From Table 7.5, we see that $\mathscr{E}(P_n^t) < \mathscr{E}(P_n^6)$ for $6 \le n \le 16$, except for $n = 7, 9, 11$ and some t. In such cases, from the data given in Table 7.6, we can check that $\mathscr{E}(P_n^t) < \mathscr{E}(C_n)$. For $n = 3, 5$, we consider all unicyclic graphs. All such graphs and their energies are shown in Fig. 7.28, by means of which our results are verified.

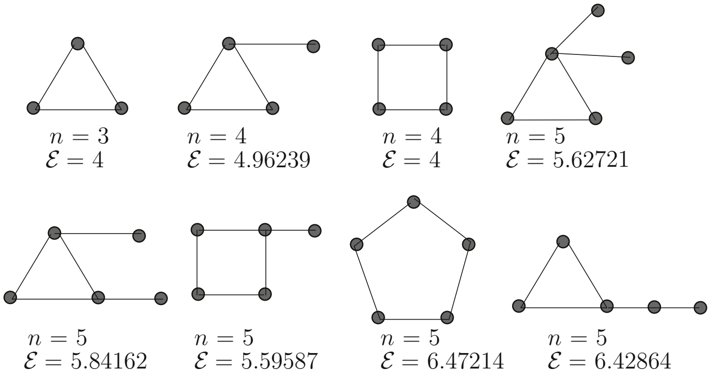


Fig. 7.28 All unicyclic graphs and their energies for $n \leq 5$

Table 7.5 Values of $\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6)$ for $n \leq 16$ and odd t

n	t	$\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6)$	n	t	$\mathscr{E}(P_n^t) - \mathscr{E}(P_n^6)$
6	3	−0.45075	6	5	−0.53412
7	3	0.22026	7	5	0.19680
8	3	−0.31283	8	5	−0.37252
8	7	−0.42994	9	3	0.08604
9	5	0.04987	9	7	0.05443
10	3	−0.26573	10	5	−0.31918
10	7	−0.35115	10	9	−0.40167
11	3	0.02396	11	5	−0.01682
11	7	−0.02469	11	9	−0.01186
12	3	−0.24081	12	5	−0.29174
12	7	−0.31698	12	9	−0.34102
12	11	−0.38894	13	3	−0.01237
13	5	−0.05536	13	7	−0.06773
13	9	−0.06719	13	11	−0.05081
14	3	−0.22520	14	5	−0.27486
14	7	−0.29740	14	9	−0.31438
14	11	−0.33517	14	13	−0.38193
15	3	−0.03635	15	5	−0.08055
15	7	−0.09506	15	9	−0.09897
15	11	−0.09481	15	13	−0.07658
16	3	−0.21447	16	5	−0.26340
16	7	−0.28459	16	9	−0.29873
16	11	−0.31223	16	13	−0.33141
16	15	−0.37761			

Table 7.6 Values of $\mathscr{E}(P_n^t)$ and $\mathscr{E}(C_n)$ for $n = 7, 9, 11, 13, 15$ and some t

n	t	$\mathscr{E}(P_n^t)$	$\mathscr{E}(C_n)$	n	t	$\mathscr{E}(P_n^t)$	$\mathscr{E}(C_n)$
7	3	8.94083	8.98792	7	5	8.91737	8.98792
9	3	11.47069	11.51754	9	5	11.43452	11.51754
9	7	11.43908	11.51754	11	3	14.00732	14.05335
n	t	$E(P_n^t)$	$E(C_n)$	n	t	$E(P_n^t)$	$E(C_n)$
7	6	8.72057	8.98792	9	6	11.38465	11.51754
10	6	12.93214	12.94427	11	6	13.98336	14.05335
13	6	16.55965	16.59246	15	6	19.12546	19.13354

Finally, we calculate the energies of C_n and P_n^6 for $n = 7, 9, 10, 11, 13, 15$ and verify that in these cases $\mathscr{E}(C_n) > \mathscr{E}(P_n^6)$. ■

7.3 Bicyclic Graphs with Extremal Energies

After considering the extremal problems on trees and unicyclic graphs, in this section we consider the extremal energies of bicyclic graphs. Let $G(n)$ be the class of connected bicyclic graphs with n vertices which contain no disjoint odd cycles of lengths k and ℓ with $k + \ell \equiv 2 \pmod 4$. Denote by $S_n^{3,3}$ the graph formed by joining $n - 4$ pendent vertices to a vertex of degree 3 of the $K_4 - e$.

7.3.1 *Minimal Energy of Bicyclic Graphs*

As mentioned in the above subsections, Conjecture 7.5 was confirmed for $m = n-1,\ 2(n-2),\ n$. Zhang and Zhou [523] and Hou [267] independently considered the conjecture for $m = n + 1$.

Let $S_n^{4,4}$ be the graph obtained by joining $n - 5$ pendent vertices to a vertex of degree three of the complete bipartite graph $K_{2,3}$. Let $S_n'^{4,4}$, $S_n'^{3,3}$ be, respectively, the graph obtained from $S_n^{4,4}$, $S_n^{3,3}$ by moving a pendent edge to the other vertex of degree three; see Fig. 7.29. Hou [267] reported that $S_n^{4,4}$ has the minimal energy among all n-vertex connected bicyclic graphs with at most one odd cycle. Note that the class of bicyclic graph with n vertices and at most one odd cycle is a proper subset of $G(n)$. In this subsection, we show that $S_n^{3,3}$, $S_n^{4,4}$, and $S_n'^{3,3}$ have, respectively, minimal, second-minimal, and third-minimal energies in $G(n)$ [523].

From the Sachs theorem, one easily obtains:

Lemma 7.56. *For any graph G, $b_4(G) = m(G, 2) - 2Q$, where Q is the number of quadrangles in G.* ■

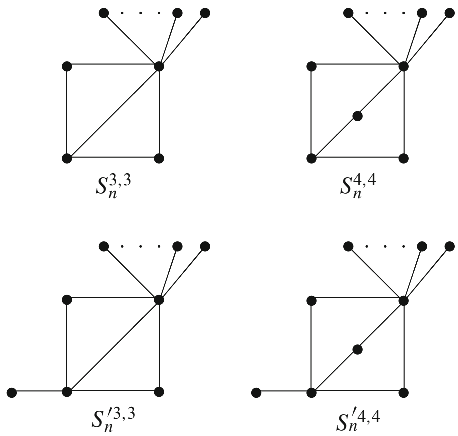


Fig. 7.29 The graphs $S_n^{3,3}$, $S_n^{4,4}$, $S_n'^{3,3}$, and $S_n'^{4,4}$

Lemma 7.57. (i) *If* $G \in G(n)$, *then* $(-1)^i a_{2i}(G) \geq 0$ *for* $1 \leq i \leq \lfloor n/2 \rfloor$. *Hence,* $b_{2i}(G) = |a_{2i}(G)| = (-1)^i a_{2i}(G)$.

(ii) *If* $G \in G(n)$ *contains* $K_4 - e$, *then* $(-1)^i a_{2i+1}(G) \geq 0$ *for* $1 \leq i \leq \lfloor n/2 \rfloor$. *Hence,* $b_{2i+1}(G) = |a_{2i+1}(G)| = (-1)^i a_{2i+1}(G)$.

Proof. Let L_i be the set of Sachs subgraphs of G with i vertices. Let $L_i^{(1)}$ be the set of graphs with no cycles in L_i and $L_i^{(2)} = L_i \setminus L_i^{(1)}$. Note that $G \in G(n)$ has exactly two or three distinct cycles and at most two odd cycles.

(i) By the Sachs theorem, $(-1)^i a_{2i}(G) = \sum_{S \in L_{2i}} (-1)^{\omega(S)+i} 2^{c(S)}$, where $\omega(G)$ and $c(G)$ denote the number of connected components of G and the number of cycles of G, respectively. If G has at most one odd cycle, then $(-1)^i a_{2i}(G) \geq 0$. So we need only to consider the case when $G \in G(n)$ has exactly two odd cycles. If no S in L_{2i} contains cycles, then $p(S) = i$, $(-1)^k a_{2k}(G) = \sum_{S \in L_{2i}^{(1)}} 1 \geq 0$. Suppose that some S_0 in L_{2i} contains at least one cycle C_s with length s. If s is odd, then S_0 contains exactly two disjoint odd cycles of lengths, say, s and t. Since $G \in G(n)$, we have $s + t \equiv 0 \pmod 4$, $\omega(S) + i = 2 + [2i - (s+t)]/2 + i \equiv 0 \pmod 2$, and then $(-1)^i a_{2i}(G) = \sum_{S \in L_{2i}^{(1)}} 1 + 4 \sum_{S \in L_{2i}^{(2)}} 1 \geq 0$. If s is even, then $|L_{2i}^{(1)}| \geq 2|L_{2i}^{(2)}|$ and so $(-1)^i a_{2i}(G) = \sum_{S \in L_{2i}^{(1)}} 1 + \sum_{S \in L_{2i}^{(2)}} 2(-1)^{s-1} \geq 0$.

(ii) If $G \in G(n)$ contains $K_4 - e$, then $L_{2i+1}^{(1)} = \emptyset$, any $S \in L_{2i+1}^{(2)}$ must contain a unique triangle, $\omega(S) = 1 + (2i + 1 - 3)/2 = i$, $c(S) = 1$, and so $(-1)^i a_{2i+1}(G) = 2 \sum_{S \in L_{2i+1}^{(2)}} 1 \geq 0$. ∎

Similarly, in view of Lemma 7.57, a quasi-order relation can be introduced as follows:

1. Let G_1 and G_2 be graphs of $G(n)$ containing $K_4 - e$. If $b_i(G_1) \geq b_i(G_2)$ holds for all $i \geq 0$, $\mathscr{E}(G_1) \geq \mathscr{E}(G_2)$ and we write $G_1 \succeq G_2$ or $G_2 \preceq G_1$.
2. Let G_1 be any graph in $G(n)$ and $G_2 \cong S_n^{4,4}$. Similarly, we also write $G_1 \succeq G_2 \cong S_n^{4,4}$, if $b_{2i}(G_1) \geq b_{2i}(G_2)$ holds for all $i \geq 0$.

In either case, if $G_1 \succeq G_2$ and there exists an i such that $b_i(G_1) > b_i(G_2)$, then we write $G_1 \succ G_2$.

Lemma 7.58. *Let $G \in G(n)$. If $b_4(G) > b_4(S_n^{4,4}) = 3n - 15$, then $G \succ S_n^{4,4}$.*

Proof. It is easy to see that $b_0(G) = b_0(S_n^{4,4})$, $b_2(G) = b_2(S_n^{4,4}) = n + 1$, $b_4(S_n^{4,4}) = 3n - 15$, and $b_i(S_n^{4,4}) = 0$ for $i = 1, 3$ or $i \geq 5$. Since $b_4(G) > 3n - 15$, we have $G \succ S_n^{4,4}$. ■

Lemma 7.59. *If $G \in G(n)$ does not contain $K_4 - e$ and $G \ncong S_n^{4,4}$, then $G \succ S_n^{4,4}$.*

Proof. Since $G \in G(n)$, G has either two or three distinct cycles. If G has three cycles, then any two must share common edges. We may choose two cycles of lengths of a and b with t common edges such that $a - t \geq t, b - t \geq t$. If G has exactly two cycles, suppose that the lengths of the two cycles are a and b. Then in any case, we choose two cycles C_a and C_b with lengths a and b, respectively. We will prove that $b_4(G) > b_4(S_n^{4,4}) = 3n - 15$.

Case 1. C_a and C_b have no common vertices. Then $n - a - b \geq 0$. We proceed by induction on $n - a - b$. If $n - a - b = 0$, then by Lemma 7.56,

$$\begin{aligned} b_4(G) &\geq m(G,2) - 4 = m(C_a,2) + m(C_b,2) + ab + (a + b - 4) - 4 \\ &= \frac{1}{2}[(a+b)^2 - (a+b) - 16] \end{aligned}$$

and so $b_4(G) - (3n - 15) \geq \frac{1}{2}(n^2 - 7n + 14) > 0$. It follows that $b_4(G) > 3n - 15$.

Suppose that the claim is true for all graphs with $n - a - b < p$ ($p \geq 1$), and let $n - a - b = p$.

Subcase 1.1. There is no pendent edge in G. Then C_a connects C_b by a path of length $p + 1$. By Lemma 7.56,

$$\begin{aligned} b_4(G) \geq m(G,2) - 4 &= m(C_a,2) + m(C_b,2) + m(P_{p+2},2) + (a-2)(n+1-a) \\ &\quad + 2(n-a) + (b-2)(n+1-a-b) + 2(n-a-b) - 4 \\ &= \frac{1}{2}(n^2 - n - 16) \end{aligned}$$

and so $b_4(G) - (3n - 15) \geq \frac{1}{2}(n^2 - 7n + 14) > 0$. It follows that $b_4(G) > 3n - 15$.

Subcase 1.2. uv is a pendent edge of G with pendent vertex v. By Theorem 1.3, $b_4(G) = b_4(G - v) + b_2(G - u - v)$ and $b_4(S_n^{4,4}) = b_4(S_{n-1}^{4,4}) + b_2(K_{1,3})$. By the induction hypothesis, $b_4(G-v) \geq b_4(S_{n-1}^{4,4})$. Since C_a and C_b have no common vertices, $b_2(G-u-v) > 3 = b_2(K_{1,3})$. We have $b_4(G) > b_4(S_n^{4,4}) = 3n-15$.

By combining Subcases 1.1 and 1.2, we conclude that in Case 1, $b_4(G) > b_4(S_n^{4,4}) = 3n-15$.

Case 2. C_a and C_b have at least one common vertex and t ($t \geq 0$) common edges. Then $n-a-b+t \geq -1$. We use induction on $n-a-b+t$. If $n-a-b+t = -1$, then G contains no vertices except vertices in the two cycles. There are four subcases.

Subcase 2.1. $t = 0$. Then $n = a+b-1$. By Lemma 7.56,

$$\begin{aligned} b_4(G) &\geq m(G,2) - 4 = m(C_a,2) + m(C_b,2) + a(b-2) + 2(a-2) - 4 \\ &= \frac{1}{2}[(a+b)^2 - 3(a+b) - 16], \end{aligned}$$

and since $a+b \geq 6$, we have $b_4(G)-(3n-15) \geq \frac{1}{2}\,[(a+b)^2-9(a+b)+20] > 0$.

Subcase 2.2. $t = 1$. Then $n = a+b-2$. If G contains quadrangles, then either $n = 6$, $b_4(G) = 7 > 3 = b_4(S_6^{4,4})$, or $n = b+2$, $b \neq 4$, $b_4(G) = b-2+\frac{1}{2}(b+2)(b-1)-2 > 3(b+2)-15 = b_4(S_{b+2}^{4,4}, 2)$. If G does not contain quadrangles, then by Lemma 7.56,

$$b_4(G) = m(G,2) = a+b-6+m(C_{a+b-2},2) = a+b-6+\frac{1}{2}[(a+b-2)(a+b-5)].$$

Since $a+b \geq 6$, we have $b_4(G)-(3n-15) = \frac{1}{2}\,[(a+b)^2-11(a+b)+40] > 0$.

Subcase 2.3. $t = 2$. Then $n = a+b-3$. If G contains a quadrangle, let $a = 4$. Then $b \neq 4$ since $G \not\cong S_n^{4,4}$. By Lemma 7.56, $b_4(G) = 2(b-2)+b(b-3)/2-2$, and so $b_4(G)-b_4(S_n^{4,4}) = \frac{1}{2}\,(b^2-5b+12) > 0$. If G does not contain quadrangles, then by Lemma 7.56, $b_4(G) = m(G,2) = 2(a+b-6) + m(C_{a+b-4},2)$, and so $b_4(G) - b_4(S_n^{4,4}) = \frac{1}{2}[(a+b)^2 - 13(a+b) + 52)] > 0$.

Subcase 2.4. $t \geq 3$. Note that $a, b \geq 2t$. Then $n = a+b-t-1$. By Lemma 7.56, $b_4(G) = m(G,2) = m(P_{t+1},2) + 2(a+b-2t-2) + (t-2)(a+b-2t) + m(C_{a+b-2t},2)$, and so

$$\begin{aligned} b_4(G) - b_4(S_n^{4,4}) &= \frac{1}{2}\,[(a+b)^2 - (2t+9)(a+b) + t^2 + 9t + 30] \\ &= \frac{1}{2}\,[(a+b)-(t+3)][(a+b)-(t+6)] + 6 > 0. \end{aligned}$$

By combining the Subcases 2.1 through 2.4, we conclude that in Case 2, $b_4(G) > b_4(S_n^{4,4})$ if $n-a-b+t = -1$. Suppose that it is true for $n-a-b+t < p$ ($p \geq 0$), and let $n-a-b+t = p$. Then G must contain a pendent edge uv with v as a pendent vertex. From Theorem 1.3, $b_4(G) = b_4(G-v) + b_2(G-u-v)$ and $b_4(S_n^{4,4}) = b_4(S_{n-1}^{4,4}) + b_2(K_{1,3})$. By the induction hypothesis, $b_4(G-v) \geq b_4(S_{n-1}^{4,4})$. Since G does not contain $K_4 - e$, $b_2(G-u-v) > 3 = b_2(K_{1,3})$. So $b_4(G) > b_4(S_{a+b-t-p}^{4,4})$. Thus, we have shown that in Case 2, $b_4(G) > b_4(S_n^{4,4}) = 3n - 15$.

Lemma 7.59 follows by combining Cases 1 and 2 and by taking into account Lemma 7.58. ■

Similarly, we have:

Lemma 7.60. *If $G \in G(n)$ does not contain $K_4 - e$ and $G \not\cong S_n^{4,4}, S_n'^{4,4}$, then $G \succ S_n'^{4,4}$.* ■

Lemma 7.61. *If $G \in G(n)$ contains $K_4 - e$ and $G \not\cong S_n^{3,3}$, then $G \succ S_n^{3,3}$.*

Proof. We demonstrate the validity of $b_i(G) \geq b_i(S_n^{3,3})$ by induction on n. If $n = 4$, the lemma holds. Suppose that it is true for $n < p$ $(p \geq 5)$, and let $n = p$. Then G contains a pendent edge uv with pendent vertex v. From Theorem 1.3, $b_i(G) = b_i(G-v) + b_{i-2}(G-u-v)$ and $b_i(S_n^{3,3}) = b_i(S_{n-1}^{3,3}) + b_{i-2}(P_3)$. By the induction hypothesis, $b_i(G-v) \geq b_i(S_{n-1}^{3,3})$. On the other hand, $b_{i-2}(G-u-v) \geq b_{i-2}(P_3)$ since

$$b_{i-2}(G-u-v) = \begin{cases} 1 & i-2 = 0 \\ > 2 & i-2 = 2 \\ \geq 0 & \text{otherwise} \end{cases}$$

and

$$b_{i-2}(P_3) = \begin{cases} 1 & i-2 = 0 \\ 2 & i-2 = 2 \\ 0 & \text{otherwise.} \end{cases}$$

Thus, $b_i(G) \geq b_i(S_n^{3,3})$ holds for all i. Since $G \not\cong S_n^{3,3}$, from the above argument, we see that $b_{i_0}(G) > b_{i_0}(S_n^{3,3})$ for some i_0. The lemma follows. ■

Similarly, we have:

Lemma 7.62. *If $G \in G(n)$ contains $K_4 - e$ and $G \not\cong S_n^{3,3}, S_n'^{3,3}$, then $G \succ S_n'^{3,3}$.* ■

Lemma 7.63. *$\mathscr{E}(S_n'^{4,4}) > \mathscr{E}(S_n'^{3,3}) > \mathscr{E}(S_n^{4,4}) > \mathscr{E}(S_n^{3,3})$ for $n \geq 9$.*

Proof. It is not difficult to verify that

$$\phi(S_n'^{3,3}) = x^n - (n+1)x^{n-2} - 4x^{n-3} + (3n-13)x^{n-4}$$
$$\phi(S_n'^{4,4}) = x^n - (n+1)x^{n-2} + (4n-21)x^{n-4}$$
$$\phi(S_n^{3,3}) = x^n - (n+1)x^{n-2} - 4x^{n-3} + (2n-8)x^{n-4}$$
$$\phi(S_n^{4,4}) = x^n - (n+1)x^{n-2} + (3n-15)x^{n-4}.$$

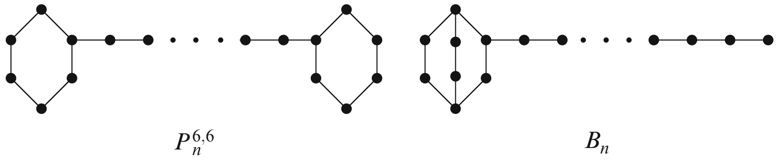


Fig. 7.30 The graphs $P_n^{6,6}$ and B_n

This implies

$$\mathscr{E}(S_n^{\prime 4,4}) - \mathscr{E}(S_n^{\prime 3,3}) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \frac{[1 + (n+1)x^2 + (4n-21)x^4]^2}{[1 + (n+1)x^{-2} + (3n-13)x^4]^2 + 16x^6} \, \mathrm{d}x.$$

Let

$$\begin{aligned} f(x) &= [1 + (n+1)x^2 + (4n-21)x^4]^2 - [1 + (n+1)x^{-2} + (3n-13)x^4]^2 - 16x^6 \\ &= (n-8)(7n-34)x^8 + 2(n^2 - 7n + 16)x^6 + 2(n-8)x^4. \end{aligned}$$

Then $f(x) > 0$ for $n \geq 9$. So $\mathscr{E}(S_n^{\prime 4,4}) > \mathscr{E}(S_n^{\prime 3,3})$. Similarly, we get $\mathscr{E}(S_n^{\prime 3,3}) > \mathscr{E}(S_n^{4,4}) > \mathscr{E}(S_n^{3,3})$. ■

Combining Lemmas 7.59 through 7.63, we obtain the following result:

Theorem 7.25. *$S_n^{3,3}$, $S_n^{4,4}$, and $S_n^{\prime 3,3}$ have, respectively, minimal, second-minimal, and third-minimal energies in $G(n)$.* ■

7.3.2 *Maximal Energy of Bicyclic Graphs*

For bicyclic graphs with maximal energy, the following conjecture was proposed in [242]. Let $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path of order $n - 10$ (see Fig. 7.30).

Conjecture 7.7. For $n = 14$ and $n \geq 16$, the bicyclic molecular graph of order n with maximal energy is $P_n^{6,6}$.

Let $\mathscr{B}_n$ be the class of all connected bipartite bicyclic graphs that are not the graph obtained from two cycles C_a and C_b ($a, b \geq 10$ and $a \equiv b \equiv 2 \pmod 4$), joined by an edge. Let $\mathscr{B}_n^1$ be a subset of $\mathscr{B}_n$ containing all graphs with exactly two edge-disjoint cycles. Let further $\mathscr{B}_n^2 = \mathscr{B}_n \setminus \mathscr{B}_n^1$ be the set of all graphs with exactly three cycles. In this subsection, we show that $P_n^{6,6}$ is the graph with maximal energy in $\mathscr{B}_n$ [340].

As before, denote by P_n^{ℓ} the unicyclic graph obtained by connecting a vertex of C_{ℓ} with a leaf of $P_{n-\ell}$ and by $C(n, \ell)$ the set of all unicyclic graphs obtained from

C_ℓ by adding to it $n-\ell$ pendent vertices. Let $P(n;s,t)$ be the tree obtained by attaching a pendent vertex of P_{t+1} to the $(s+1)$-th vertex of P_{n-t}. The following results are applied in the proof of our result: If T is a tree with n vertices and $T \not\cong P_n$, $P(n;2,2)$, then $P(n;2,2) \succ T$, which follows from Theorem 4.12 since $P(n;2,2) = n-2(3)2$.

The following lemma is an easy consequence of Theorem 1.3:

Lemma 7.64. *Let uv be an edge of a bipartite graph G, then*

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) + 2\sum_{C_\ell \in \mathscr{C}(uv)} (-1)^{1+\ell/2}\, b_{2i-\ell}(G-C_\ell)$$

where $\mathscr{C}(uv)$ is the set of cycles containing uv. In particular, if uv is a pendent edge of G with pendent vertex v, then $b_{2i}(G) = b_{2i}(G-v) + b_{2i-2}(G-u-v)$. ■

Lemma 7.65. *Let $G \in \mathscr{B}_n^1$ $(n \geq 16)$ and $G \not\cong P_n^{6,6}$. Then $G \prec P_n^{6,6}$.*

Proof. Since $G \in \mathscr{B}_n^1$, G contains exactly two cycles, say C_a and C_b, that are connected by a path P_t $(t \geq 1)$. This subgraph is called the *central structure* of G, denoted by $\Theta(a,b;t)$. In this way, G is also viewed as the graph obtained from $\Theta(a,b;t)$ by planting some trees on it.

Case 1. $t \geq 2$.

Subcase 1.1. There is no edge uv of P_t such that $G-uv$ contains two components whose orders are at least 6. Then G contains the central structure $\Theta(4,a;2)$ (or $\Theta(4,a;3)$), and there is at most one edge planted on the C_4 of $\Theta(4,a;2)$ (or no tree is planted on C_4 of $\Theta(4,a;3)$).

If G contains $\Theta(4,a;2)$ and no tree is planted on C_4, let uv be an edge of C_a and u be the vertex of degree 3 in $\Theta(4,a;2)$. By Lemma 7.64,

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) + (-1)^{1+a/2}\, 2\, b_{2i-a}(G-C_a)$$

$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2\, b_{2i-6}(P_{n-6}^6).$$

Observe that $P_n^6 \succ G-uv$ and $b_{2i-6}(P_{n-6}^6) > b_{2i-6}(P_{n-6}^4) > b_{2i-8}(P_{n-8}^4) > \cdots > b_{2i-a}(G-C_a)$ for $a \equiv 2 \pmod 4$. If $a \equiv 0 \pmod 4$, then the result is obvious.

It suffices to prove that $G-u-v \prec P_{n-6}^6 \cup P_4$. Clearly, $G-u-v \prec C_4 \cup P_{n-6}$. By Lemma 7.64,

$$\begin{aligned} b_{2k}(G-u-v) &\leq b_{2k}(C_4 \cup P_{n-6}) \\ &= b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_{n-6}) - 2b_{2k-4}(P_{n-6}) \\ &= b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-10}) \\ &\quad + b_{2k-4}(P_2 \cup P_3 \cup P_{n-11}) - 2b_{2k-4}(P_{n-6}) \end{aligned}$$

$$\leq b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-10}) - b_{2k-4}(P_{n-6})$$
$$= b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(2P_2 \cup P_4 \cup P_{n-12})$$
$$+ b_{2k-4}(P_2 \cup P_4 \cup P_1 \cup P_{n-13}) - b_{2k-4}(P_{n-6})$$
$$< b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_4 \cup P_4 \cup P_{n-12}) + 2b_{2k-6}(P_4 \cup P_{n-12})$$
$$= b_{2k}(P_{n-6}^6 \cup P_4).$$

If G contains $\Theta(4, a; 2)$ and only one pendent edge is planted on C_4 or G contains $\Theta(4, a; 3)$ and no tree is planted on C_4, similar to the above proof, we can also prove that $G \prec P_n^{6,6}$.

Subcase 1.2. There exists an edge uv of P_t such that $G - uv$ contains two components with orders at least 6.

If there is at least one cycle C_4, suppose that G is the graph obtained from $\Theta(4, a; t)$ by planting some trees on it and uv is an edge of C_a that is incident to P_t. By Lemma 7.64,

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) + (-1)^{1+a/2}\, 2\, b_{2i-a}(G - C_a)$$

and

$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2\, b_{2i-6}(P_{n-6}^6).$$

In a similar manner as in the above discussion, it suffices to prove that $b_{2i-2}(G-u-v) < b_{2i-2}(P_{n-6}^6 \cup P_4)$. Since the component containing C_4 in $G-u-v$ has at least 6 vertices and $a \geq 4$, we denote the component as G_x $(x \geq 6)$. From Lemma 7.43, we have $G_x \preceq P_x^4$ (or $G_x \in C(x, 4)$, the proof of this case is similar). We are reduced to the following claim:

Claim 1. $P_{n-x}^4 \cup P_x \preceq P_{n-2}^4 \cup P_2 \prec P_{n-4}^6 \cup P_4$, where $n - x \geq 6$ and $x \geq 1$.

Deleting the edge of P_{n-x-3} that is incident to C_4 in $P_{n-x}^4 \cup P_x$ and the edge of P_{n-5} that is incident to C_4 in $P_{n-2}^4 \cup P_2$ and combining Lemmas 7.64 and 4.6, we obtain the first inequality.

By Lemma 7.64,

$$b_{2i}(P_{n-2}^4 \cup P_2) = b_{2i}(P_{n-2} \cup P_2) + b_{2i-2}(2P_2 \cup P_{n-6}) - 2b_{2i-4}(P_{n-6} \cup P_2)$$
$$= b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(P_1 \cup P_2 \cup P_{n-5}) + b_{2i-2}(2P_2 \cup P_{n-6}) - 2b_{2i-4}(P_{n-6} \cup P_2)$$
$$< b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(2P_2 \cup P_4 \cup P_{n-10}) + b_{2i-2}(3P_1 \cup P_{n-5})$$
$$< b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(2P_4 \cup P_{n-10}) + b_{2i-2}(2P_1 \cup P_{n-4}) + 2b_{2i-6}(P_4 \cup P_{n-10})$$
$$= b_{2i}(P_4 \cup P_{n-4}) + b_{2i-2}(2P_4 \cup P_{n-10}) + 2b_{2i-6}(P_4 \cup P_{n-10}) = b_{2i}(P_{n-4}^6 \cup P_4).$$

Thus, we complete the proof of the claim.

In the following cases, we assume that G contains two cycles C_a and C_b $(a, b \geq 6)$.

Subcase 1.2.1. $G \cong \Theta(a, b; 2)$ $(a, b \geq 6)$. Thus, $n = a + b$.

If there is a cycle of length 6, then $a \geq 10$. Let xy be an edge of C_a that is incident to the P_2 of $\Theta(a, 6; 2)$. By Lemma 7.64,

$$b_{2i}(G) = b_{2i}(P_n^6) + b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+a/2}\, 2\, b_{2i-a}(C_6)$$

and

$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6).$$

It suffices to prove that

$$b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) \geq b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+a/2}\, 2\, b_{2i-a}(C_6).$$

By the Sachs theorem, for $i = 1, 2, 3$,

$$b_{2i-2}(P_{n-6}^6 \cup P_4) + 2\, b_{2i-6}(P_{n-6}^6) = 1,\ n-3,\ (n^2 - 9n + 22)/2,$$

respectively, whereas

$$b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+a/2}\, 2\, b_{2i-a}(C_6) = 1,\ n-3,\ (n^2 - 9n + 20)/2,$$

respectively. Assuming that $i \geq 4$, we obtain

$$\begin{aligned} b_{2i-2}(C_6 \cup P_{n-8}) &= b_{2i-2}(P_6 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_{n-8}) + 2\, b_{2i-8}(P_4 \cup P_{n-12}) \\ &\quad + 2\, b_{2i-10}(P_3 \cup P_{n-13}) \end{aligned}$$

$$b_{2i-2}(P_{n-6}^6 \cup P_4) = b_{2i-2}(P_{n-6} \cup P_4) + b_{2i-4}(2P_4 \cup P_{n-12}) + 2\, b_{2i-8}(P_{n-12} \cup P_4)$$

and

$$\begin{aligned} 2b_{2i-6}(P_{n-6}^6) &= 2b_{2i-6}(P_{n-6}) + 2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}) \\ &= b_{2i-6}(P_4 \cup P_3 \cup P_{n-13}) + b_{2i-8}(P_3 \cup P_{n-11}) + b_{2i-8}(P_4 \cup P_2 \cup P_{n-14}) \\ &\quad + b_{2i-6}(P_{n-6}) + 2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}). \end{aligned}$$

Since

$$\begin{aligned} b_{2i-4}(P_4 \cup P_{n-8}) &= b_{2i-4}(2P_4 \cup P_{n-12}) + b_{2i-6}(P_4 \cup P_3 \cup P_{n-13}) \\ b_{2i-8}(P_3 \cup P_{n-11}) &= b_{2i-8}(P_1 \cup P_3 \cup P_{n-12}) + b_{2i-10}(P_3 \cup P_{n-13}) \\ b_{2i-8}(P_4 \cup P_2 \cup P_{n-14}) &= b_{2i-8}(P_4 \cup 2P_1 \cup P_{n-14}) + b_{2i-10}(P_4 \cup P_{n-14}), \end{aligned}$$

we have

$$\begin{aligned} &b_{2i-2}(P_{n-6}^{6} \cup P_4) + 2b_{2i-6}(P_{n-6}^{6}) \\ &\quad \geq b_{2i-2}(C_6 \cup P_{n-8}) + b_{2i-8}(P_1 \cup P_3 \cup P_{n-12}) + b_{2i-8}(P_4 \cup 2P_1 \cup P_{n-14}) \\ &\qquad + b_{2i-6}(P_{n-6}) + 2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}). \end{aligned}$$

For $a \equiv 0 \pmod 4$, the result is obvious. We thus assume that $a \equiv 2 \pmod 4$ and since $2b_{2i-a}(C_6) = 0$ for $2i < a$, $2b_{2i-a}(C_6) = 2$ for $2i = a$, $2b_{2i-a}(C_6) = 12$ for $2i = a+2$, $2b_{2i-a}(C_6) = 18$ for $2i = a+4$, and $2b_{2i-a}(C_6) = 8$ for $2i = a+6 = n$, by simple computation, we get

$$b_{2i-2}(P_{n-6}^{6} \cup P_4) + 2b_{2i-6}(P_{n-6}^{6}) > b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+a/2}\, 2b_{2i-a}(C_6).$$

If there is a cycle of length congruent to 0 (mod 4), say $b \equiv 0 \pmod 4$, then it must be $b \geq 8$. Similarly, we have $b_{2i}(G) = b_{2i}(P_n^a) + b_{2i-2}(C_a \cup P_{b-2}) - 2b_{2i-b}(C_a)$. Deleting an edge of C_a in $C_a \cup P_{b-2}$ and an edge of C_6 in $C_6 \cup P_{n-8}$ and applying Lemma 4.6, we get that $C_6 \cup P_{n-8} \succ C_a \cup P_{b-2}$. Thus, we also have $b_{2i-2}(P_{n-6}^{6} \cup P_4) + 2b_{2i-6}(P_{n-6}^{6}) > b_{2i-2}(C_6 \cup P_{n-8}) > b_{2i-2}(C_a \cup P_{b-2})$ and $P_n^a \prec P_n^6$, which completes the proof of the subcase.

Subcase 1.2.2. $t \geq 6$. We can choose an edge rs of P_t such that $G-rs$ and $G-r-s$ contain two components of orders at least 6 that are either unicyclic graphs or trees and each component is not isomorphic to a cycle. Thus, we choose an edge uv of P_{n-10} in $P_n^{6,6}$ such that $P_n^{6,6} - uv$ contains two components with the same valencies as those of $G - rs$. Note that if $G - r - s$ has at least three components, then we can obtain a larger graph G' with exactly two components, by adding some edges to $G - r - s$. We thus have $b_{2i}(G) = b_{2i}(G - rs) + b_{2i-2}(G - r - s) \leq b_{2i}(P_n^{6,6} - uv) + b_{2i-2}(P_n^{6,6} - u - v) = b_{2i}(P_n^{6,6})$ and $G \prec P_n^{6,6}$.

Subcase 1.2.3. $2 \leq t \leq 5$. If there are some trees planted on both cycles, similar to the proof of Subcase 1.2.2, we can obtain the result. Let C_a, C_b $(a, b \geq 6)$ be two cycles of G. Assume that there is no tree planted on C_a. In order to prove the result, we first give the following claim:

Claim 2. (a) For b being even and $b \geq 8$, $P_{b+x}^{b} \cup P_y \prec P_{b+x}^{6} \cup P_y \preceq P_{n-4}^{6} \cup P_4$, where $n = b + x + y$ and $x \geq 1, y \geq 4$. (b) $P_{n-t}^{6} \cup P_t \preceq P_{n-4}^{6} \cup P_4$ for $n - t \neq 8, n - t \geq 7$, and $t \geq 4$.

The first inequality in (a) is obvious. In the following, we prove the second inequality. It is reduced to proving (b). By Lemma 7.64,

$$b_{2i}(P_{n-t}^{6} \cup P_t) = b_{2i}(P_{n-t} \cup P_t) + b_{2i-2}(P_4 \cup P_t \cup P_{n-t-6}) + 2b_{2i-6}(P_{n-t-6} \cup P_t)$$

$$b_{2i}(P_{n-4}^{6} \cup P_4) = b_{2i}(P_{n-4} \cup P_4) + b_{2i-2}(P_4 \cup P_4 \cup P_{n-10}) + 2b_{2i-6}(P_{n-10} \cup P_4).$$

By Lemma 4.6, we obtain the result. Now we turn to the proof of Subcase 1.2.3.

If $t = 2$, then there must be some trees planted on C_b. Let uv be an edge of C_a and u be a vertex of P_t. By Lemma 7.64, we have

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) + (-1)^{1+a/2}\, 2\, b_{2i-a}(G-C_a)$$

and

$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}\left(P_{n-6}^6\right).$$

Similar as in the previous proof, it suffices to show that

$$b_{2i-2}(G-u-v) \le b_{2i-2}\left(P_{n-6}^6 \cup P_4\right).$$

If $b \ge 8$, by Claim 2 the result follows. If $b = 6$ and $G-u-v \cong P_8^6 \cup P_{n-10}$, then G is the graph obtained from $\Theta(6, n-8, 2)$ by attaching P_3 to C_6. In a similar manner as above, we prove that $G \prec \Theta(6, n-8, 4)$.

If $3 \le t \le 5$, let uv be the edge as above. If $G-u-v \ncong P_8^6 \cup P_{n-10}$, the result is obtained similarly. If $G-u-v \cong P_8^6 \cup P_{n-10}$, then $G \cong \Theta(6, n-8, 4)$. Deleting the edge of C_6 that is incident to P_4 and applying Lemma 7.64, we can also obtain the result.

Case 2. $t = 1$. Then G contains two cycles C_a and C_b $(a \ge b)$ which have exactly one common vertex w. Let wl be an edge of C_a. Deleting it, we have

$$\begin{aligned}
b_{2i}(G) &= b_{2i}(G-wl) + b_{2i-2}(G-w-l) + (-1)^{1+a/2} 2b_{2i-a}(G-C_a)\\
&\le b_{2i}(P_n^b) + b_{2i-2}(P_2 \cup P_{n-4}) + 2b_{2i-a}(P_{n-a}) \quad (\text{where } a \equiv 2 \pmod 4)\\
&\le b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) = b_{2i}(P_n^{6,6})
\end{aligned}$$

in which $P_2 \cup P_{n-4} \prec P(n-2; 2, 2) \prec P_{n-6}^6 \cup P_4$ and the second inequality is proven in Claim 3.

Claim 3. $P(n; 2, 2) \prec P_{n-4}^6 \cup P_4$.

It is clear that $b_0(P(n; 2, 2)) = b_0(P_{n-4}^6 \cup P_4) = 1$, $b_2(P(n; 2, 2)) = b_2(P_{n-4}^6 \cup P_4) = n-1$, $b_4(P(n; 2, 2)) = m(P(n; 2, 2), 2) = (n^2-5n+4)/2$, and $b_4(P_{n-4}^6 \cup P_4) = m(P_{n-4} \cup P_4, 2) = (n^2-5n+4)/2$.

In the following, we suppose that $i \ge 3$. By Lemma 7.64,

$$\begin{aligned}
b_{2i}(P(n; 2, 2)) &= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_{n-6})\\
&= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_4 \cup P_{n-10}) + b_{2i-4}(2P_2 \cup P_3 \cup P_{n-11})\\
&= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_4 \cup P_{n-10})\\
&\quad + b_{2i-4}(2P_1 \cup P_2 \cup P_3 \cup P_{n-11}) + b_{2i-6}(P_2 \cup P_3 \cup P_{n-11}).
\end{aligned}$$

Thus,

$$\begin{aligned}
b_{2i}(P(n;2,2)) &\leq b_{2i}(P_{n-4}\cup P_4)+b_{2i-2}(P_2\cup P_2\cup P_4\cup P_{n-10})\\
&\quad + b_{2i-4}(2P_1\cup P_4\cup P_{n-10})+b_{2i-6}(P_{n-10}\cup P_4)\\
&\leq b_{2i}(P_{n-4}\cup P_4)+b_{2i-2}(P_4\cup P_4\cup P_{n-10})+2b_{2i-6}(P_{n-10}\cup P_4)\\
&= b_{2i}(P^6_{n-4}\cup P_4)
\end{aligned}$$

which completes the proof of Claim 3.

Combining all above cases, the proof is completed. ■

Lemma 7.66. *Let $G\in\mathscr{B}^2_n$ $(n\geq 16)$. Then $G\prec P^{6,6}_n$.*

Proof. Since $G\in\mathscr{B}^2_n$, G also has a central structure which can be viewed as the graph obtained from three paths P_x, P_y, and P_z by identifying three pendent vertices (each from one path) into one vertex, and the other three pendent vertices into another vertex. We write it as $\Omega(x,y,z)$ $(x\geq y\geq z)$. Then G contains three cycles C_{x+y-2}, C_{x+z-2}, and C_{y+z-2}.

Case 1. There is no cycle of length congruent to 0 (mod 4). Suppose that C_a, C_b, and C_c are the three cycles of G.

Subcase 1.1. The length of a longest cycle equals 10. Then G contains the central structure that is isomorphic to one of $\Omega(6,6,2)$, $\Omega(6,6,6)$, and $\Omega(8,4,4)$.

If G contains the central structure $\Omega(6,6,2)$, since $n\geq 16$, we can always find an edge uv of C_{10} with vertex u of degree 3 in $\Omega(6,6,2)$ such that $G-u-v$ is not a path and $G-C_6$ is disconnected and is not isomorphic to $P_{n-8}\cup P_2$, where uv is an edge of C_6.

By Lemma 7.64,

$$b_{2i}(G)=b_{2i}(G-uv)+b_{2i-2}(G-u-v)+2b_{2i-10}(G-C_{10})+2b_{2i-6}(G-C_6)$$
$$b_{2i}(P^{6,6}_n)=b_{2i}(P^6_n)+b_{2i-2}(P^6_{n-6}\cup P_4)+2b_{2i-6}(P^6_{n-6}).$$

Evidently, $b_{2i}(G-uv)\leq b_{2i}(P^6_n)$. By Claim 3 and Lemma 4.6, $b_{2i-2}(G-u-v)\leq b_{2i-2}(P(n-2;2,2))\leq b_{2i-2}(P^6_{n-6}\cup P_4)$.

It suffices to prove that $b_{2i-6}(P^6_{n-6})\geq b_{2i-10}(G-C_{10})+b_{2i-6}(G-C_6)$. Since uv is the edge such that $G-C_6\ncong P_2\cup P_{n-8}$, it is easy to see that $G-C_6\preceq P_4\cup P_{n-10}$.

We thus have

$$\begin{aligned}
b_{2i-6}(P^6_{n-6}) &\geq b_{2i-6}(P_{n-6})+b_{2i-8}(P_4\cup P_{n-12})\\
&= b_{2i-6}(P_4\cup P_{n-10})+b_{2i-8}(P_3\cup P_{n-11})+b_{2i-8}(P_4\cup P_{n-12})\\
&\geq b_{2i-6}(P_4\cup P_{n-10})+b_{2i-10}(P_3\cup P_{n-13})+b_{2i-8}(P_4\cup P_{n-12})\\
&= b_{2i-6}(P_4\cup P_{n-10})+b_{2i-8}(P_{n-8})\\
&\geq b_{2i-6}(P_4\cup P_{n-10})+b_{2i-10}(P_{n-10})\\
&\geq b_{2i-6}(G-C_6)+b_{2i-10}(G-C_{10}).
\end{aligned}$$

If G contains the central structure $\Omega(6,6,6)$ or $\Omega(8,4,4)$, we choose the edge uv such that u is the vertex of degree 3 in the central structure and is contained in two C_{10}'s, say C_{10}^1 and C_{10}^2. Similar to above proof, we obtain

$$b_{2i-6}(P_{n-6}^6) > b_{2i-10}(G - C_{10}^1) + b_{2i-10}(G - C_{10}^2)$$

from which the result follows.

Subcase 1.2. There is a cycle of length at least 14. Then

$$b_{2i-6}(P_{n-6}^6) \geq b_{2i-6}(P_{n-6}) + b_{2i-8}(P_4 \cup P_{n-12}) \geq b_{2i-6}(P_{n-6}) + b_{2i-14}(P_{n-14}).$$

The result follows in a similar way as in Subcase 1.1.

Subcase 1.3. The central structure of G is $\Omega(4,4,4)$.

Let B_n be the graph obtained by attaching a pendent vertex of P_{n-7} to a vertex of degree 2 in $\Omega(4,4,4)$ (see Fig. 7.30).

Claim 4. If G contains the central structure $\Omega(4,4,4)$, then $G \preceq B_n$ with equality if and only if $G \cong B_n$.

We apply induction on n. By simple computation, the result is found to be true for $n = 8$ and $n = 9$. We suppose that $n \geq 10$ and that the result is true for smaller values. Assume that uv is a pendent edge with pendent vertex v.

If u is a vertex of $\Omega(4,4,4)$, then $b_{2i}(G) = b_{2i}(G-v) + b_{2i-2}(G-u-v) \leq b_{2i}(B_{n-1}) + b_{2i-2}(P_{n-2}^6) \leq b_{2i}(B_{n-1}) + b_{2i-2}(B_{n-2}) = b_{2i}(B_n)$. If u is not a vertex of $\Omega(4,4,4)$, then $b_{2i}(G) = b_{2i}(G-v) + b_{2i-2}(G-u-v) \leq b_{2i}(B_{n-1}) + b_{2i-2}(B_{n-2}) = b_{2i}(B_n)$, in which case we obtain $b_{2i}(G-v) < b_{2i}(B_{n-1})$ by the induction hypothesis. This completes the proof of the claim.

Claim 5. $B_n \prec P_n^{6,6}$.

By Lemma 7.64,

$$\begin{aligned}
b_{2i}(P_n^{6,6}) &= b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) \\
&\geq b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_{n-6}) + b_{2i-4}(2P_4 \cup P_{n-12}) \\
&\quad + 4b_{2i-8}(P_4 \cup P_{n-12}) + 2b_{2i-6}(P_{n-6}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_1 \cup P_{n-9}) + 2b_{2i-6}(P_{n-6}) \\
&\quad + b_{2i-4}(2P_2 \cup P_4 \cup P_{n-12}) + b_{2i-6}(2P_1 \cup P_4 \cup P_{n-12}) + 4b_{2i-8}(P_4 \cup P_{n-12}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_1 \cup P_2 \cup P_{n-11}) + 2b_{2i-6}(P_{n-6}) \\
&\quad + b_{2i-4}(2P_2 \cup P_4 \cup P_{n-12}) + 2b_{2i-6}(2P_1 \cup P_4 \cup P_{n-12}) + 4b_{2i-8}(P_4 \cup P_{n-12})
\end{aligned}$$

and

$$\begin{aligned}
b_{2i}(B_n) &= b_{2i}(P_n^6) + b_{2i-2}(P(6;2,1) \cup P_{n-8}) + 4b_{2i-6}(P_2 \cup P_{n-8}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) \\
&\quad + b_{2i-4}(2P_1 \cup P_2 \cup P_{n-8}) + 4b_{2i-6}(P_2 \cup P_{n-8}).
\end{aligned}$$

Since $2[b_{2i-6}(2P_1 \cup P_4 \cup P_{n-12}) + 2b_{2i-8}(P_4 \cup P_{n-12})] = 2[b_{2i-6}(P_2 \cup P_4 \cup P_{n-12}) + b_{2i-8}(P_4 \cup P_{n-12})] \geq 2b_{2i-6}(P_2 \cup P_{n-8})$, it follows that $b_{2i}(P_n^{6,6}) \geq b_{2i}(B_n)$, which completes the proof of the claim.

Case 2. There is a cycle, say C_a, such that $a \equiv 0 \pmod 4$. If $G \ncong \Omega(n-2,3,3)$, we can always find a cycle of length congruent to $0 \pmod 4$, say C_a and an edge uv of it such that u is the vertex of degree 3 of $\Omega(x,y,z)$ and $G-u-v$ is not a path. Deleting it and applying Lemma 7.64, we have $b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) - 2\,b_{2i-a}(G-C_a) + (-1)^{1+b/2}\,2\,b_{2i-b}(G-C_b)$ and $b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2\,b_{2i-6}(P_{n-6}^6)$. Similar to the above proof, it suffices to show that $G-u-v \prec P_{n-6}^6 \cup P_4$. Since $G-u-v$ is not a path, $G-u-v \preceq P(n-2;2,2)$. By Claim 3, we obtain the result.

If $G \cong \Omega(n-2,3,3)$, then there are two cycles of lengths $n-1$ in G, since $n \geq 16$. The result is proven in a similar way as in the Subcase 1.2.

Combining all cases, we complete the proof of the lemma. ■

Lemmas 7.65 and 7.66 imply:

Theorem 7.26. *Let $G \in \mathscr{B}_n$ $(n \geq 16)$. Then $G \preceq P_n^{6,6}$. Moreover, $\mathscr{E}(G) \leq \mathscr{E}(P_n^{6,6})$, with equality if and only if $G \cong P_n^{6,6}$.* ■

Remark 7.7. Let $R_{a,b}$ be the graph obtained from two cycles C_a and C_b $(a,b \geq 10$ and $a \equiv b \equiv 2 \pmod 4))$ joined by an edge. Recall that, as shown in Theorem 7.26, Li and Zhang [340] proved that $P_n^{6,6}$ has maximal energy among all graphs in $\mathscr{B}_n$. However, they could not determine which of the two graphs $R_{a,b}$ and $P_n^{6,6}$ has the maximal value of energy, since these two graphs are quasi-order incomparable. In [121], computer-generated numerical results up to $a+b=50$ were reported, supporting the conjecture. So, it was still necessary to have a mathematical proof to this conjecture. By using the Coulson integral formula, similar to the method in Sect. 4.4, Huo et al. [280] proved the following result:

Theorem 7.27. *For any bipartite bicyclic graph G, $\mathscr{E}(G) \leq \mathscr{E}(P_n^{6,6})$, with equality if and only if $G \cong P_n^{6,6}$.*

This proves Conjecture 7.7 for bipartite bicyclic graphs. However, for nonbipartite bicyclic graphs, the conjecture is still open.

7.4 Bipartite Graphs with Minimal Energy

Let $A(n,m)$ be the bipartite (n,m)-graph with two vertices on one side, one of which is connected to all vertices on the other side. Let $A'(n,m)$ be the graph obtained from $A(n-1,m-1)$ by adding a pendent edge to the vertex of second-maximal degree in $A(n-1,m-1)$.

In this subsection, we show [341] that $A(n,m)$ is the unique graph with minimal energy among all connected bipartite (n,m)-graphs for $n \leq m \leq 2(n-2)$, giving a solution to Conjecture 7.5. Moreover, we prove that $A'(n, m)$ is the unique graph with the second-minimal energy among all connected bipartite (n, m)-graphs for $n \le m \le 2n - 5$.

Lemma 7.67. *Let uv be a cut edge in G and $e(G)$ the number of edges of G. Then $b_4(G) = b_4(G - uv) + e(G - u - v)$. In particular, let uv be a pendent edge of G with pendent vertex v. Then $b_4(G) = b_4(G - v) + e(G - u - v)$.*

Proof. Since uv is a cut edge, we have that the number of quadrangles $Q(G) = Q(G - uv)$. By Lemma 7.56, $b_4(G - uv) = m(G - uv, 2) - 2Q(G - uv)$ and $b_4(G) = m(G, 2) - 2Q(G) = m(G - uv, 2) + m(G - u - v, 1) - 2Q(G) = b_4(G - uv) + e(G - u - v)$. ■

Theorem 7.28. *$A(n, m)$ $(n \le m \le 2(n - 2))$ is the unique graph with minimal energy among all bipartite connected (n, m)-graphs.*

Proof. Let G be a bipartite connected (n, m)-graph. Then $\Delta(G) \le n - 2$.

Since $b_i(A(n, m)) = 0$ for $i \ne 0, 2, 4$, we have that $b_0(G) = 1$ and $b_2(G) = m$. It suffices to prove that $b_4(G) \ge b_4(A(n, m))$. We apply induction on n to prove it. From the table of [80], the result is true for $n = 7$. So we suppose that $n \ge 8$ and the result is true for smaller n.

Case 1. There is a pendent edge uv with pendent vertex v. If $m = 2n - 4$, then $b_4(G) \ge b_4(A(n, 2n - 4)) = 0$. We thus assume that $m \le 2n - 5$, and then $m - 1 \le 2(n - 1) - 4$. By Lemma 7.67, $b_4(G) = b_4(G - v) + e(G - u - v)$ and $b_4(A(n, m)) = b_4(A(n - 1, m - 1)) + e(S_{m-n+3})$. Since $\Delta(G) \le n - 2$, we have $e(G - u - v) \ge m - \Delta(G) \ge m - n + 2 = e(S_{m-n+3})$. Combined with the induction hypothesis, the result follows.

Case 2. There is no pendent vertex in G.

Claim 6. Let G be a connected bipartite (n, m)-graph for $n \le m \le 2(n - 2)$. Then $Q(G) \le \binom{m-n+2}{2}$.

We apply induction on m. The result is obvious for $m = n$. So we suppose that $n < m \le 2(n - 2)$ and that the result is true for smaller m. Let e be an edge of a cycle in G. Then G contains at most $m - n + 1$ quadrangles containing the edge e. Otherwise, we suppose that there are $m - n + a$ $(a \ge 2)$ quadrangles containing $e = uv$. Let U be the set of neighbor vertices of u except v, and let V be the set of neighbor vertices of v except u. Then there are exactly $m - n + a$ edges between U and V. Let X be a subset of U such that each vertex in X is incident to some of the above $m - n + a$ edges and Y be a subset of V defined similarly as X. Assume that $|X| = x$ and $|Y| = y$. Let G_0 be a subgraph of G induced by $V(G_0) = \{u\} \cup \{v\} \cup X \cup Y$. Then G_0 has $m - n + a + x + y + 1$ edges and $x + y + 2$ vertices. In order to make the remaining vertices connected to G_0, the number of remaining edges must be at least that of the remaining vertices, i.e.,

$$m - (m - n + a + x + y + 1) \ge n - (x + y + 2) \tag{7.48}$$

that is, $n-a-1 \geq n-2$, which contradicts $a \geq 2$. Note that Ineq. (7.48) still holds when there are no remaining vertices. Let $Q_G(e)$ denote the number of quadrangles in G containing the edge e. Then,

$$Q(G) = Q_G(e) + Q(G-e) \leq m-n+1+\binom{m-1-n+2}{2} = \binom{m-n+2}{2}$$

where $Q(G-e) \leq \binom{m-1-n+2}{2}$, obtained by the induction hypothesis.

A nonincreasing sequence $(d)_G = (d_1, d_2, \ldots, d_n)$ of positive integers is said to be graphic if there exist a simple graph G having degree sequence $(d)_G$.

Claim 7. Let G be a bipartite connected (n,m)-graph. If G has no pendent vertex, then

$$\sum_{v \in V(A(n,m))} \binom{d(v)}{2} \geq \sum_{v \in V(G)} \binom{d(v)}{2}.$$

In fact, let

$$(d)_G = (d_1, d_2, \ldots, d_{i-1}, d_i, \ldots, d_j, d_{j+1}, \ldots, d_n)$$

and

$$(d)' = (d_1, d_2, \ldots, d_{i-1}, d_i+1, \ldots, d_j-1, d_{j+1}, \ldots, d_n)$$

where $d_i \geq d_j$. By writing

$$(d)' = (d'_1, d'_2, \ldots, d'_{i-1}, d'_i, \ldots, d'_j, d'_{j+1}, \ldots, d'_n),$$

we obtain

$$\sum_{t=1}^{n} \binom{d'_t}{2} > \sum_{t=1}^{n} \binom{d_t}{2}$$

because

$$\sum_{t=1}^{n} \binom{d'_t}{2} - \sum_{t=1}^{n} \binom{d_t}{2} = \binom{d_i+1}{2} + \binom{d_j-1}{2} - \binom{d_i}{2} - \binom{d_j}{2} = d_i - d_j + 1 > 0.$$

Notice that $d_1 \geq d_2 \geq \cdots \geq d_n \geq 2$ and $d_1 + d_2 + \cdots + d_n = 2m$. Repeating this operation, we obtain the sequence

$$(d)'' = \left(d''_1, d''_2, d_3, \ldots, d_{m-n+4}, \overbrace{1, 1, \ldots, 1}^{2n-m-4}\right)$$

where $d''_1 \leq n-2$ and $d''_2 \geq d_2$ if $d''_1 = n-2$ and $d''_2 = d_2$ if $d''_1 < n-2$. Since $d''_1 \geq d''_2 \geq d_3 \geq \cdots \geq d_{m-n+4} \geq 2$, by doing the above operation repeatedly, we finally obtain the degree sequence $(d)_{A(n,m)}$:

$$(d)_{A(n,m)} = \left(n-2, m-n+2, \overbrace{2, 2, \ldots, 2}^{m-n+2}, \overbrace{1, 1, \ldots, 1}^{2n-m-4} \right)$$

which has the maximal value of $\sum\limits_{v \in V(G)} \binom{d(v)}{2}$. The proof of the claim is thus complete.

For a simple graph G, we have $m(G,2) = \binom{m}{2} - \sum_{v \in V(G)} \binom{d(v)}{2}$. From Lemma 7.56, we know that $b_4(G) = \binom{m}{2} - \sum\limits_{v \in V(G)} \binom{d(v)}{2} - 2Q(G)$. By Claims 6 and 7, we easily obtain the result.

Combining all the above cases, we thus complete the proof. ■

Since $\phi(A(n,m)) = x^{n-4}\left[x^4 - mx^2 + (m-n+2)(2n-m-4)\right]$, by simple computation, we arrive at:

Corollary 7.9. *Let G be a bipartite connected (n,m)-graph with $n \le m \le 2n-4$. Then $\mathscr{E}(G) \ge 2\sqrt{m + 2\sqrt{(m-n+2)(2n-m-4)}}$, with equality if and only if $G \cong A(n,m)$.* ■

Theorem 7.29. *$A'(n,m)$ $(n \le m \le 2n-5)$ is the unique graph with second-minimal energy among all connected bipartite (n,m)-graphs.*

Proof. Since $b_0(A'(n,m)) = 1$, $b_2(A'(n,m)) = m$, $b_4(A'(n,m)) = (m-n+3)(2n-m-4)-1$, and $b_i(A'_{n,m}) = 0$ for other positive integers i, we can proceed similarly as in the proof of Theorem 7.28. ■

Analogously, $\phi(A'(n,m)) = x^{n-4}\left[x^4 - mx^2 + (m-n+3)(2n-m-4) - 1\right]$, and therefrom, we arrive at:

Corollary 7.10. *Let G be a connected bipartite (n,m)-graph with $n \le m \le 2n-5$. If $G \ncong A(n,m)$, then $\mathscr{E}(G) \ge 2\sqrt{m + 2\sqrt{(m-n+3)(2n-m-4)-1}}$, with equality if and only if $G \cong A'(n,m)$.* ■

7.5 Concluding Remarks

In this lengthy chapter, we have outlined only the most relevant results on graphs with extremal energy and/or the typical proof techniques. Details of numerous other results from the literature are omitted, quoting only the respective references.

There are a few works on the extremal-energy tricyclic [329] and tetracyclic graphs [325]. However, the methods used in these works are essentially same as those employed for trees, unicyclic graphs, and bicyclic graphs. The main difference is that these considerations are much more complicated than those outlined in this chapter. For this reason, we have skipped their details.

On the other hand, some results on extremal-energy graphs are described in other parts of this book. For instance, the presently known (few) results concerning the maximum-energy graphs on n vertices have been stated in Theorems 5.9 and 5.10, in Sect. 5.2.1. Thus, by the works of Koolen and Moulton [305] and Haemers [252, 253], the maximum-energy n-vertex graphs have been characterized for n being the square of an even integer, in particular for $n = 4, 16, 36, 64, 100$, and 144. At the present moment, the main unsolved problem of the theory of graph energy seems to be the following:

Grand Open Problem. *Characterize the maximum-energy graph(s) of order n, for $n \neq (2k)^2$, $k = 1, 2, \ldots$.*

Chapter 8
Hyperenergetic and Equienergetic Graphs

8.1 Hyperenergetic Graphs

The energy of the n-vertex complete graph K_n is equal to $2(n-1)$. We call an n-vertex graph G *hyperenergetic* if $\mathscr{E}(G) > 2(n-1)$. From Theorem 5.24, we know that for almost all graphs, $\mathscr{E}(G) > \left(\frac{1}{4} + o(1)\right) n^{3/2}$, which means that almost all graphs are hyperenergetic. Therefore, any search for hyperenergetic graphs nowadays is a futile task. Yet, before Theorem 5.24 was discovered, a number of such results were obtained. We outline here some of them; for surveys, see [41, 178].

In [149], it was conjectured that the complete graph K_n has the greatest energy among all n-vertex graphs. This conjecture was soon shown to be false [84]. The first systematic construction of hyperenergetic graphs was proposed by Walikar et al. [478], who showed that the line graphs of K_n, $n \geq 5$ and of $K_{\frac{n}{2},\frac{n}{2}}$, $n \geq 8$ are hyperenergetic. These results were eventually extended to other graphs with large number of edges [212, 308, 440, 476, 477].

Hou et al. [269] showed that the line graph of any (n,m)-graph, $n \geq 5$, $m \geq 2n$ is hyperenergetic. Also, the line graph of any bipartite (n,m)-graph, $n \geq 7$, $m \geq 2(n-1)$ is hyperenergetic. Some classes of circulant graphs [35, 438, 453] as well as Kneser graphs and their complements [12] are hyperenergetic. In fact, almost all circulant graphs are hyperenergetic [453].

Graphs on n vertices with fewer than $2n-1$ edges are not hyperenergetic [192, 475]. This, in particular, implies that Hückel graphs (graphs representing conjugated molecules [133, 216, 238], in which the vertex degrees do not exceed 3) cannot be hyperenergetic. More results on hyperenergetic molecular graphs can be found in [170, 437].

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8.2 Equienergetic Graphs

Two nonisomorphic graphs are said to be *equienergetic* if they have the same energy. There exist numerous pairs of graphs with identical spectra, so-called cospectral graphs [81]. In a trivial manner, such graphs are equienergetic. Therefore, in what follows, we will be interested only in noncospectral equienergetic graphs.

It is also trivial that the graphs G and $G \cup \overline{K_p}$ (which are not cospectral) are equienergetic. Namely, the spectrum of the graph whose components are G and additional p isolated vertices consists of the eigenvalues of G and of p zeros.

The smallest triplet of nontrivial equienergetic graphs (all having $\mathscr{E} = 4$) is shown in Fig. 8.1. The smallest pair of equienergetic noncospectral connected graphs with equal number of vertices is shown in Fig. 8.2. A pair of 4-regular such graphs of order 9 was given in Example 4.1. These examples indicate that there exist many (nontrivial) families of equienergetic graphs and that the construction/finding of such families will not be particularly difficult.

The concept of equienergetic graphs was put forward independently and almost simultaneously by Brankov et al. [47] and Balakrishnan [26]. Since 2004, a plethora of papers were published on equienergetic graphs [14,42,292,293,296,349,359,403, 404,407–410,442,496] as well as a not-easy-to-read review [180].

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Take another set of vertices $U = \{u_1, u_2, \ldots, u_n\}$. Define a graph DG whose vertex set is $V(DG) = V(G) \cup U$ and whose edge set consists only of the edges joining u_i to the neighbors of v_i in G for $i = 1, 2, \ldots, n$. The resulting graph DG is called the identity duplication graph of G [292,427].

With the same notation as above, let $u_1, u_2, \ldots, u_n$ be vertices of another copy of G. Make u_i adjacent to the neighbors of v_i in G for $i = 1, 2, \ldots, n$. The resulting graph [292] is denoted by D_2G.

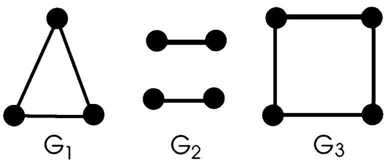

Fig. 8.1 Three noncospectral equienergetic graphs with $\mathscr{E} = 4$. The respective spectra are $\mathrm{Spec}(G_1) = \{2, -1, -1\}$, $\mathrm{Spec}(G_2) = \{1, 1, -1, -1\}$, and $\mathrm{Spec}(G_3) = \{2, 0, 0, -2\}$

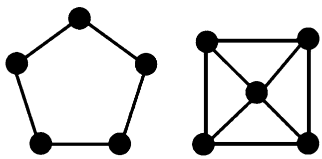

Fig. 8.2 The smallest pair of equienergetic noncospectral connected graphs of the same order

One can readily see that the adjacency matrix of DG is

$$\mathbf{A}(DG) = \begin{pmatrix} \mathbf{0} & \mathbf{A}(G) \\ \mathbf{A}(G) & \mathbf{0} \end{pmatrix} = \mathbf{A} \bigotimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Thus, if $\mathrm{Spec}(G) = \{\lambda_i \ , \ i = 1, \ldots, n\}$, then $\mathrm{Spec}(DG) = \{\lambda_i, -\lambda_i \ , \ i = 1, \ldots, n\}$. It is also easily seen that the adjacency matrix of D_2G is

$$\mathbf{A}(D_2G) = \begin{pmatrix} \mathbf{A}(G) & \mathbf{A}(G) \\ \mathbf{A}(G) & \mathbf{A}(G) \end{pmatrix} = \mathbf{A} \bigotimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

and thus $\mathrm{Spec}(D_2G) = \{2\lambda_1, 2\lambda_2 \ldots, 2\lambda_n, 0, 0, \ldots, 0\}$. Therefore, we deduce the following:

Theorem 8.1. *DG and D_2G are a pair of noncospectral equienergetic graphs.* ■

Furthermore, Indulal and Vijayakumar [292] proved another result concerning noncospectral equienergetic graphs.

Theorem 8.2. *There exists a pair of n-vertex noncospectral equienergetic graphs for $n = 6, 14, 18$, and $n \geq 20$.* ■

In order to prove Theorem 8.2, we first introduce some lemmas:

Lemma 8.1. *Let $\mathbf{M}$ be a nonsingular matrix, and let $\mathbf{N}$, $\mathbf{P}$, and $\mathbf{Q}$ be matrices. Then*

$$\begin{vmatrix} \mathbf{M} & \mathbf{N} \\ \mathbf{P} & \mathbf{Q} \end{vmatrix} = |\mathbf{M}| \left| \mathbf{Q} - \mathbf{P}\mathbf{M}^{-1}\mathbf{N} \right|.$$ ■

Lemma 8.2 [81]. *Let G be a connected r-regular graph of order n and A the adjacency matrix of G with m distinct eigenvalues $\lambda_1 = r, \lambda_2, \ldots, \lambda_m$. Then the polynomial*

$$\varphi(x) = n \frac{(x - \lambda_2)(x - \lambda_3) \cdots (x - \lambda_m)}{(r - \lambda_2)(r - \lambda_3) \cdots (r - \lambda_m)}$$

satisfies $\varphi(A) = J$, where J is the square matrix of order n whose all entries are 1, called all-one matrix, so that $\varphi(r) = n$, $\varphi(\lambda_i) = 0 \ \forall \lambda_i \neq r$. ■

Let G be an r-regular graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$. Introduce a set of n isolated vertices $\{u_1, u_2, \ldots, u_n\}$ and make each u_i adjacent to the neighbors of v_i in G for every i. Then, introduce a set of k $(k \geq 0)$ isolated vertices and make all of them adjacent to all vertices of G. The resultant graph is denoted by $H_k(G)$.

Lemma 8.3. *Let G be a connected r-regular graph of order n, and let $H_k(G)$ be the graph obtained by the above operation. Then*

$$\mathscr{E}(H_k(G)) = \sqrt{5} \left(\mathscr{E}(G) - r + \sqrt{r^2 + \frac{4}{5} nk} \right). \tag{8.1}$$

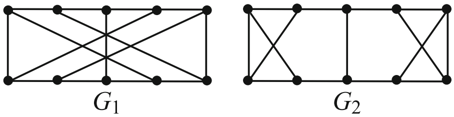

Fig. 8.3 The cubic graphs G_1 and G_2 used in the proof of Theorem 8.2

Proof. Let $\mathbf{A}$ be the adjacency matrix of G and $\mathbf{J}$ the all-one matrix. Then the adjacency matrix of $H_k(G)$ is given by

$$\begin{pmatrix} \mathbf{A} & \mathbf{A} & \mathbf{J}_{n\times k} \\ \mathbf{A} & 0 & 0 \\ \mathbf{J}_{k\times n} & 0 & 0 \end{pmatrix}.$$

Thus, the characteristic polynomial of $H_k(G)$ is

$$\begin{vmatrix} x\,\mathbf{I}-\mathbf{A} & -\mathbf{A} & -\mathbf{J}_{n\times k} \\ -\mathbf{A} & x\,\mathbf{I} & 0 \\ -\mathbf{J}_{k\times n} & 0 & x\,\mathbf{I}_k \end{vmatrix}.$$

According to Lemma 8.1,

$$\begin{aligned} \begin{vmatrix} x\,\mathbf{I}-\mathbf{A} & -\mathbf{A} & -\mathbf{J}_{n\times k} \\ -\mathbf{A} & x\,\mathbf{I} & 0 \\ -\mathbf{J}_{k\times n} & 0 & x\,\mathbf{I}_k \end{vmatrix} &= x^k \left| \begin{pmatrix} x\,\mathbf{I} & -\mathbf{A} \\ -\mathbf{A} & x\,\mathbf{I}-\mathbf{A} \end{pmatrix} - \begin{pmatrix} 0 \\ -\mathbf{J}_{n\times k} \end{pmatrix} \frac{\mathbf{I}_k}{x} \begin{pmatrix} 0 & -\mathbf{J}_{k\times n} \end{pmatrix} \right| \\ &= x^{k-2n} \begin{vmatrix} x^2\,\mathbf{I} & -\mathbf{A}\,x \\ -\mathbf{A}\,x & x^2\,\mathbf{I}-\mathbf{A}\,x-k\mathbf{J} \end{vmatrix} \\ &= x^k \left| x^2\,\mathbf{I}-\mathbf{A}\,x-k\mathbf{J}-\mathbf{A}^2 \right| \\ &\Longrightarrow x^k \prod_{i=1}^{n} [x^2-\lambda_i x-k\varphi(\lambda_i)-\lambda_i^2] = 0\,. \end{aligned}$$

Thus, we can characterize the spectrum of $H_k(G)$ as follows:

- $x = 0$ k times
- $x = \frac{1}{2}(r \pm \sqrt{5r^2+4nk})$
- $x = \frac{1}{2}(1 \pm \sqrt{5})\lambda_i\ ,\ i = 2, \ldots, n$

Therefore, Eq. (8.1) holds. ■

Proof of Theorem 8.2. For $n = 6, 14, 18$, by Theorem 8.1, we deduce that DC_ℓ and D_2C_ℓ ($\ell = 3, 7, 9$) are a pair of noncospectral equienergetic graphs.

The cubic graphs G_1 and G_2, as shown in Fig. 8.3, are a pair of noncospectral equienergetic graphs of order 10 due to Cvetković et al. [81]. Let $H_k(G_i)$ be the graph obtained from G_i, $i = 1, 2$ by the operation defined above. Then by Lemma 8.3, $H_k(G_1)$ and $H_k(G_2)$ are noncospectral equienergetic graphs of order $n = 20 + k$ $(k \geq 0)$. ■

The *join* $G_1 \vee G_2$ of two graphs G_1 and G_2 is the graph obtained by joining each vertex of G_1 with every vertex of G_2. We first investigate some basic properties of this product for regular graphs.

Lemma 8.4. [81] *Let G_i be an r_i-regular graph of order n_i, $i = 1, 2$. Then*

$$\phi(G_1 \vee G_2) = \frac{\phi(G_1)\,\phi(G_2)}{(x - r_1)(x - r_2)}\big[(x - r_1)(x - r_2) - n_1 n_2\big]. \qquad ■$$

Lemma 8.5. *Let G_i be an r_i-regular graph of order n_i, $i = 1, 2$. Then*

$$\mathscr{E}(G_1 \vee G_2) = \mathscr{E}(G_1) + \mathscr{E}(G_2) + \sqrt{(r_1 + r_2)^2 + 4(n_1 n_2 - r_1 r_2)} - (r_1 + r_2)\,.$$

Proof. According to Lemma 8.4,

$$(x - r_1)(x - r_2)\phi(G_1 \vee G_2) = \phi(G_1)\,\phi(G_2)\big((x - r_1)(x - r_2) - n_1 n_2\big)\,.$$

We use $P_1(x)$ and $P_2(x)$ to denote, respectively, the left-hand and the right-hand sides of the above equation. One can readily see that the sum of the absolute values of the roots of $P_1(x) = 0$ is $\mathscr{E}(G_1 \vee G_2) + r_1 + r_2$. Moreover, the roots of $P_2(x) = 0$ are the eigenvalues of G_1 and G_2 and $\frac{1}{2}\Big(r_1 + r_2 \pm \sqrt{(r_1 + r_2)^2 + 4(n_1 n_2 - r_1 r_2)}\Big)$. Therefore,

$$\mathscr{E}(G_1 \vee G_2) = \mathscr{E}(G_1) + \mathscr{E}(G_2) + \sqrt{(r_1 + r_2)^2 + 4(n_1 n_2 - r_1 r_2)} - (r_1 + r_2)$$

which completes the proof. ■

Ramane and Walikar [407] proved a stronger result concerning connected noncospectral equienergetic graphs stated below:

Theorem 8.3. *There exists a pair of connected noncospectral equienergetic n-vertex graphs for every $n \geq 9$.*

Proof. Consider the graphs H_1 and H_2 depicted in Fig. 4.1. From Example 4.1, $\mathscr{E}(H_1) = \mathscr{E}(H_2) = 16$. It is well known that $\phi(K_t, x) = (x - t + 1)(x + 1)^{t-1}$, and thus $\mathscr{E}(K_t) = 2(t - 1)$. Using Lemma 8.5, we have $\mathscr{E}(H_1 \vee K_t) = \mathscr{E}(H_2 \vee K_t) = t + 11 + \sqrt{(t + 3)^2 + 4(5t + 4)}$. Therefore, $H_1 \vee K_t$ and $H_2 \vee K_t$ are equienergetic. Moreover, $H_1 \vee K_t$ and $H_2 \vee K_t$ are noncospectral since H_1 and H_2 are noncospectral. Obviously, $H_1 \vee K_t$ and $H_2 \vee K_n$ are connected graphs. Hence, $H_1 \vee K_t$ and $H_2 \vee K_t$ are connected noncospectral equienergetic of order $n = 9 + t, t = 0, 1, \ldots$. ■

Let $L(G) = L^1(G)$ be the line graph of G. In addition, we recursively define $L^k(G) = L(L^{k-1}(G))$, $k = 2, 3, \ldots$, which are called *the iterated line graphs* of G.

If G is an r-regular graph of order n, size m, and degree $r \geq 3$, then the characteristic polynomials of G and $L^1(G)$ are related as follows [81]: $\phi(L^1(G), x) = (x+2)^{m-n}\phi(G, x-r+2)$. Thus, if $\mathrm{Spec}(G) = \{r, \lambda_2, \ldots, \lambda_n\}$, then $\mathrm{Spec}(L^1(G)) = \{r+r-2, \lambda_2+r-2, \ldots, \lambda_n+r-2, -2, \ldots, -2\}$ and $\mathrm{Spec}(L^2(G)) = \{2r-6, \ldots, 2r-6, r+3r-6, \lambda_2+3r-6, \ldots, \lambda_n+3r-6, -2, \ldots, -2\}$. Since the eigenvalues of any r-regular graph G obey the condition $|\lambda_i| \leq r$, we see that the only negative eigenvalues of $L^2(G)$ are those equal to -2, whose multiplicity is equal to $nr(r-2)/2$. Consequently, $\mathcal{E}(L^2(G)) = 2 \cdot 2 \cdot [nr(r-2)/2] = 2nr(r-2)$. In a similar manner, one can easily see that for any $k \geq 1$, $\mathcal{E}(L^{k+1}(G)) = 2n(r-2)\prod_{i=0}^{k-1}(2^i\, r - 2^{i+1} + 2)$, i.e., the energy of $L^{k+1}(G)$, $k \geq 1$, depends only on n and r. Hence, we obtain the following theorem [410]:

Theorem 8.4. *Let G_1 and G_2 be two noncospectral regular graphs of the same order and the same degree $r \geq 3$. Then for $k \geq 2$, the iterated line graphs $L^k(G_1)$ and $L^k(G_2)$ form a pair of noncospectral equienergetic graphs of the same order and the same size. If, in addition, G_1 and G_2 are chosen to be connected, then also $L^k(G_1)$ and $L^k(G_2)$ are connected.* ■

Let G_1 and G_2 be two r-regular graphs of order n with $r \geq 3$. From [403], we know that $\overline{L^2(G_1)}$ and $\overline{L^2(G_2)}$ are also equienergetic, and $\mathcal{E}(\overline{L^2(G_1)}) = \mathcal{E}(\overline{L^2(G_2)}) = (nr-4)(2r-3)-2$, where $\overline{G}$ denotes the complement of the graph G.

Let G be a simple graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The extended double cover of G, denoted by G^*, is the bipartite graph with bipartition (X, Y) where $X = \{x_1, x_2, \ldots, x_n\}$ and $Y = \{y_1, y_2, \ldots, y_n\}$, in which x_i and y_j are adjacent if and only if either $i = j$ or v_i and v_j are adjacent in G. Further, G^* is regular of degree $r+1$ if and only if G is regular of degree r. Then we have:

Theorem 8.5 [496]. *Let G_1, G_2 be two r-regular graphs of order n with $r \geq 3$. Then:*

(i) $(L^2(G_1))^*$ *and* $(L^2(G_2))^*$ *are equienergetic bipartite graphs, and*

$$\mathcal{E}((L^2(G_1))^*) = \mathcal{E}((L^2(G_2))^*) = nr(3r-5)\,.$$

(ii) $(\overline{L^2(G_1)})^*$ *and* $(\overline{L^2(G_2)})^*$ *are equienergetic bipartite graphs, and*

$$\mathcal{E}((\overline{L^2(G_1)})^*) = \mathcal{E}((\overline{L^2(G_2)})^*) = (5nr-16)(r-2)+nr-8\,.$$

(iii) $\overline{(L^2(G_1))^*}$ *and* $\overline{(L^2(G_2))^*}$ *are equienergetic bipartite graphs, and*

$$\mathcal{E}(\overline{(L^2(G_1))^*}) = \mathcal{E}(\overline{(L^2(G_2))^*}) = (2nr-4)(2r-3)-2\,.$$ ■

The authors of [311] were interested in constructing pairs of equienergetic graphs, such that one is a subgraph of the other, i.e., the energy of a graph is the same as the energy of a subgraph obtained by deleting some of its edges. Formally, we have the following problem:

Problem 8.1. Characterize graph G and a subset F of $E(G)$ such that $\mathscr{E}(G) = \mathscr{E}(G - F)$. ■

Example 8.1. Let F consist of two independent edges of the cycle C_4. Then F is an edge cut of C_4 and $\mathscr{E}(C_4) = \mathscr{E}(C_4 - F) = 4$.

Example 8.2. Let G be a simple graph obtained by deleting two independent edges from the complete graph K_5. Then the cycle C_5 is an equienergetic subgraph of G. Note that $\mathscr{E}(G) = 2 + 2\sqrt{5} = \mathscr{E}(C_5)$ and $C_5 = G - F$, where F is not an edge cut.

For $n \geq 2$ and $1 \leq s, r \leq n$, define $KK(n, s, r)$ as a simple connected graph with two copies of complete graph K_n connected via a vertex in the middle. The left complete graph is joined to the middle vertex with s edges, and the right complete graph is joined to the middle vertex with r edges. Hence, $KK(n, s, r)$ has $2n + 1$ vertices and $n^2 - n + s + r$ edges. Li and So [311] proved the following results:

Theorem 8.6. *Suppose that G is a simple graph with an edge cut F such that*

$$\mathbf{A}(G) = \begin{pmatrix} \mathbf{J}_n - \mathbf{I}_n & \mathbf{X} \\ \mathbf{X}^{\mathrm{T}} & \mathbf{J}_m - \mathbf{I}_m \end{pmatrix} \quad \text{and} \quad \mathbf{A}(G - F) = \begin{pmatrix} \mathbf{J}_n - \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_m - \mathbf{I}_m \end{pmatrix}.$$

Then $\mathscr{E}(G) = \mathscr{E}(G - F)$ if and only if (i) $n = m$ and (ii) $X = \mathbf{I}_n$ or $X = \mathbf{J}_n - \mathbf{I}_n$. ■

Theorem 8.7. *For $n \geq 2$ and $1 \leq r, s \leq n$, $\mathscr{E}(KK(n, s, r)) = \mathscr{E}(KK(n, s, r - 1))$ if and only if $n < 2r$, $s^2 + r^2 < (n - 1)(s + r)$ and $s^2 - (2r - 1)s + 2n^2 r - 8nr^2 + 8r^3 - n^2 + 6nr - 9r^2 - n + 3r = 0$.* ■

Corollary 8.1. *Let $s = n$. Then $\mathscr{E}(KK(n, s, r)) = \mathscr{E}(KK(n, s, r - 1))$ if and only if $n = s = 4k^2 - 9k + 6$ and $r = 2k^2 - 4k + 3$ for $k \geq 3$.* ■

Corollary 8.2. *Let $s = 1$. Then $\mathscr{E}(KK(n, 1, r)) = \mathscr{E}(KK(n, 1, r - 1))$ if and only if $n = 4$ and $r = 3$.* ■

8.3 Equienergetic Trees

Very little theoretical results are known for noncospectral equienergetic trees. By means of a computer search, it was shown that there are numerous pairs of noncospectral equienergetic trees [47]. Some of these are depicted in Fig. 8.4.

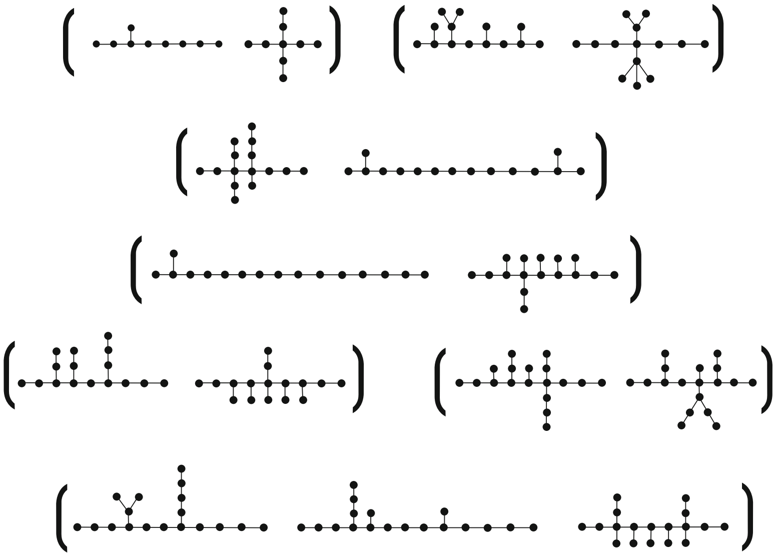

Fig. 8.4 Equienergetic trees [47]. Of the three 18-vertex trees at the bottom of this figure, the first two are cospectral but not cospectral with the third tree

Numerical calculations, no matter how accurate they are, cannot be considered as a proof that two graphs are equienergetic. In the case of equienergetic trees, this problem can, sometimes, be overcome as in the following example.

Consider the trees T_A, T_B, and T_C depicted at the bottom of Fig. 8.4. Using standard recursive methods [81, 216], one computes their characteristic polynomials as

$$\phi(T_A) = x^{18} - 17\,x^{16} + 117\,x^{14} - 421\,x^{12} + 853\,x^{10} - 973\,x^8 + 588\,x^6 - 164\,x^4 + 16\,x^2$$

$$\phi(T_B) = x^{18} - 17\,x^{16} + 117\,x^{14} - 421\,x^{12} + 853\,x^{10} - 973\,x^8 + 588\,x^6 - 164\,x^4 + 16\,x^2$$

$$\phi(T_C) = x^{18} - 17\,x^{16} + 111\,x^{14} - 359\,x^{12} + 632\,x^{10} - 632\,x^8 + 359\,x^6 - 111\,x^4 + 17\,x^2 - 1\,.$$

The trees T_A and T_B have identical characteristic polynomials and, consequently, they are cospectral. The characteristic polynomial of T_C is different, implying that T_C is not cospectral with T_A and T_B.

Now, if we are lucky, the above characteristic polynomials can be factored. In this particular case, we are lucky, and by easy calculation, we find that

$$\phi(T_A) = x^2\,(x^2-1)(x^2-2)^2\,(x^2-4)(x^4-3\,x^2+1)(x^4-5\,x^2+1)$$
$$\phi(T_C) = (x^2-1)^3\,(x^4-3\,x^2+1)(x^4-5\,x^2+1)(x^4-6\,x^2+1)\,.$$

It is now an elementary exercise in algebra to verify that $E(T_A) = E(T_B) = E(T_C) = 6 + 4\sqrt{2} + 2\sqrt{5} + 2\sqrt{7}$.

If, however, the characteristic polynomials cannot be properly factored, then at the present time, there is no way to prove that the underlying trees are equienergetic. Note that until now, no general method (different from computer search) for finding equienergetic trees has been discovered. More results on equienergetic trees can be found in [374].

We conclude this chapter by (re)stating some of the major open problems related to equienergetic trees.

Open Problems

1. Suppose that by numerical calculation we find that (up to the accuracy of the calculation) two noncospectral graphs G' and G'' have equal energies. In the general case, the eigenvalues of these graphs cannot be expressed in radicals. How to prove (mathematically) that G' and G'' are equienergetic?
2. If two noncospectral graphs are equienergetic, which structural features they have in common?
3. Construct pairs (or larger families) of noncospectral equienergetic trees with equal number of vertices by a method different from trial-and-error computer search.
4. Suppose that two graphs G' and G'' with equal number n of vertices have different energies. How small the difference $|\mathscr{E}(G') - \mathscr{E}(G'')|$ can be? Find a lower bound (possibly as function of n) for $|\mathscr{E}(G') - \mathscr{E}(G'')|$. (Recall that trees were discovered [374] for which this difference is remarkably small.)

Chapter 9
Hypoenergetic and Strongly Hypoenergetic Graphs

A graph on n vertices, whose energy is less than n, i.e., $\mathcal{E}(G) < n$, is said to be *hypoenergetic*. Graphs for which $\mathcal{E}(G) \geq n$ are said to be *nonhypoenergetic*. In [441], a *strongly hypoenergetic* graph is defined to be a (connected) graph G of order n satisfying $\mathcal{E}(G) < n - 1$. In what follows, for obvious reasons, we assume that all graphs considered are connected.

For a survey on hypoenergetic graphs, see [178].

In the chemical literature it has been noticed long time ago that for the vast majority of (molecular) graphs, the energy exceeds the number of vertices. In 1973 the theoretical chemists England and Ruedenberg published a paper [106] 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."

9.1 Some Nonhypoenergetic Graphs

Recall that in connection with the chemical applications of $\mathcal{E}$, a "molecular graph" means a connected graph in which there are no vertices of degree greater than three [216]. The authors of [106] were, indeed, quite close to the truth. Today, we know that only five such graphs violate the relation $\mathcal{E}(G) \geq n$; see below. On the other hand, there are large classes of graphs for which the condition $\mathcal{E}(G) \geq n$ is satisfied. We first mention some elementary results of this kind. For more results, we refer to [3, 197, 362, 363].

Theorem 9.1. *If the graph G is nonsingular (i.e., no eigenvalue of G is equal to zero), then G is nonhypoenergetic.*

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_9,

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

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

The determinant of the adjacency matrix is necessarily an integer. Because G is nonsingular, $|\det A(G)| \geq 1$. Therefore, also $|\det A(G)|^{1/n} \geq 1$, implying $\mathscr{E}(G) \geq n$. ■

From Theorem 5.2, we know that for any graph G, $\mathscr{E}(G) \geq 2\sqrt{m}$, from which follows:

Theorem 9.2. *If G is a graph with n vertices and m edges and if $m \geq n^2/4$, then G is nonhypoenergetic.* ■

Theorem 9.3. *If the graph G is regular of any nonzero degree, then G is nonhypoenergetic.*

Proof. Let λ_1 be the greatest graph eigenvalue. Then $\lambda_1|\lambda_i| \geq \lambda_i^2$ holds for $i = 1, 2, \ldots, n$, which summed overall i yields $\mathscr{E}(G) \geq 2m/\lambda_1$. For a regular graph of degree r, $\lambda_1 = r$ and $2m = nr$. ■

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

Theorem 9.4. [177] *All hexagonal systems are nonhypoenergetic.* ■

There are reasons to believe (cf. Theorem 5.24) that there are few hypoenergetic graphs.

9.2 Hypoenergetic and Strongly Hypoenergetic Trees

We first outline the results for hypoenergetic trees and then in the second subsection, turn our attention to the strongly hypoenergetic species.

9.2.1 Hypoenergetic Trees

Our first computer-aided and chemistry-related studies of hypoenergetic graphs were communicated in the paper [218]. Soon thereafter [199], it was shown that there exist hypoenergetic trees for any number of vertices and any value of the maximum vertex degree Δ, except for the case of $\Delta = 4$ and $n \equiv 2 \pmod 4$. Eventually, that such trees exist also for $n \equiv 2 \pmod 4$, $n > 2$ was demonstrated by Li and Ma [336] and, independently, by Liu and Liu [352].

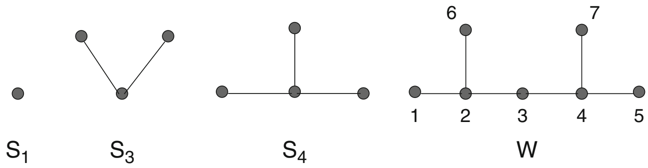

Fig. 9.1 The hypoenergetic trees with maximum vertex degree not exceeding 3

Let T denote a tree of order n and maximum degree Δ. Then of course, $n \geq \Delta + 1$. For $\Delta \leq 2$, the situation with regard to hypoenergeticity is simple: If $\Delta = 0$, then there exists a single one-vertex tree whose energy is equal to zero. This tree is, in a trivial manner, hypoenergetic. If $\Delta = 1$, then there exists a single two-vertex tree whose energy is equal to two. This tree is not hypoenergetic. For each value of n , $n \geq 3$, there exists a unique n-vertex tree with $\Delta = 2$, the path P_n whose energy is well known (see Sect. 4.1). Only P_3 is hypoenergetic.

Theorem 9.5. *(a) There exist hypoenergetic trees of order n with maximum degree* $\Delta \leq 3$ *only for* $n = 1, 3, 4, 7$ *(a single such tree for each value of n, see Fig. 9.1); (b) If* $\Delta \geq 4$*, then there exist hypoenergetic trees for all* $n \geq \Delta + 1$. ∎

The theorem will be proven in the sequel by means of three lemmas.

The nullity (= multiplicity of zero in the spectrum) of T will be denoted by n_0. For any graph G with n vertices and m edges, an upper bound for the energy is $\mathscr{E}(G) \leq \sqrt{2mn}$, cf. Theorem 5.1. Theorem 4.5 provides a simple improvement of this bound: $\mathscr{E}(G) \leq \sqrt{2m(n-n_0)}$. For a tree T of order n and nullity n_0,

$$\mathscr{E}(T) \leq \sqrt{2(n-1)(n-n_0)}. \tag{9.1}$$

Equality in Ineq. (9.1) is attained if and only if T is the n-vertex star. For $n \geq 3$, the n-vertex star is hypoenergetic. Therefore, in what follows, without loss of generality, we may assume that T is not the star, in which case the inequality in Ineq. (9.1) is strict. Now, if

$$\sqrt{2(n-1)(n-n_0)} \leq n \tag{9.2}$$

then the tree T will necessarily be hypoenergetic. Condition (9.2) can be rewritten as

$$n_0 \geq \frac{n(n-2)}{2(n-1)}. \tag{9.3}$$

Fiorini et al. [116] proved that the maximum nullity of a tree with given values of n and maximum vertex degree Δ is

$$n - 2\left\lceil \frac{n-1}{\Delta} \right\rceil \tag{9.4}$$

and showed how trees with such nullity can be constructed.

Combining Ineqs. (9.3) and (9.4), we arrive at the condition

$$n - 2\left\lceil \frac{n-1}{\Delta} \right\rceil \geq \frac{n(n-2)}{2(n-1)} \tag{9.5}$$

which, if satisfied, implies the existence of at least one hypoenergetic tree with n vertices and maximum degree Δ. Finding the solutions of Ineq. (9.5) is elementary, and we only sketch the reasoning that leads to the following:

Lemma 9.1. *(a) If $\Delta = 3$, then there exist hypoenergetic trees for $n = 4$ and $n = 7$. (b) If $\Delta = 4$, then there exist hypoenergetic trees for all $n \geq 5$, such that $n \equiv k \pmod 4$, $k = 0, 1, 3$. (c) If $\Delta \geq 5$, then there exist hypoenergetic trees for all $n \geq \Delta + 1$.*

Proof. We first observe that

$$\left\lceil \frac{n-1}{\Delta} \right\rceil = \begin{cases} n/\Delta & \text{if } n \equiv 0 \pmod \Delta \\ (n-1)/\Delta & \text{if } n \equiv 1 \pmod \Delta \\ (n-k)/\Delta + 1 & \text{if } n \equiv k \pmod \Delta\ ,\ k = 2, 3, \ldots, \Delta - 1 \end{cases} \tag{9.6}$$

by means of which Ineq. (9.5) is transformed into

$$n^2 - \frac{4n(n-1)}{\Delta} \geq 0 \qquad \text{if } n \equiv 0 \pmod \Delta \tag{9.7}$$

$$n^2 - \frac{4(n-1)^2}{\Delta} \geq 0 \qquad \text{if } n \equiv 1 \pmod \Delta \tag{9.8}$$

$$n^2 - 4(n-1)\left(\frac{n-k}{\Delta} + 1\right) \geq 0 \quad \text{if } n \equiv k \pmod \Delta\ ,\ k = 2, 3, \ldots, \Delta - 1 \tag{9.9}$$

Setting $\Delta = 3$ into the above relations, it is elementary to verify that Ineq. (9.7) is satisfied only for $n = 3$ and Ineq. (9.8) only for $n = 1, 4, 7$, whereas Ineq. (9.9) only for $n = 2$. This implies part (a) of the lemma.

Assume now that $\Delta \geq 4$ and first consider the case $n \equiv 2 \pmod \Delta$. Then Ineq. (9.9) is applicable (for $k = 2$) and is transformed into $(n-2)\,[(\Delta - 4)(n-2) - 4] \geq 0$. This inequality is evidently satisfied for $n = 2$. If $n > 2$, then we arrive at $(\Delta - 4)(n-2) - 4 \geq 0$, which does not hold for $\Delta = 4$ but holds for $\Delta > 4$.

If $n \equiv 0 \pmod \Delta$ and $n \equiv 1 \pmod \Delta$, then Ineqs. (9.7) and (9.8) are transformed into

$$n(\Delta - 4) + 4 \geq 0 \qquad \text{and} \qquad n^2\,(\Delta - 4) + 8n - 4 \geq 0$$

respectively, which are obeyed by all n. If $\Delta = 4$ and $n \equiv 3 \pmod 4$, then Ineq. (9.9) holds for all respective values of n. By this, we arrive at part (b) of the lemma.

It remains to verify that for $\Delta \geq 5$ and $3 \leq k \leq \Delta - 1$, the relation (9.9) is always satisfied. In order to do this, rewrite Ineq. (9.9) as $(\Delta - 4)\, n^2 - 4(\Delta - k - 1)\, n + 4(\Delta - k) \geq 0$, in which case the left-hand side is a quadratic polynomial in variable n. Its value will be nonnegative if the discriminant $D = [-4(\Delta - k - 1)]^2 - 16(\Delta - 4)(\Delta - k)$ is nonpositive. Now, D is a quadratic polynomial in variable k. For both $k = 3$ and $k = \Delta - 1$, $D = -16\,(\Delta - 4)$, implying that the value of D is negative for all k , $3 \leq k \leq \Delta - 1$.

By this, the proof has been completed. ■

In what follows, we prove that hypoenergetic trees with $\Delta = 3$ exist only for $n = 4$ and $n = 7$ (a single such tree for each such n). Let S_n denote the star on n vertices and W the 7-vertex tree, obtained from P_5 by adding a pendent vertex to the second vertex and to the fourth vertex, respectively. The tree W is depicted in Fig. 9.1, where also the numbering of its vertices is indicated.

By computer search, it was shown [218] that among trees with maximum degree at most 3 and order at most 22, S_1, S_3, S_4 and W are the only hypoenergetic trees.

Lemma 9.2. *There are no hypoenergetic trees with maximum degree at most* 3*, except* S_1*,* S_3*,* S_4 *and* W*.*

Proof. As mentioned above, by checking all trees with n vertices, $n \leq 22$, and maximum degree at most 3, it was found that S_1, S_3, S_4 and W are the only hypoenergetic trees of order at most 22.

Our proof is based on the following observation. From Corollary 4.6, we know that the energy will strictly decrease by deleting edges from a tree. By deleting k edges, $e_1, \ldots, e_k$, $k \geq 1$, from a tree T, it will be decomposed into $k+1$ connected components $T_1, T_2, \ldots, T_{k+1}$, each being a tree. If none of these components are hypoenergetic, i.e., if $\mathscr{E}(T_i) \geq n(T_i)$ for all $i = 1, 2, \ldots, k+1$, then

$$\begin{aligned} \mathscr{E}(T) > \mathscr{E}(T - e_1 - \cdots - e_k) &= \mathscr{E}(T_1) + \mathscr{E}(T_2) + \cdots + \mathscr{E}(T_{k+1}) \\ &\geq n(T_1) + n(T_2) + \cdots + n(T_{k+1}) = n(T) \end{aligned} \tag{9.10}$$

and, consequently, T is also not hypoenergetic.

Now, we divide the trees with the maximum degree at most 3 into two classes:

Class 1 contains the trees T that have an edge e, such that $T - e \cong T' \cup T''$ and $T', T'' \ncong S_1, S_3, S_4, W$.

Class 2 contains the trees T in which there exists no edge e, such that $T - e \cong T' \cup T''$ and $T', T'' \ncong S_1, S_3, S_4, W$, i.e., for any edge e of T, at least one of T' or T'' is isomorphic to a tree in $\{S_1, S_3, S_4, W\}$.

Then we distinguish between the following two cases and proceed by induction on the number n of vertices.

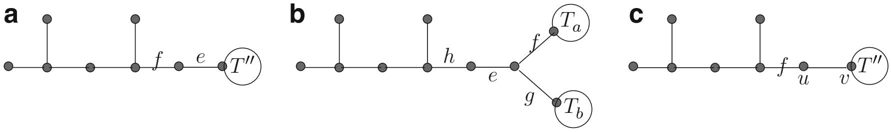

Fig. 9.2 Explanation of the notation used in the proof of Lemma 9.2

Case 1. The tree T belongs to Class 2. Consider the center of T. There are two subcases: either T has a (unique) center edge e or a (unique) center vertex v.

Subcase 1.1. T has a center edge e. The two fragments attached to e will be denoted by T' and T''. If so, then consider $T - e \cong T' \cup T''$.

Subsubcase 1.1.1. T' is isomorphic to a tree in $\{S_1, S_3, S_4, W\}$, and if $T' \cong W$, then it is attached to the center edge e through the vertex 3 but not through a pendent vertex (these are vertices $1, 5, 6, 7$; see Fig. 9.1). Then it is easy to see that the order of T is at most 14. Hence, if T is not isomorphic to an element of $\{S_1, S_3, S_4, W\}$, then T is not hypoenergetic.

Subsubcase 1.1.2. W is attached to the center edge e through a pendent vertex. Then we need to distinguish between the situations shown in Fig. 9.2.

If the other end vertex of the center edge e is of degree 2 (see diagram A in Fig. 9.2), then T'' has at least 5 and at most 16 vertices. Consequently, T has at least 12 and at most 23 vertices. If the number of vertices is between 12 and 22, we know that T is not hypoenergetic. If $n = 23$, then by deleting the edge f from T, we get a 6-vertex and a 17-vertex fragment, neither of which being hypoenergetic. Then T is not hypoenergetic because of Ineq. (9.10).

If the other end vertex of the center edge e is of degree 3, then the structure of the tree T is as shown in diagram B in Fig. 9.2. Each fragment T_a, T_b must have at least 4 and at most 15 vertices. If neither $T_a \cong W$ nor $T_b \cong W$, then the subgraph $T - f - g$ consists of three components, each having not more than 15 vertices, none of which being hypoenergetic. Then $\mathscr{E}(T - f - g) > n$ and we are done. If $T_a \cong W$, but $T_b \ncong W$, then we have to delete the edges g and h, resulting, again, in three nonhypoenergetic fragments. Finally, if both $T_a, T_b \cong W$, then T has 22 vertices and is thus not hypoenergetic.

Subcase 1.2. T has a center vertex v. If v is of degree two, then the two fragments attached to it will be denoted by T' and T''. If v is of degree three, then the three fragments attached to it will be denoted by T', T'', and T'''.

Subsubcase 1.2.1. T' is isomorphic to a tree in $\{S_1, S_3, S_4, W\}$. If $T' \cong W$, then it is attached to the center vertex v through the vertex 3 but not through a pendent vertex. Then it is easy to see that the order of T is at most 22. Hence, if T is not isomorphic to an element of $\{S_1, S_3, S_4, W\}$, then T is not hypoenergetic.

Subsubcase 1.2.2. W is attached to the center vertex v through a pendent vertex, as shown in diagram C in Fig. 9.2. Since T belongs to Class 2, by deleting the edge f, we see that $T'' \cup uv$ is isomorphic to a tree in $\{S_1, S_3, S_4, W\}$, which contradicts to the fact that v is the center vertex of T.

Case 2. The tree T belongs to Class 1. For the first few values of n, this is confirmed by direct calculation. Then by the induction hypothesis, assuming that $\mathscr{E}(T') \geq n(T')$ and $\mathscr{E}(T'') \geq n(T'')$ from $\mathscr{E}(T) > \mathscr{E}(T-e) = \mathscr{E}(T') + \mathscr{E}(T'') \geq n(T') + n(T'') = n(T)$, we conclude that also $\mathscr{E}(T) > n(T)$.

By this, all possible cases have been exhausted, and the proof is complete. ■

From Lemmas 9.1 and 9.2, one easily obtains Theorem 9.5 except for the case of $\Delta = 4$ and $n \equiv 2 \pmod 4$.

Lemma 9.3. *There exist n-vertex hypoenergetic trees with $\Delta = 4$ for any $n \equiv 2 \pmod 4$, $n > 2$.*

Proof. Suppose that $n \equiv 2 \pmod 4$, $n > 2$. If $n = 6$, then from Table 2 of [81] (Table 2), we see that there exists a unique tree (denoted by T_6) of order 6 with $\Delta = 4$ and $\mathscr{E}(T_6) = 5.818 < 6$, i.e., T_6 is hypoenergetic. Let S_5 be the 5-vertex star. Then $\Delta(S_5) = 4$ and $\mathscr{E}(S_5) = 4$. Let u be a leaf vertex in T_6 and v be a leaf vertex in S_5. Then by Theorem 4.18, for the coalescence $T_{10} = T_6 \circ S_5$ of T_6 and S_5 with respect to u and v, we have $\mathscr{E}(T_{10}) < 10$. Obviously, T_{10} is a tree of order 10 with $\Delta = 4$. By consecutively doing the coalescence operations $(\cdots((T_6 \circ S_5) \circ S_5)\cdots) \circ S_5$, we can construct hypoenergetic trees with $\Delta = 4$ for any $n \geq 10$ such that $n \equiv 2 \pmod 4$. ■

Proof of Theorem 9.5. Combine Lemmas 9.1–9.3. ■

9.2.2 *Strongly Hypoenergetic Trees*

In the previous subsection, we discussed the existence of hypoenergetic trees. Now, we establish the existence of strongly hypoenergetic trees, following the work of Li and Ma [337].

In order to state our result, we use the notion of complete d-ary trees (see Fig. 7.1) and the definition of $T^*_{n,d}$ (see Definition 7.1). Let $\mathscr{T}_{n,d}$ be the set of all trees with n vertices and maximum degree at most $d+1$. We will use Theorem 7.2 to obtain strongly hypoenergetic trees with $\Delta = 4$.

By Theorem 9.5, we know that the only hypoenergetic trees with maximum degree at most 3 are S_1, S_3, S_4 and W. Then from Table 2 of [81], we have that $\mathscr{E}(S_1) = 0$, $\mathscr{E}(S_3) = 2.828$, $\mathscr{E}(S_4) = 3.464$, and $\mathscr{E}(W) = 6.828$. Thus, we arrive at:

Theorem 9.6. *There do not exist any strongly hypoenergetic trees with maximum degree at most* 3. ■

For trees with maximum degree at least 4, we have the following results:

Lemma 9.4. *(1) If $\Delta = 4$, then there exist n-vertex strongly hypoenergetic trees for all $n > 5$ such that $n \equiv 1 \pmod 4$; (2) If $\Delta = 5$, then there exist n-vertex strongly hypoenergetic trees for $n = 6$ and all $n \geq 9$, but there do not exist any strongly hypoenergetic trees for $n = 7$ and 8; (3) If $\Delta \geq 6$, then there exist n-vertex strongly hypoenergetic trees for all $n \geq \Delta + 1$.*

Proof. The first half of the proof is similar to that of Lemma 9.1. Let T be a tree of order n. By Ineq. (9.1), $\mathscr{E}(T) \leq \sqrt{2(n-1)(n-n_0)}$, and equality holds if and only if T is the n-vertex star S_n. Note that $\mathscr{E}(S_n) = 2\sqrt{n-1} < n-1$ for $n > 5$ and $\mathscr{E}(S_5) = 4 = n-1$, i.e., S_n is strongly hypoenergetic for $n > 5$. Therefore, in what follows, without loss of generality, we may assume that T is not a star, which implies that the inequality in (9.1) is strict. Now, if $\sqrt{2(n-1)(n-n_0)} \leq n-1$ or, equivalently,

$$n_0 \geq \frac{n+1}{2} \tag{9.11}$$

then the tree T will necessarily be strongly hypoenergetic.

Combining Ineqs. (9.11) and (9.4), we arrive at the condition

$$n - 2\left\lceil \frac{n-1}{\Delta} \right\rceil \geq \frac{n+1}{2}$$

or, equivalently,

$$\left\lceil \frac{n-1}{\Delta} \right\rceil \leq \frac{n-1}{4} \tag{9.12}$$

which, if satisfied, implies the existence of at least one strongly hypoenergetic tree with n vertices and maximum degree Δ.

Similarly, by observing Eq. (9.6), we get that in the case $n \equiv 1 \pmod{\Delta}$, Ineq. (9.12) holds for all $\Delta \geq 4$.

If $n \equiv 0 \pmod{\Delta}$, then Ineq. (9.12) is transformed into $(\Delta-4)n - \Delta \geq 0$, which is always valid for all $n \geq \Delta \geq 5$.

Consider now the case $n \equiv k \pmod{\Delta}$, $k = 2, 3, \ldots, \Delta - 1$. Since T is a tree, we only need to consider $n \geq \Delta + k$. Then Ineq. (9.12) is transformed into

$$\frac{n-k}{\Delta} \leq \frac{n-5}{4}. \tag{9.13}$$

If $\Delta \geq 7$, then $(n-k)/\Delta \leq (n-2)/7$, and it is easy to check that the inequality $(n-2)/7 \leq (n-5)/4$ holds for all $n \geq 9$.

If $\Delta = 6$, then $(n-k)/\Delta \leq (n-2)/6$, and it is easy to check that the inequality $(n-2)/6 \leq (n-5)/4$ holds for all $n \geq 11$. For $n = 9$ or $n = 10$, we have $n = \Delta + k$, and therefore Ineq. (9.13) also holds. Although Ineq. (9.13) does not hold for $n = 8$, we know that there exists a unique tree of order 8 with $\Delta = 6$. The energy of this tree is 6.774 (see Table 2 in [81]), which is less than $n - 1 = 7$.

Suppose that $\Delta = 5$. If $k = 4$, then $(n-k)/\Delta = (n-4)/5$, and it is easy to check that the inequality $(n-4)/5 \leq (n-5)/4$ holds for all $n \geq 9$. If $k = 3$, then

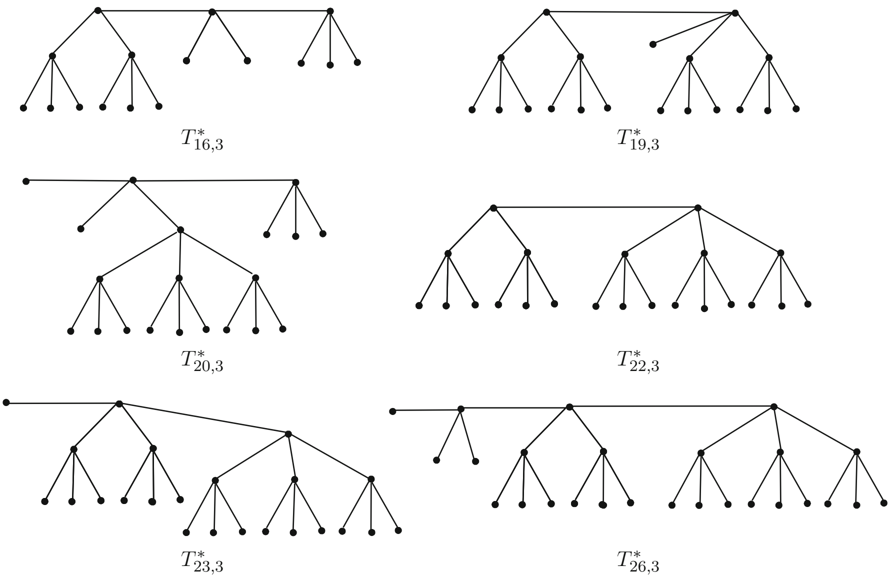

Fig. 9.3 The trees $T^*_{n,3}$ for $n = 16, 19, 20, 22, 23$, and 26

$(n-k)/\Delta = (n-3)/5$, and the inequality $(n-3)/5 \leq (n-5)/4$ holds for all $n \geq 13$. From Table 2 of [81], there are three trees of order 8 and with $\Delta = 5$, whose energies are 7.114, 7.212, and 8.152. Hence, there do not exist any strongly hypoenergetic trees of order $n = 8$ with $\Delta = 5$. If $k = 2$, then $(n-k)/\Delta = (n-2)/5$, and it is easy to check that the inequality $(n-2)/5 \leq (n-5)/4$ holds for all $n \geq 17$. From Table 2 of [81], we see that there exists a unique tree of order 7 with $\Delta = 5$. Its energy is 6.324, which is to say that the tree is not strongly hypoenergetic. Finally, we construct a strongly hypoenergetic tree of order 12 with $\Delta = 5$. As stated above, there exists a tree, denoted by T_{11}, of order 11 with $\Delta = 5$, and its nullity is $n_0 = n - 2\lceil (n-1)/\Delta \rceil = 11 - 2\lceil (10)/5 \rceil = 7$. Then by Ineq. (9.1), $\mathscr{E}(T_{11}) \leq \sqrt{2(n-1)(n-n_0)} = \sqrt{2(11-1)(11-7)} < 9$. Let T_2 be the tree of order 2, $v \in V(T_2)$, and u a leaf vertex in T_{11}. Clearly, $\mathscr{E}(T_2) = 2$. Let $T_{11} \circ T_2$ be the coalescence of T_{11} and T_2 with respect to u and v. Thus, by Theorem 4.18, $\mathscr{E}(T_{11} \circ T_2) \leq \mathscr{E}(T_{11}) + \mathscr{E}(T_2) < 9 + 2 = 11$. Obviously, $T_{11} \circ T_2$ is a tree of order 12 with maximum degree 5, and so it is a desired tree. The proof is now complete. ∎

In the following, we consider strongly hypoenergetic trees for the remaining case $\Delta = 4$ and $n \equiv k \pmod 4$, $k = 0, 2, 3$. From Table 2 of [81], we conclude that there does not exist any strongly hypoenergetic tree with $\Delta = 4$ for $n = 6, 7, 8$. By Theorem 7.2, $T^*_{n,3}$ is the unique tree in $\mathscr{T}_{n,3}$ that minimizes the energy. Obviously, $\Delta(T^*_{n,3}) = 4$. Trees $T^*_{16,3}$, $T^*_{19,3}$, $T^*_{20,3}$, $T^*_{22,3}$, $T^*_{23,3}$, and $T^*_{26,3}$ are shown in Fig. 9.3. From Table 9.1, we know that there do not exist any strongly hypoenergetic tree with $\Delta = 4$ for $n = 10, 11, 12, 14, 15, 16, 18, 19, 22$ and that $T^*_{20,3}$, $T^*_{23,3}$, and $T^*_{26,3}$ are strongly hypoenergetic.

Table 9.1 The energy of $T^*_{n,3}$

n	$\mathscr{E}(T^*_{n,3})$	n	$\mathscr{E}(T^*_{n,3})$	n	$\mathscr{E}(T^*_{n,3})$
10	9.61686	11	10.36308	12	11.13490
14	13.39786	15	14.26512	16	15.01712
18	17.24606	19	18.13157	20	18.86727
22	21.06862	23	21.96975		
26	24.87008				

Then starting from the strongly hypoenergetic trees $T^* = T^*_{20,3}$, $T^*_{23,3}$, and $T^*_{26,3}$, we do the coalescence operation of T^* and the 5-vertex star S_5 at a leaf of each of the two trees. Like in the proof of Lemma 9.3, $T^* \circ S_5$ is strongly hypoenergetic, which follows from Theorem 4.18 and the fact that $\mathscr{E}(S_5) = 4$ and T^* is strongly hypoenergetic. By consecutively doing the coalescence operation $(\cdots((T^* \circ S_5) \circ S_5)\cdots) \circ S_5$, we get

Lemma 9.5. *If $\Delta = 4$, then there exist n-vertex strongly hypoenergetic trees for all n such that $n \equiv 0 \pmod 4$ and $n \geq 20$ or $n \equiv 2 \pmod 4$ and $n \geq 26$ or $n \equiv 3 \pmod 4$ and $n \geq 23$.* ■

Hence, the result (1) of Lemma 9.4 can now be extended as follows:

Corollary 9.1. *Suppose that $\Delta = 4$ and $n \geq 5$. Then there exist n-vertex strongly hypoenergetic trees only for $n = 9, 13, 17, 20, 21$ and $n \geq 23$.* ■

Combining Lemma 9.4 and Corollary 9.1, we finally arrive at:

Theorem 9.7. *(1) If $\Delta = 4$ and $n \geq 5$, then there exist n-vertex strongly hypoenergetic trees only for $n = 9, 13, 17, 20, 21$ and $n \geq 23$. (2) If $\Delta = 5$, then there exist n-vertex strongly hypoenergetic trees for $n = 6$ and all $n \geq 9$, but there do not exist any strongly hypoenergetic trees for $n = 7$ and 8. (3) If $\Delta \geq 6$, then there exist n-vertex strongly hypoenergetic trees for all $n \geq \Delta + 1$.* ■

Remark 9.1. Nonhypoenergetic biregular trees, unicyclic, and bicyclic graphs were investigated by Majstorović et al. [363] (see also [197]). Triregular graphs of this kind were considered by Majstorović et al. [363] (see also [361, 362]) and Li et al. [328] (see also [494]).

9.3 Hypoenergetic and Strongly Hypoenergetic k-Cyclic Graphs

You and Liu [507] proved the existence of hypoenergetic unicyclic and bicyclic graphs with large maximum degrees. They did not discuss the case of such graphs with small maximum degrees. Later, You et al. [508] established the existence of

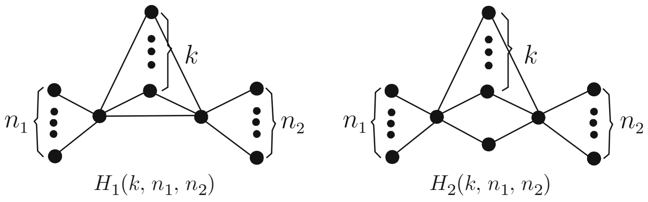

Fig. 9.4 The graphs $H_1(k,n_1,n_2)$ and $H_2(k,n_1,n_2)$

hypoenergetic k-cyclic graphs. Li and Ma [336], followed by Hui and Deng [276], obtained then more general results on hypoenergetic and strongly hypoenergetic k-cyclic graphs, which are outlined in this section.

The following results [43, 59, 83] are needed in the sequel. Let, as before, $n_0(G)$ denote the number of zero eigenvalues in the spectrum of the graph G:

Lemma 9.6. *Suppose that G is a simple graph on n vertices without isolated vertices. Then*

(1) $n_0(G) = n-2$ if and only if G is isomorphic to a complete bipartite graph K_{n_1,n_2}, where $n_1+n_2=n$ and $n_1,n_2>0$.
(2) $n_0(G) = n-3$ if and only if G is isomorphic to a complete tripartite graph K_{n_1,n_2,n_3}, where $n_1+n_2+n_3=n$ and $n_1,n_2,n_3>0$. ■

Lemma 9.7. *Let v be a pendent vertex of a graph G and u the vertex in G adjacent to v. Then $n_0(G)=n_0(G-u-v)$.* ■

Let $H_i(k,n_1,n_2)$ $(i=1,2)$ (or simply H_i) be the graph of order n depicted in Fig. 9.4, where $k \geq 1$, $n_1 \geq 0, n_2 \geq 0$. Obviously, H_1 and H_2 are k-cyclic, and $|V(H_1)| \geq k+2$, $|V(H_2)| \geq k+3$. If $n_1=n_2=0$, then by Lemma 9.6, $n_0(H_1) = n-3$, $n_0(H_2)=n-2$. Otherwise, by Lemma 9.7, $n_0(H_1)=n_0(H_2)=n-4$. Hence, $n_0(H_1) \geq n-4$ and $n_0(H_2) \geq n-4$.

By Theorem 4.5, we have $\mathscr{E}(H_i) \leq \sqrt{2m(n-n_0)} = \sqrt{2(n+k-1)(n-n_0)} \leq \sqrt{8(n+k-1)}$. If $\sqrt{8(n+k-1)} < n$, then H_i is hypoenergetic, i.e., if $(n-4)^2 - 8k-8 > 0$, which is satisfied by all $n > 4+\sqrt{8(k+1)}$. It is easy to check that

$$\max\left\{k+1, 4+\sqrt{8(k+1)}\right\} = \begin{cases} 4+\sqrt{8(k+1)} & \text{if } 1 \leq k \leq 13 \\ k+1 & \text{if } k \geq 14 \end{cases}$$

and

$$\max\left\{k+2, 4+\sqrt{8(k+1)}\right\} = \begin{cases} 4+\sqrt{8(k+1)} & \text{if } 1 \leq k \leq 12 \\ k+2 & \text{if } k \geq 13 \end{cases}.$$

Hence, we have:

Lemma 9.8. *(1) If*

$$n > \max\left\{k+1, 4+\sqrt{8(k+1)}\right\} = \begin{cases} 4+\sqrt{8(k+1)} & \textit{if } 1 \le k \le 13 \\ k+1 & \textit{if } k \ge 14 \end{cases}$$

then H_1 is hypoenergetic.
(2) If

$$n > \max\left\{k+2, 4+\sqrt{8(k+1)}\right\} = \begin{cases} 4+\sqrt{8(k+1)} & \textit{if } 1 \le k \le 12 \\ k+2 & \textit{if } k \ge 13 \end{cases}$$

then H_2 is hypoenergetic. ■

Notice that the inequality $\sqrt{8(k+1)} \le k+3$ holds for any $k \ge 1$, so we have the following result. It was also communicated by You et al. [508].

Theorem 9.8. *There exist hypoenergetic k-cyclic graphs for all $n \ge k+8$.* ■

If $\sqrt{8(n+k-1)} < n-1$ holds, then H_i is strongly hypoenergetic. The latter inequality can be transformed into $(n-5)^2 - 8k - 16 > 0$, which is obeyed by all $n > 5 + \sqrt{8(k+2)}$. It is easy to check that

$$\max\left\{k+1, 5+\sqrt{8(k+2)}\right\} = \begin{cases} 5+\sqrt{8(k+2)} & \text{for } 1 \le k \le 15 \\ k+1 & \text{for } k \ge 16 \end{cases}$$

and

$$\max\left\{k+2, 5+\sqrt{8(k+2)}\right\} = \begin{cases} 5+\sqrt{8(k+2)} & \text{for } 1 \le k \le 14 \\ k+2 & \text{for } k \ge 15 \end{cases}.$$

Lemma 9.9. *(1) If*

$$n > \max\left\{k+1, 5+\sqrt{8(k+2)}\right\} = \begin{cases} 5+\sqrt{8(k+2)} & \textit{for } 1 \le k \le 15 \\ k+1 & \textit{for } k \ge 16 \end{cases}$$

then H_1 is strongly hypoenergetic.
(2) If

$$n > \max\left\{k+2, 5+\sqrt{8(k+2)}\right\} = \begin{cases} 5+\sqrt{8(k+2)} & \textit{for } 1 \le k \le 14 \\ k+2 & \textit{for } k \ge 15 \end{cases}$$

then H_2 is strongly hypoenergetic. ■

In the following, we consider hypoenergetic and strongly hypoenergetic k-cyclic graphs with order n and maximum degree Δ.

Theorem 9.9. *(1) If $n-k$ is even and $\Delta \in [\frac{n+k}{2}, n-1]$ or $n-k$ is odd and $\Delta = n-1$, then there exist hypoenergetic k-cyclic graphs of order n with maximum degree Δ for all $n > \max\left\{k+1, 4+\sqrt{8(k+1)}\right\}$.*

(2) If $n-k$ is odd and $\Delta \in [\frac{n+k-1}{2}, n-2]$, then there exist hypoenergetic k-cyclic graphs of order n with maximum degree Δ for all $n > \max\{k+2, 4+\sqrt{8(k+1)}\}$.

Proof. (1) Suppose that $n-k$ is even and $\Delta \in [\frac{n+k}{2}, n-1]$ or $n-k$ is odd and $\Delta = n-1$. Let $G = H_1(k, \Delta-k-1, n-\Delta-1)$. Then by Lemma 9.8, G is hypoenergetic when $n > \max\left\{k+1, 4+\sqrt{8(k+1)}\right\}$.

(2) Suppose that $n-k$ is odd and $\Delta \in [\frac{n+k-1}{2}, n-2]$. Let $G = H_2(k, \Delta-k-1, n-\Delta-2)$. Then from Lemma 9.8 follows that G is hypoenergetic when $n > \max\left\{k+2, 4+\sqrt{8(k+1)}\right\}$. ■

By Lemma 9.9, similar to the proof of Theorem 9.9, we obtain:

Theorem 9.10. *(1) If $n-k$ is even and $\Delta \in [\frac{n+k}{2}, n-1]$ or $n-k$ is odd and $\Delta = n-1$, then there exist strongly hypoenergetic k-cyclic graphs of order nwith maximum degree Δ for all $n > \max\left\{k+1, 5+\sqrt{8(k+2)}\right\}$.*

(2) If $n-k$ is odd and $\Delta \in [\frac{n+k-1}{2}, n-2]$, then there exist strongly hypoenergetic k-cyclic graphs of order n with maximum degree Δ for all $n > \max\{k+2, 5+\sqrt{8(k+2)}\}$. ■

Theorem 9.11. *(1) If $n-k$ is even and $\max\left\{\frac{2k+1}{2}, \frac{5+k+\sqrt{8(k+2)}}{2}\right\} < \Delta \le n-1$, then there exist hypoenergetic k-cyclic graphs of order n with maximum degree Δ for all $n > \max\left\{k+3, 7+\sqrt{8(k+2)}\right\}$.*

(2) If $n-k$ is odd and $\max\left\{\frac{2k+1}{2}, \frac{4+k+\sqrt{8(k+2)}}{2}\right\} < \Delta \le n-1$, then there exist hypoenergetic k-cyclic graphs of order n with maximum degree Δ for all $n > \max\left\{k+4, 7+\sqrt{8(k+2)}\right\}$. ■

Similar to the proof of Lemma 9.3, we obtain the following result, which provides a useful method for constructing additional hypoenergetic k-cyclic graphs:

Theorem 9.12. *If there exists a t-vertex hypoenergetic k-cyclic graph with $\Delta \ge 4$ and at least one vertex of degree at most $\Delta - 1$, then there exist hypoenergetic k-cyclic graphs with Δ for all $n \ge t$, such that $n \equiv t \pmod 4$.* ■

In Sect. 9.2.1, we determined all hypoenergetic trees. In the following subsections, we characterize hypoenergetic unicyclic, bicyclic, and tricyclic graphs.

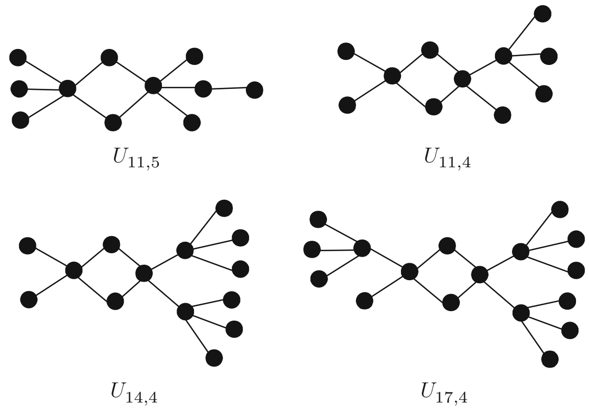

Fig. 9.5 The graphs $U_{11,5}$, $U_{11,4}$, $U_{14,4}$, and $U_{17,4}$

9.3.1 Hypoenergetic Unicyclic Graphs

You and Liu [507] got the following result for the existence of hypoenergetic unicyclic graphs.

Lemma 9.10. *(1) If $n \leq 6$, then there does not exist any hypoenergetic unicyclic graph. (2) There exist hypoenergetic unicyclic graphs for all $n \geq 7$. (3) If n is even and $\Delta \in [n/2, n-1]$ or n is odd and $\Delta \in [(n+1)/2, n-1]$, then there exist hypoenergetic unicyclic graphs with maximum degree Δ for all $n \geq 9$.* ■

Eventually, Li and Ma [336] extended the interval for the maximum degree Δ:

Lemma 9.11 [336]. *If n is even and $\Delta \in [5, n-1]$ or n is odd and $\Delta \in [6, n-1]$, then there exist hypoenergetic unicyclic graphs of order n with maximum degree Δ for all $n \geq 9$.*

Proof. Notice that if $k = 1$, then $n > \max\left\{k+2, 4+\sqrt{8(k+1)}\right\}$ implies $n \geq 9$, $n > \max\left\{k+4, 7+\sqrt{8(k+2)}\right\}$ implies $n \geq 12$, $\Delta > \max\left\{\frac{2k+1}{2}, \frac{5+k+\sqrt{8(k+2)}}{2}\right\}$ implies $\Delta \geq 6$, and $\Delta > \max\left\{\frac{2k+1}{2}, \frac{4+k+\sqrt{8(k+2)}}{2}\right\}$ implies $\Delta \geq 5$. Hence, the result follows from Theorem 9.9 for $9 \leq n \leq 11$ and from Theorem 9.11 for $n \geq 12$. ■

In the following, we consider the case $4 \leq \Delta \leq 7$. Let $U_{7,5} = H_2(1,3,0)$, $U_{7,6} = H_1(1,4,0)$, $U_{8,4} = H_2(1,2,2)$, $U_{8,5} = H_2(1,3,1)$, $U_{8,6} = H_2(1,4,0)$, $U_{8,7} = H_1(1,5,0)$, and $U_{9,5} = H_2(1,3,2)$. Let $U_{11,5}, U_{11,4}, U_{14,4}$, and $U_{17,4}$ be the graphs depicted in Fig. 9.5. From the data given in Table 9.2, we see that the graphs $U_{n,\ell}$ are hypoenergetic unicyclic graphs of order n with $\Delta = \ell$. Since by Theorem 9.12, $U_{8,4}, U_{11,4}, U_{14,4}, U_{17,4}, U_{9,5}$, and $U_{11,5}$ are hypoenergetic, we obtain:

Table 9.2 Energies of the graphs $U_{n,\ell}$ for $\Delta = \ell$

n	Δ	$\mathscr{E}(U_{n,\Delta})$	n	Δ	$\mathscr{E}(U_{n,\Delta})$	n	Δ	$\mathscr{E}(U_{n,\Delta})$
7	5	6.89898	8	6	7.39104	11	5	10.58501
7	6	6.64681	8	7	7.07326	14	4	13.90827
8	4	7.72741	9	5	8.24621	17	4	16.96885
8	5	7.65069	11	4	10.87716			

Lemma 9.12. *(1) If $\Delta = 4$, then there exist hypoenergetic unicyclic graphs of order n for all $n = 8, 11, 12$ and $n \geq 14$; (2) If $\Delta = 5$, then there exist hypoenergetic unicyclic graphs of order n for all odd $n \geq 9$.* ■

Combining Lemmas 9.11, 9.12, and the data from Table 9.2, we get:

Theorem 9.13. *If (a) $n = 8, 11, 12$ or $n \geq 14$ and $\Delta = 4$ or (b) $n \geq 7$ and $\Delta \in [5, n-1]$, then there exist hypoenergetic unicyclic graphs with order n and maximum degree Δ.* ■

If $n \leq 6$, then by Lemma 9.10, there exists no hypoenergetic unicyclic graph. From [80], there are 12 unicyclic graphs with $n = 7$ and $\Delta = 4$. In these graphs, the minimal energy is $\mathscr{E} = 7.1153 > n = 7$, and the extremal graph is $H_2(1,1,2)$. We can also show that there are no hypoenergetic unicyclic graphs with $n = 9$ or 10 and $\Delta = 4$. In [276], it was shown that there are no hypoenergetic unicyclic graphs with $n = 13$ and $\Delta = 4$.

At the end of this subsection, we consider the remaining case $\Delta \leq 3$. The following notation and results [385] are needed:

Lemma 9.13. *Let G be a graph of order n with at least n edges and with no isolated vertices. If G is quadrangle-free and $\Delta(G) \leq 3$, then $\mathscr{E}(G) > n$.* ■

Lemma 9.14. *If there exists an edge-cut F of a connected graph G, such that $G-F$ has two components G_1 and G_2, and both G_1 and G_2 are nonhypoenergetic, then G is also nonhypoenergetic.*

Proof. From Theorem 4.20, it follows that $\mathscr{E}(G) \geq \mathscr{E}(G-F) = \mathscr{E}(G_1)+\mathscr{E}(G_2) \geq |V(G_1)| + |V(G_2)| = n$. ■

Theorem 9.14. *There does not exist any hypoenergetic unicyclic graph with $\Delta \leq 3$.*

Proof. Let G be an n-vertex unicyclic graph with $\Delta \leq 3$. We show that G is nonhypoenergetic. If $n \leq 6$, then G is nonhypoenergetic by Lemma 9.10. If G is quadrangle-free, then G is nonhypoenergetic by Lemma 9.13. So in what follows, we assume that $n \geq 7$ and G contain a quadrangle $C = x_1x_2x_3x_4x_1$. We only need to consider the following four cases:

Case 1. There exists an edge e on C, such that the end vertices of e are of degree 2.

Without loss of generality, assume that $d(x_1) = d(x_4) = 2$. Let $F = \{x_1x_2, x_4x_3\}$, then $G - F$ has two components, say G_1 and G_2, where G_1 is the tree of order 2 with $x_1 \in V(G_1)$ and G_2 is a tree of order at least 5 since $n \geq 7$.

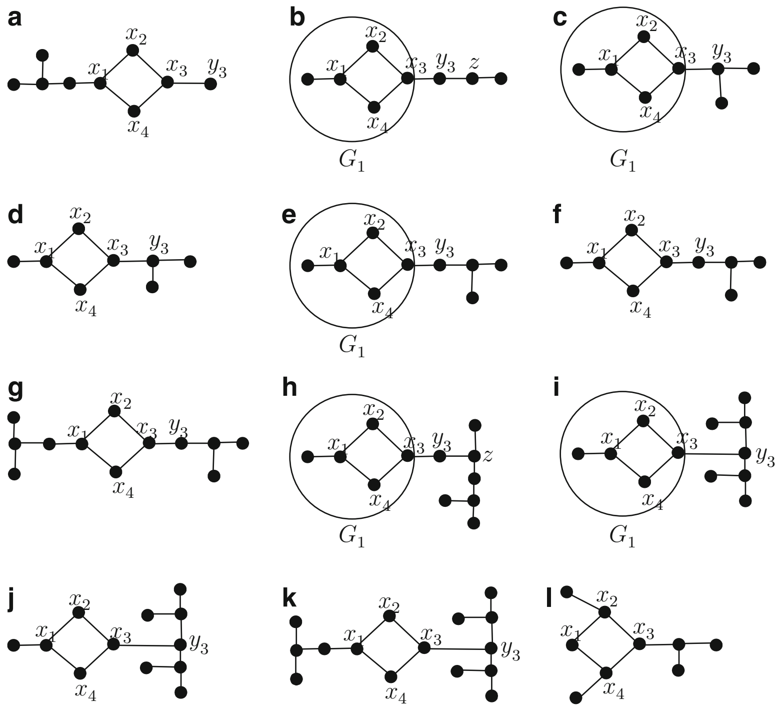

Fig. 9.6 The graphs used in the proof of Theorem 9.14

Since $\Delta(G) \leq 3$, G_2 cannot be isomorphic to the graph W (depicted in Fig. 9.1). Therefore, by Theorem 9.5 (a), G_1, G_2 are nonhypoenergetic. The result follows from Lemma 9.14.

Case 2. There exist exactly two nonadjacent vertices x_i and x_j on C such that $d(x_i) = d(x_j) = 2$.

Without loss of generality, assume that $d(x_2)=d(x_4)=2$, $d(x_1)=d(x_3)=3$. Let y_3 be the vertex adjacent to x_3 lying outside C. Then $G-x_3y_3$ has two components, say G_1 and G_2, where G_1 is a unicyclic graph and G_2 is a tree. Notice that G_1 is nonhypoenergetic by Case 1. If $G_2 \ncong S_1, S_3, S_4, W$ (see Fig. 9.1), then by Theorem 9.5 (a) and Lemma 9.14, we are done. So, we only need to consider the following four cases:

Subcase 2.1. $G_2 \cong S_1$.

Let $F = \{x_2x_3, x_3x_4\}$, then $G - F$ has two components, say G_1' and G_2', where G_1' is a tree of order at least 4 and G_2' is a tree of order 2. If $G_1' \ncong S_4, W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong S_4$, then $n = 6$, a contradiction. If $G_1' \cong W$, then G must be the graph shown in Fig. 9.6a. By direct computing, we have $\mathscr{E}(G) = 9.78866 > 9 = n$.

Subcase 2.2. $G_2 \cong S_3$.

Then G must have the structure shown in Fig. 9.6b or c. In the former case, $G - y_3z$ has two components, say G_1' and G_2', where G_1' is a unicyclic graph and G_2' is a tree of order 2. From Subcase 2.1 follows that G_1' is nonhypoenergetic. Therefore, by Theorem 9.5 (a) and Lemma 9.14, we are done. In the latter case, $G - \{x_1x_2, x_4x_3\}$ has two components, say G_1' and G_2', where G_1' is a tree of order at least 3 and G_2' is a tree of order 5. If $G_1' \ncong S_3, S_4, W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. Since $\Delta(G) \leq 3$, G_1' cannot be isomorphic to S_4 or W. If $G_1' \cong S_3$, then G must be the graph shown in Fig. 9.6d. By direct computing, we have $\mathscr{E}(G) = 8.81463 > 8 = n$.

Subcase 2.3. $G_2 \cong S_4$.

G must have the structure shown in Fig. 9.6e. Let $F = \{x_2x_3, x_3x_4\}$, then $G - F$ has two components, say G_1' and G_2', where G_1' is a tree of order at least 4 and G_2' is a tree of order 5. If $G_1' \ncong S_4, W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong S_4$, then G must be the graph shown in Fig. 9.6f. By direct computing, we get $\mathscr{E}(G) = 9.78866 > 9 = n$. If $G_1' \cong W$, then G must be the graph shown in Fig. 9.6g. Now, $G - \{x_1x_2, x_3x_4\}$ has two components, say G_1'' and G_2'', where G_i'' is a tree of order 6, $i = 1, 2$. Therefore, we are done by Theorem 9.5 (a) and Lemma 9.14.

Subcase 2.4. $G_2 \cong W$.

Then G must have the structure shown in Fig. 9.6h or i. In the former case, $G - y_3z$ has two components, say G_1' and G_2', where G_1' is a unicyclic graph and G_2' is a tree of order 6. It follows from Subcase 2.1 that G_1' is nonhypoenergetic. Therefore, we are done by Theorem 9.5 (a) and Lemma 9.14. In the latter case, $G - \{x_2x_3, x_3x_4\}$ has two components, say G_1' and G_2', where G_1' is a tree of order at least 4 and G_2' is a tree of order 8. If $G_1' \ncong S_4, W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong S_4$, then G must be the graph shown in Fig. 9.6j, and by direct computing, we obtain $\mathscr{E}(G) = 13.05749 > 12 = n$. If $G_1' \cong W$, then G must be the graph shown in Fig. 9.6k. Now, $G - \{x_1x_2, x_3x_4\}$ has two components, say G_1'' and G_2'', where G_1'' is a tree of order 6 and G_2'' is a tree of order 9. Therefore, we are done by Theorem 9.5 (a) and Lemma 9.14.

Case 3. There exists exactly one vertex x_i on C, such that $d(x_i) = 2$.

Without loss of generality, assume that $d(x_1) = 2$. Let $F = \{x_1x_4, x_2x_3\}$. Then $G - F$ has two components, say G_1 and G_2, where G_1 is a tree of order at least 3 with $x_1 \in V(G_1)$ and G_2 is a tree of order at least 4. Since $\Delta(G) \leq 3$, the graphs G_1, G_2 cannot be isomorphic to S_4 or W. So, if $G_1 \ncong S_3$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1 \cong S_3$, then $G - \{x_1x_2, x_2x_3\}$ has two components, say G_1' and G_2', where G_1' is the tree of order at least 5 with $x_1 \in V(G_1')$ and G_2' is the tree of order 2. If $G_1' \ncong W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong W$, then G must be the graph shown in Fig. 9.6l. By direct computing, we have $\mathscr{E}(G) = 9.80028 > 9 = n$.

Case 4. $d(x_1) = d(x_2) = d(x_3) = d(x_4) = 3$.

Let $F = \{x_1x_4, x_2x_3\}$. Then $G - F$ has two components, say G_1 and G_2, where G_1 and G_2 are trees of order at least 4. It is easy to check that G_1, G_2 cannot be isomorphic to S_4 or W. Therefore, we are done by Theorem 9.5 (a) and Lemma 9.14.

By this, all possibilities have been exhausted and the proof is thus complete. ■

9.3.2 Hypoenergetic Bicyclic Graphs

You and Liu [507] obtained the following results for the existence of hypoenergetic bicyclic graphs:

Lemma 9.15 (1). *If $n = 4, 6, 7$, then there does not exist any hypoenergetic bicyclic graph. (2) There exist hypoenergetic bicyclic graphs for all $n \geq 8$. (3) 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 there exist hypoenergetic bicyclic graphs with maximum degree Δ for all $n \geq 9$.* ■

Lemma 9.16. *If n is even and $\Delta \in [7, n - 1]$ or n is odd and $\Delta \in [6, n - 1]$, then there exist hypoenergetic bicyclic graphs of order n with maximum degree Δ for all $n \geq 9$.*

Proof. Note that when $k = 2$, then $n > \max\left\{k + 2, 4 + \sqrt{8(k + 1)}\right\}$ which implies $n \geq 9$ and $n > \max\left\{k + 4, 7 + \sqrt{8(k + 2)}\right\}$ which implies $n \geq 13$, as well as $\Delta > \max\left\{\frac{2k+1}{2}, \frac{5+k+\sqrt{8(k+2)}}{2}\right\}$ implying $\Delta \geq 7$ and $\Delta > \max\left\{\frac{2k+1}{2}, \frac{4+k+\sqrt{8(k+2)}}{2}\right\}$ implying $\Delta \geq 6$. Hence, the result follows from Theorem 9.9 for $9 \leq n \leq 12$ and from Theorem 9.11 for $n \geq 13$. ■

In the following, we consider the case $4 \leq \Delta \leq 7$. Let $B(8, 5) = H_2(2, 1, 2)$, $B(8, 6) = H_2(2, 0, 3)$, $B(8, 7) = H_1(2, 0, 4)$, $B(9, 5) = H_2(2, 2, 2)$, and $B(10, 6) = H_2(2, 2, 3)$. Let $B(10, 5)$, $B(11, 5)$, $B(9, 4)$, $B(16, 4)$, $B(18, 4)$, and $B(19, 4)$ be the graphs depicted in Fig. 9.7. As seen from Table 9.3, these graphs are bicyclic, of order n, with $\Delta = \ell$ and are hypoenergetic. By Theorem 9.12, we obtain:

Lemma 9.17. *(1) If $\Delta = 4$, then there exist hypoenergetic bicyclic graphs of order n for $n = 9, 13$ and all $n \geq 16$. (2) If $\Delta = 5$, then there exist hypoenergetic bicyclic graphs of order n for all $n \geq 8$. (3) If $\Delta = 6$, then there exist hypoenergetic bicyclic graphs of order n for all even $n \geq 8$.* ■

Combining Lemmas 9.16, 9.17, and Table 9.3, we arrive at:

Theorem 9.15. *If (a) $n = 9, 13$ or $n \geq 16$ and $\Delta = 4$ or (b) $n \geq 8$ and $\Delta \in [5, n - 1]$, then there exist hypoenergetic bicyclic graphs of order n and with maximum degree Δ.* ■

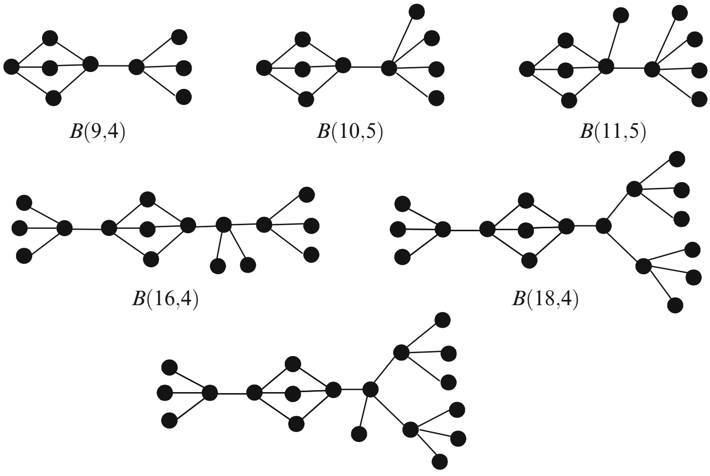

Fig. 9.7 Graphs $B(9,4)$, $B(10,5)$, $B(11,5)$, $B(16,4)$, $B(18,4)$, and $B(19,4)$

Table 9.3 Energies of the graphs $B(n,\ell)$ for $\Delta = \ell$

n	Δ	$\mathscr{E}(B(n,\Delta))$	n	Δ	$\mathscr{E}(B(n,\Delta))$	n	Δ	$\mathscr{E}(B(n,\Delta))$
8	5	7.90778	9	5	8.48528	16	4	15.77861
8	6	7.74597	10	5	9.25036	18	4	17.94188
8	7	7.68165	10	6	8.98112	19	4	18.87354
9	4	8.75560	11	5	10.74799			

If $n = 4, 6, 7$, then by Lemma 9.15, there exist no hypoenergetic bicyclic graphs. From Table 1 of [81], we see that there are two bicyclic graphs with $n = 5$ and $\Delta = 4$, and the smallest of their energies is $\mathscr{E} = 6.04090 > n = 5$. The respective extremal graph is $H_1(2,0,1)$. Thus, for $\Delta = 4$, $n = 8, 10, 11, 12, 14, 15$ are the only few cases for which we cannot determine whether or not there exist hypoenergetic bicyclic graphs. Fortunately, in [276], it was shown that there are no such hypoenergetic bicyclic graphs.

At the end of this subsection, we consider the remaining case $\Delta \leq 3$.

Theorem 9.16. *The complete bipartite graph $K_{2,3}$ is the only hypoenergetic bicyclic graph with $\Delta \leq 3$.*

Proof. Let G be an n-vertex bicyclic graph with $\Delta \leq 3$. If $n = 4, 6, 7$, then by Lemma 9.15, G is nonhypoenergetic. If $n = 5$, from Table 1 of [81], it is seen that there are three bicyclic graphs with $\Delta \leq 3$. Direct calculation reveals that $K_{2,3}$ is the only hypoenergetic species among them, $\mathscr{E}(K_{2,3}) = 4.8990$. If G is quadrangle-free, then by Lemma 9.13, G is nonhypoenergetic. So, in the following, we assume that G contains a quadrangle and that $n \geq 8$. We show that under these conditions, G is nonhypoenergetic.

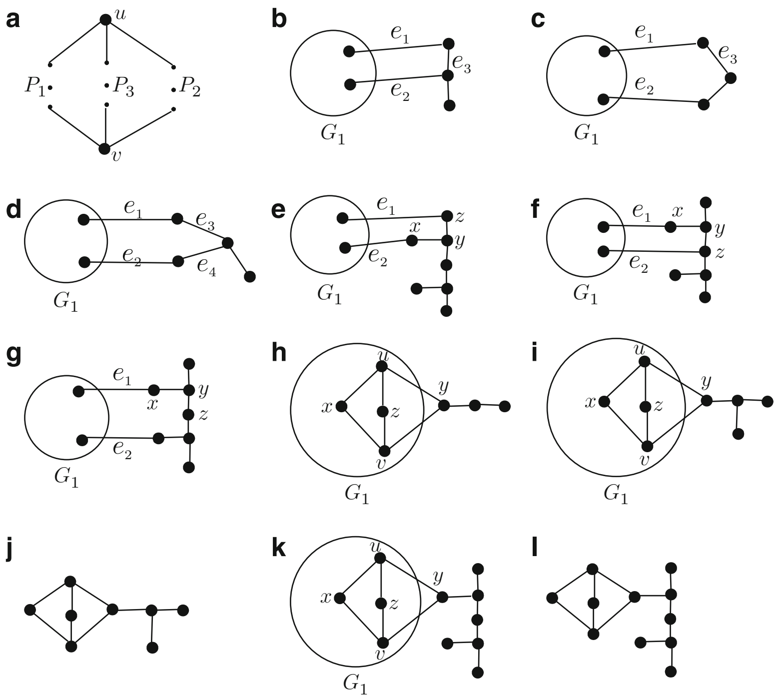

Fig. 9.8 The graphs used in the proof of Theorem 9.16

If the cycles in G are disjoint, then it is clear that there exists a path P connecting the two cycles. Obviously, for any edge e on P, $G-e$ has two components which are unicyclic graphs. Thus, G is nonhypoenergetic by Lemma 9.14 and Theorem 9.14. Otherwise, the cycles in G have two or more common vertices. Then we may assume that G contains a subgraph shown in Fig. 9.8a, where P_1, P_2, P_3 are paths in G.

We distinguish between the following three cases:

Case 1. At least one of P_1, P_2, and P_3 has length not less than 3. Let this be the path P_2.

Let e_1 and e_2 be the edges on P_2 incident with vertices u and v, respectively. Then $G-\{e_1, e_2\}$ has two components, say G_1 and G_2, such that G_1 is unicyclic and G_2 is a tree of order at least 2. From Theorem 9.14, it follows that G_1 is nonhypoenergetic. If $G_2 \not\cong S_3, S_4, W$ (see Fig. 9.1), then we are done by Theorem 9.5 (a) and Lemma 9.14. So, we only need to consider the following three subcases:

Subcase 1.1. $G_2 \cong S_3$.

Then G must have the structure shown in Fig. 9.8b or c. In either case, $G-\{e_2, e_3\}$ has two components, say G_1' and G_2', such that G_1' is a unicyclic graph and G_2' is the tree of order 2. By Theorem 9.14, G_1' is nonhypoenergetic. Therefore, the result follows from Theorem 9.5 (a) and Lemma 9.14.

Subcase 1.2. $G_2 \cong S_4$.

Then G must have the structure shown in Fig. 9.8d. Obviously, $G - \{e_3, e_4\}$ has two components, say G_1' and G_2', where G_1' is a unicyclic graph and G_2' is the tree of order 2. Therefore, the result follows from Theorems 9.14 and 9.5 (a) and Lemma 9.14.

Subcase 1.3. $G_2 \cong W$.

Then G must have the structure shown in Fig. 9.8e, f or g. Obviously, $G - \{xy, yz\}$ has two components, say G_1' and G_2', such that G_1' is a unicyclic graph and G_2' is a tree of order 5 or 2. Therefore, the result follows from Theorems 9.14 and 9.5 (a) and Lemma 9.14.

Case 2. All paths P_1, P_2 and P_3 have length 2.

Assume that $P_1 = uxv$, $P_3 = uzv$, and $P_2 = uyv$. Let $F = \{uy, vy\}$. Then $G - F$ has two components, say G_1 and G_2, where G_1 is a unicyclic graph and G_2 is a tree. It follows from Theorem 9.14 that G_1 is nonhypoenergetic. If $G_2 \ncong S_1, S_3, S_4, W$, then we are done by Theorem 9.5 (a) and Lemma 9.14. So, we only need to consider the following four cases:

Subcase 2.1. $G_2 \cong S_1$.

Let $F' = \{uy, zv, xv\}$. Then $G - F'$ has two components, say G_1' and G_2', such that G_2' is the tree of order 2 with $y \in V(G_2')$, whereas G_1' is a tree of order at least 6 since $n \geq 8$. Since $\Delta(G) \leq 3$, G_1' cannot be isomorphic to W. Therefore, by Theorem 9.5 (a), G_1', G_2' are nonhypoenergetic. The result follows from Lemma 9.14.

Subcase 2.2. $G_2 \cong S_3$.

Then G must have the structure shown in Fig. 9.8h. Let $F' = \{uy, zv, xv\}$. Then $G - F'$ has two components, say G_1' and G_2', where G_2' is the path of order 4 with $y \in V(G_2')$, and G_1' is a tree of order at least 4 since $n \geq 8$. Since $\Delta(G) \leq 3$, G_1' cannot be isomorphic to S_4 or W. Therefore, by Theorem 9.5 (a), G_1', G_2' are nonhypoenergetic. The result follows from Lemma 9.14.

Subcase 2.3. $G_2 \cong S_4$.

Then G must have the structure shown in Fig. 9.8i. Let $F' = \{uy, zv, xv\}$. Then $G - F'$ has two components, say G_1' and G_2', such that G_2' is the tree of order 5 with $y \in V(G_2')$, whereas G_1' is a tree of order at least 3. Since $\Delta(G) \leq 3$, G_1' cannot be isomorphic to S_4 or W. If $G_1' \ncong S_3$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong S_3$, then G must be the graph depicted in Fig. 9.8j. By direct computing, we get $\mathscr{E}(G) = 8.24621 > 8 = n$.

Subcase 2.4. $G_2 \cong W$.

Then G must have the structure shown in Fig. 9.8k. Let $F' = \{uy, zv, xv\}$. Then $G - F'$ has two components, say G_1' and G_2', where G_2' is a tree of order 8 with $y \in V(G_2')$ and G_1' is a tree of order at least 3. Since $\Delta(G) \leq 3$, G_1' cannot be isomorphic to S_4 or W. If $G_1' \ncong S_3$, then we are done by Theorem 9.5 (a) and Lemma 9.14. If $G_1' \cong S_3$, then G must be the graph depicted in Fig. 9.8l. By direct computing, we get $\mathscr{E}(G) = 11.60185 > 11 = n$.

Case 3. One of the paths P_1, P_2 and P_3 has length 1.

Then the other two paths must have length 2 since our graph has no multiple edges. Without loss of generality, we assume that $P_1 = uxv$, $P_3 = uv$, and $P_2 = uyv$. Then in a similar way as in the proof of Case 2, we can show that G is nonhypoenergetic.

The proof is thus complete. ■

9.3.3 Hypoenergetic Tricyclic Graphs

You and Liu [507] obtained the following results for the existence of hypoenergetic tricyclic graphs.

Lemma 9.18. *(1) If $n = 4, 5, 7$, then there does not exist any hypoenergetic tricyclic graph. (2) There exist hypoenergetic tricyclic graphs for all $n \geq 8$. (3) If n is even and $\Delta \in [n/2 + 1, n - 1]$ or n is odd and $\Delta \in [(n + 3)/2, n - 1]$, then there exist hypoenergetic tricyclic graphs with maximum degree Δ for all $n \geq 10$.* ■

Lemma 9.19. *If n is even and $\Delta \in [7, n - 1]$ or n is odd and $\Delta \in [8, n - 1]$, then there exist hypoenergetic tricyclic graphs of order n with maximum degree Δ for all $n \geq 10$.*

Proof. Note that when $k = 3$, then $n > \max\left\{k + 2, 4 + \sqrt{8(k + 1)}\right\}$ which implies $n \geq 10$ and $n > \max\left\{k + 4, 7 + \sqrt{8(k + 2)}\right\}$ which implies $n \geq 14$, as well as $\Delta > \max\left\{\frac{2k+1}{2}, \frac{5+k+\sqrt{8(k+2)}}{2}\right\}$ implying $\Delta \geq 8$ and $\Delta > \max\left\{\frac{2k+1}{2}, \frac{4+k+\sqrt{8(k+2)}}{2}\right\}$ implying $\Delta \geq 7$. Hence, the result follows from Theorem 9.9 for $10 \leq n \leq 13$ and from Theorem 9.11 for $n \geq 14$. ■

We now consider hypoenergetic tricyclic graphs with $4 \leq \Delta \leq 8$. Denote $T_{6,4} = H_2(3, 0, 0)$, $T_{8,6} = H_2(3, 0, 2)$, $T_{9,6} = H_2(3, 1, 2)$, $T_{9,7} = H_2(3, 0, 3)$, $T_{9,8} = H_1(3, 0, 4)$, $T_{10,6} = H_2(3, 2, 2)$, and $T_{11,7} = H_2(3, 2, 3)$. The graphs $T_{9,5}$, $T_{10,5}$, $T_{11,5}$, $T_{12,5}$, $T_{11,6}$, $T_{13,4}$, $T_{16,4}$, and $T_{19,4}$ are depicted in Fig. 9.9. From the data given in Table 9.4, we see that $T_{n,\ell}$ are hypoenergetic tricyclic graphs of order n with $\Delta = \ell$. By Theorem 9.12, we obtain:

Lemma 9.20. *(1) If $\Delta = 4$, then there exist hypoenergetic tricyclic graphs of order n for $n = 6, 10, 13, 14$ and $n \geq 16$. (2) If $\Delta = 5$, then there exist hypoenergetic tricyclic graphs of order n for all $n \geq 9$. (3) If $\Delta = 6$, then there exist hypoenergetic tricyclic graphs of order n for all $n \geq 8$. (4) If $\Delta = 7$, then there exist hypoenergetic tricyclic graphs of order n for all odd $n \geq 9$.* ■

Combining Lemmas 9.19 and 9.20 and Table 9.4, we arrive at:

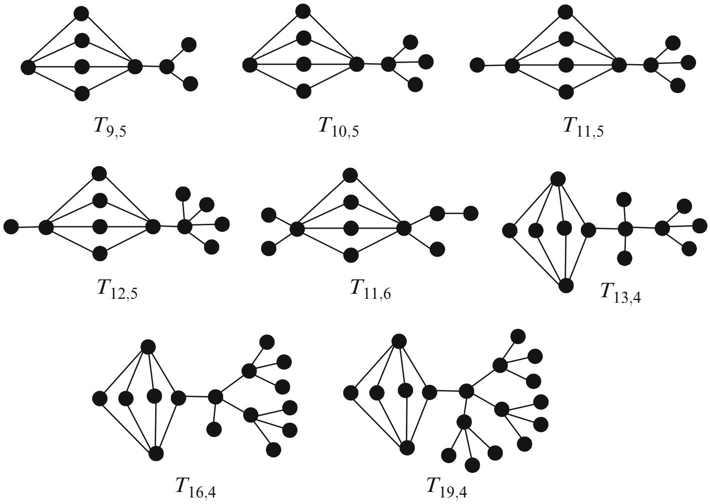

Fig. 9.9 The graphs $T_{9,5}$, $T_{10,5}$, $T_{11,5}$, $T_{12,5}$, $T_{11,6}$, $T_{13,4}$, $T_{16,4}$, and $T_{19,4}$

Table 9.4 Energies of the graphs $T_{n,\ell}$ for $\Delta = \ell$

n	Δ	$\mathscr{E}(T_{n,\Delta})$	n	Δ	$\mathscr{E}(T_{n,\Delta})$	n	Δ	$\mathscr{E}(T_{n,\Delta})$
6	4	5.65685	9	8	8.50189	11	7	9.63287
8	6	7.91375	10	5	9.50432	12	5	11.50305
9	5	8.93180	10	6	9.15298	13	4	12.78001
9	6	8.59845	11	5	10.00000	16	4	15.90909
9	7	8.46834	11	6	10.94832	19	4	18.88809

Theorem 9.17. *If (a) $n = 6, 10, 13, 14$ or $n \geq 16$ and $\Delta = 4$ or (b) $n \geq 9$ and $\Delta = 5$ or (c) $n \geq 8$ and $\Delta = 6$ or (d) $n \geq 9$ and $\Delta \in [7, n-1]$, then there exist hypoenergetic tricyclic graphs of order n and with maximum degree Δ.* ■

If $n = 4, 5, 7$, then by Lemma 9.18, there exist no hypoenergetic tricyclic graphs. By Table 1 from [87], there are four tricyclic graphs with $n = 6$ and $\Delta = 5$. The smallest energy of these graphs is $\mathscr{E} = 6.89260 > n = 6$, and the extremal graph is $H_1(3,0,1)$. When $n = 8$ and $\Delta = 7$, it is easy to check that there are five tricyclic graphs, that the smallest energy among them is $\mathscr{E} = 8.04552 > n = 8$, and that the extremal graph is $H_1(3,0,3)$. We also found that the minimal energy among tricyclic graphs with $n = 8$ and $\Delta = 5$ is $\mathscr{E} = 8 = n$, and the extremal graph is $H_2(3,1,1)$. Thus, for $\Delta = 4$, $n = 8, 9, 11, 12, 15$ are the only few cases for which we could not determine whether or not there exist hypoenergetic tricyclic graphs. In [276], it was demonstrated that there are no such hypoenergetic tricyclic graphs.

9.4 All Hypoenergetic Graphs with Maximum Degree at Most 3

From Theorem 9.5, we know that there exist only four hypoenergetic trees with $\Delta \leq 3$, depicted in Fig. 9.1. In [338], all connected hypoenergetic graphs with maximum degree at most 3 were considered, and the following results were obtained:

Theorem 9.18. *The complete bipartite graph $K_{2,3}$ is the only hypoenergetic connected cycle-containing (or cyclic) graph with $\Delta \leq 3$.* ■

Therefore, combining Theorems 9.5 and 9.18, all connected hypoenergetic graphs with maximum degree at most 3 have been characterized.

Theorem 9.19. *S_1, S_3, S_4, W (see Fig. 9.1) and $K_{2,3}$ are the only five hypoenergetic connected graphs with $\Delta \leq 3$.* ■

By means of Theorems 9.14 and 9.16, we obtain:

Lemma 9.21. *$K_{2,3}$ is the only hypoenergetic graph with $\Delta \leq 3$ among all unicyclic and bicyclic graphs.* ■

Proof of Theorem 9.18. Notice that by Lemma 9.21, $K_{2,3}$ is hypoenergetic. Let G be a connected cyclic graph with $G \ncong K_{2,3}$, $\Delta \leq 3$, and cyclomatic number $c(G) = m - n + 1 \geq 1$. In the following, by induction on $c(G)$, we show that G is nonhypoenergetic. From Lemma 9.21, it follows that the result is true if $c(G) \leq 2$. We assume that G is nonhypoenergetic for $1 \leq c(G) < k$. Now, let G be a graph with $c(G) = k \geq 3$. In the following, we will repeatedly make use of the following claim:

Claim 1. *If there exists an edge cut F of G such that $G - F$ has exactly two components G_1, G_2 with $0 \leq c(G_1), c(G_2) < k$, and $G_1, G_2 \ncong S_1, S_3, S_4, W, K_{2,3}$, then we are done.*

Proof. It follows from Theorem 9.5 and the induction hypothesis that G_1 and G_2 are nonhypoenergetic. The claim follows from Lemma 9.14. ■

For convenience, we call an edge cut F of G a *good edge cut* if F satisfies the conditions in Claim 1. In what follows, we use $\hat{G}$ to denote the graph obtained from G by repeatedly deleting pendent vertices. Clearly, $c(\hat{G}) = c(G)$. Denote by $\kappa'(\hat{G})$ the edge connectivity of $\hat{G}$. Since $\Delta(\hat{G}) \leq 3$, we have $1 \leq \kappa'(\hat{G}) \leq 3$. Therefore, we only need to consider the following three cases.

Case 1. $\kappa'(\hat{G}) = 1$.

Let e be an edge cut of $\hat{G}$. Then $\hat{G} - e$ has exactly two components, say, H_1 and H_2. It is clear that $c(H_1) \geq 1$, $c(H_2) \geq 1$, and $c(H_1) + c(H_2) = k$. Consequently, $G - e$ has exactly two components G_1 and G_2 with $c(G_1) \geq 1$, $c(G_2) \geq 1$, and $c(G_1) + c(G_2) = k$, where H_i is a subgraph of G_i for $i = 1, 2$. If neither G_1 nor G_2 is isomorphic to $K_{2,3}$, then we are done by Claim 1. Otherwise, by symmetry,

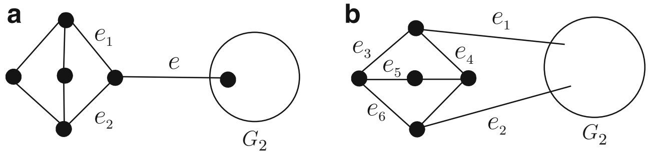

Fig. 9.10 The graphs used in Case 1 and Subcase 2.1 of Theorem 9.18

we assume that $G_1 \cong K_{2,3}$. Then G must have the structure shown in Fig. 9.10a. Now, let $F = \{e_1, e_2\}$. Then $G - F$ has exactly two components G_1' and G_2', where G_1' is a quadrangle and G_2' is a graph obtained from G_2 by adding a pendent edge. Therefore, $c(G_2') = k - 2$ and $G_2' \ncong K_{2,3}$, and so we are done by Claim 1.

Case 2. $\kappa'(\hat{G}) = 2$.

Let $F = \{e_1, e_2\}$ be an edge cut of $\hat{G}$. Then $\hat{G} - F$ has exactly two components, say, H_1 and H_2. Clearly, $c(H_1) + c(H_2) = k - 1 \geq 2$.

Subcase 2.1. $c(H_1) \geq 1$ and $c(H_2) \geq 1$.

Then $G - F$ has exactly two components G_1 and G_2 with $c(G_1) \geq 1$, $c(G_2) \geq 1$, and $c(G_1) + c(G_2) = k - 1$, where H_i is a subgraph of G_i for $i = 1, 2$. If neither G_1 nor G_2 is isomorphic to $K_{2,3}$, then we are done by Claim 1. Otherwise, by symmetry, we assume that $G_1 \cong K_{2,3}$. Then G must have the structure shown in Fig. 9.10b. Let $F' = \{e_2, e_3, e_4\}$. Then it is easy to see that F' is a good edge cut. The proof is thus complete.

Subcase 2.2. One of H_1 and H_2 is a tree. Let this be H_2.

Now, H_1 has at most 2 pendent edges since $\kappa'(\hat{G}) = 2$. Assume that e_3 is a pendent edge of H_1, and e_3 and e_2 are adjacent. Then $\{e_1, e_3\}$ is also an edge cut of $\hat{G}$, and $\hat{G} - \{e_1, e_3\}$ has exactly two components H_1' and H_2' satisfying $c(H_1') = c(H_1)$, $c(H_2') = 0$, and $|V(H_1')| < |V(H_1)|$. Thus, we finally get a 2-edge cut F', such that the component of $\hat{G} - F'$, which is not a tree, has no pendent edges. Without loss of generality, assume that $F = \{e_1, e_2\}$ is such an edge cut.

Therefore, $G - F$ has exactly two components G_1 and G_2 with $c(G_1) = k - 1$ and $c(G_2) = 0$. If $G_1 \ncong K_{2,3}$ and $G_2 \ncong S_1, S_3, S_4, W$, then we are done by Claim 1. So, we assume that this is not true. We only need to consider the following five cases.

Subsubcase 2.2.1. $G_2 \cong S_1$.

Let $V(G_2) = \{x\}$. Ten $e_1 = xx_1$ and $e_2 = xx_2$ since H_1 has no pendent vertices. We may assume that $N_{G_1}(x_2) = \{y_1, y_2\}$ (see Fig. 9.11a, where one of y_1 and y_2 may be equal to x_1). Let $F' = \{e_1, x_2y_1, x_2y_2\}$. Then $G - F'$ has exactly two components G_1' and G_2' such that G_1' is a graph obtained from G_1 by deleting a vertex of degree 2 and G_2' is a tree of order 2. Therefore, $c(G_1') = k - 2$. If $G_1' \ncong K_{2,3}$, then we are done by Claim 1. Otherwise, G must be the graph depicted in Fig. 9.11b. It is easy to see that $F'' = \{e_1, e_3, e_4, e_5\}$ is a good edge cut.

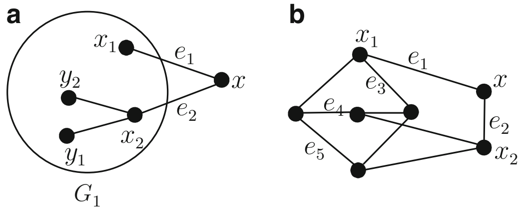

Fig. 9.11 The graphs used in Subsubcase 2.2.1 of Theorem 9.18

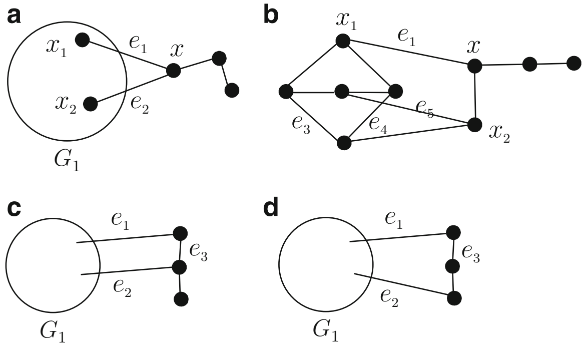

Fig. 9.12 The graphs used in Subsubcase 2.2.2 of Theorem 9.18

Subsubcase 2.2.2. $G_2 \cong S_3$.

If e_1 and e_2 are incident with a common vertex in G_2, then G must have the structure shown in Fig. 9.12a. In a similar way as in the proof of Subsubcase 2.2.1, we conclude that there exists an edge cut F' such that $G - F'$ has exactly two components G_1' and G_2' satisfying the conditions that $c(G_1') = k - 2$, and G_2' is a path of order 4. If $G_1' \ncong K_{2,3}$, then we are done by Claim 1. Otherwise, G must be the graph shown in Fig. 9.12b. It is easy to see that $F'' = \{e_1, e_3, e_4, e_5\}$ is a good edge cut.

If e_1 and e_2 are incident with two different vertices in G_2, then G must have the structure shown in Fig. 9.12c or d. It is easy to see that $F' = \{e_2, e_3\}$ is a good edge cut. The proof is thus complete.

Subsubcase 2.2.3. $G_2 \cong S_4$.

If e_1 and e_2 are incident with a common vertex in G_2, then G must have the structure shown in Fig. 9.13a. Similarly as in the proof of Subsubcase 2.2.1, we find that there exists an edge cut F' such that $G - F'$ has exactly two components G_1' and G_2' satisfying the conditions that $c(G_1') = k - 2$ and G_2' is a tree of order 5. If $G_1' \ncong K_{2,3}$, then we are done by Claim 1. Otherwise, G is the graph given in Fig. 9.13b. It is easy to see that $F'' = \{e_1, e_3, e_4, e_5\}$ is a good edge cut.

If e_1 and e_2 are incident to two different vertices in G_2, then G must have the structure shown in Fig. 9.13c. It is easy to see that $F' = \{xy, yz\}$ is a good edge cut. The proof is thus complete.

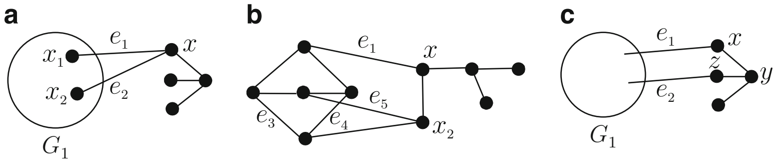

Fig. 9.13 The graphs used in Subsubcase 2.2.3 of Theorem 9.18

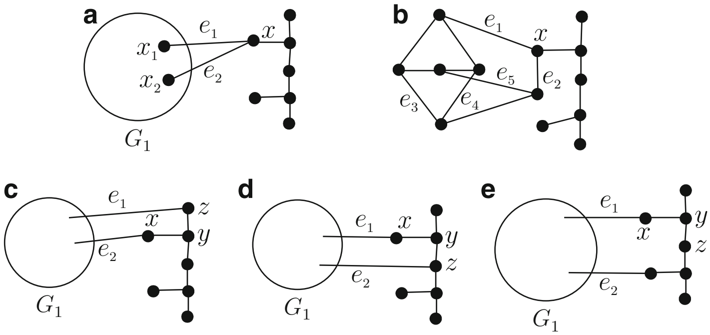

Fig. 9.14 The graphs used in Subsubcase 2.2.4 of Theorem 9.18

Subsubcase 2.2.4. $G_2 \cong W$.

If e_1 and e_2 are incident to a common vertex in G_2, then G must have the structure shown in Fig. 9.14a. Similarly as in the proof of Subsubcase 2.2.1, we obtain that there exists an edge cut F' such that $G - F'$ has exactly two components G_1' and G_2' satisfying the conditions $c(G_1') = k-2$ and that G_2' is a tree of order 8. If $G_1' \ncong K_{2,3}$, then we are done by Claim 1. Otherwise, G is the graph given in Fig. 9.14b. It is easy to see that $F'' = \{e_1, e_3, e_4, e_5\}$ is a good edge cut.

If e_1 and e_2 are incident to two different vertices in G_2, then G must have the structure shown in Fig. 9.14c, d or e. It is easy to see that $F' = \{xy, yz\}$ is a good edge cut. The proof is thus complete.

Subsubcase 2.2.5. $G_1 \cong K_{2,3}$ and $G_2 \ncong S_1, S_3, S_4, W$.

It is easy to see that G must have the structure shown in Fig. 9.10b. Let $F' = \{e_1, e_4, e_5, e_6\}$. Then $G - F'$ has exactly two components G_1' and G_2', where G_1' is a tree of order 2 and G_2' is a tree of order at least 4. It is easy to see that G_2' cannot be isomorphic to S_4 or W. Therefore, we are done by Claim 1. The proof is thus complete.

Case 3. $\kappa'(\hat{G}) = 3$.

Noticing that $\Delta(\hat{G}) \leq 3$ and $\Delta(G) \leq 3$, we obtain that $G = \hat{G}$ is a connected 3-regular graph.

Let $F = \{e_1, e_2, e_3\}$ be an edge cut of G. Then $G - F$ has exactly two components, say, G_1 and G_2. Clearly, $c(G_1) + c(G_2) = k - 2 \geq 1$.

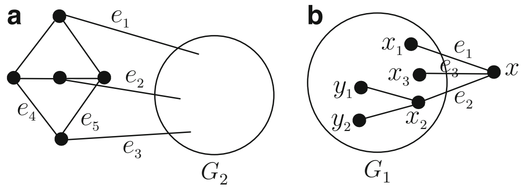

Fig. 9.15 The graphs used in Case 3 of Theorem 9.18

Subcase 3.1. $c(G_1) \geq 1$ and $c(G_2) \geq 1$.

If neither G_1 nor G_2 is isomorphic to $K_{2,3}$, then we are done by Claim 1. Otherwise, by symmetry, we assume that $G_1 \cong K_{2,3}$. Then G must have the structure shown in Fig. 9.15a.

Let $F' = \{e_1, e_2, e_4, e_5\}$. Then it is easy to see that F' is a good edge cut. The proof is thus complete.

Subcase 3.2. One of G_1 and G_2, say G_2, is a tree.

Let $|V(G_2)| = n_2$. Then we have $3n_2 = \sum_{v \in V(G_2)} d_G(v) = 2(n_2-1)+3 = 2n_2+1$. Therefore, $n_2 = 1$, i.e., $G_2 = S_1$. Let $V(G_2) = \{x\}$. Then $e_1 = xx_1$, $e_2 = xx_2$, and $e_3 = xx_3$. Let $N_{G_1}(x_2) = \{y_1, y_2\}$ (see Fig. 9.15b). Let $F' = \{e_1, e_3, x_2y_1, x_2y_2\}$. Since $\kappa'(G) = 3$, $G - F'$ has exactly two components G_1' and G_2', where G_1' is a graph obtained from G_1 by deleting a vertex of degree 2 and G_2' is the tree of order 2. Therefore, $c(G_1') = k - 3$. It is easy to check that $G_1' \ncong K_{2,3}$. If G_1' is a tree, then we have $|V(G_1')| = 2$ since $3|V(G_1')| = \sum_{v \in V(G_1')} d_G(v) = 2(|V(G_1')| - 1) + 4 = 2|V(G_1')| + 2$. Therefore, we are done by Claim 1. ■

Remark 9.2. Let W^* be the 6-vertex tree obtained by attaching two pendent vertices to each of the vertices of S_2. Majstorović et al. [363] proposed:

Conjecture 9.1. The star S_2, the graph W^*, and the complete bipartite graphs $K_{2,2}$ and $K_{3,3}$ are the only four connected graphs with maximum degree $\Delta \leq 3$ whose energies are equal to the number of vertices.

Li and Ma gave a confirmative proof of this conjecture. The proof is similar to that of Theorem 9.18; for details, see [335].

Chapter 10
Miscellaneous

In this chapter we have collected results on graph energy that could not be outlined elsewhere.

Characterizing the set of positive numbers that can occur as the energy of a graph has been a problem of interest. In this connection, Rao [412] asked whether the energy of a graph can ever be an odd integer. We first prove that such a case cannot happen, i.e., if $\mathscr{E}$ is an integer, then it is an even integer [28]. In fact, we show that if the energy is rational, then it must be an even integer. The proof is based on the concept of the additive compound introduced by Fiedler [114, 115].

Let $\mathbf{A}$ be the adjacency matrix of a graph G with order n. Let $\mathbf{B}$ be an $n \times n$ matrix, and let $1 \leq k \leq n$ be an integer. The *k-th additive compound* $\mathscr{A}_k(\mathbf{B})$ is a matrix of order $\binom{n}{k} \times \binom{n}{k}$ defined as follows. The rows and the columns of $\mathscr{A}_k(\mathbf{B})$ are indexed by the k-subsets of $\{1, 2, \ldots, n\}$, arranged in an arbitrary, but fixed, order. Let S and T be subsets of $\{1, 2, \ldots, n\}$. The (S, T)-entry of $\mathscr{A}_k(\mathbf{B})$ is the coefficient of x in the expansion of the determinant of the submatrix of $\mathbf{B} + x\,\mathbf{I}$ indexed by the rows in S and the columns in T.

As an example, let

$$\mathbf{B} = \begin{bmatrix} 2 & 3 & 1 \\ -1 & 0 & 2 \\ 4 & 1 & 3 \end{bmatrix}.$$

Let the 2-subsets of $\{1, 2, 3\}$ be arranged as $\{1, 2\}, \{1, 3\}, \{2, 3\}$. The submatrix of $\mathbf{B} + x\,\mathbf{I}$, indexed by the rows and the columns in $\{1, 2\}$, is given by $\begin{bmatrix} 2 + x & 3 \\ -1 & x \end{bmatrix}$. The coefficient of x in the determinant of this matrix is 2, and hence, the $(1, 1)$-entry of $\mathscr{A}_2(\mathbf{B})$ is 2. It can be checked that the second additive compound of $\mathbf{B}$ is given by

$$\mathscr{A}_2(\mathbf{B}) = \begin{bmatrix} 2 & 2 & -1 \\ 1 & 5 & 3 \\ -4 & -1 & 3 \end{bmatrix}.$$

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_10,

The main result of Fiedler on additive compounds is the following: If $\mu_1, \ldots, \mu_n$ are the eigenvalues of $\mathbf{B}$, then the eigenvalues of $\mathscr{A}_k(\mathbf{B})$ are given by $\mu_{i_1} + \cdots + \mu_{i_k}$, for all $1 \le i_1 < \cdots < i_k \le n$.

Consider now the graph G with the $n \times n$ adjacency matrix $\mathbf{A}$. As before, let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $\mathbf{A}$. Without loss of generality, we assume that $\lambda_1, \ldots, \lambda_k$ are positive and the rest are nonpositive. Since the trace of $\mathbf{A}$ is zero, the energy of G is $2\sum_{i=1}^{k} \lambda_i$. Note that the characteristic polynomial of $\mathscr{A}_k(\mathbf{A})$ is a monic polynomial with integer coefficients. Also, $\sum_{i=1}^{k} \lambda_i$ is an eigenvalue of $\mathscr{A}_k(\mathbf{A})$ by the result of Fiedler mentioned above. It follows that if $\sum_{i=1}^{k} \lambda_i$ is rational, then it must be an integer. Thus, if the energy of G is rational, then it must be an even integer.

Theorem 10.1. *The energy of a graph cannot be an odd integer.* ■

We conclude this consideration with some remarks. Clearly, the above technique yields the more general result that if $\mathbf{A}$ is any $n \times n$ symmetric matrix with integer entries, then the sum of the moduli of its eigenvalues cannot be an odd integer. This was also conjectured by Rao in a personal communication. It may also be noted that every positive even integer is the energy of a graph. In fact, the energy of the complete bipartite graph K_{1,p^2} is $2p$.

In what follows, we demonstrate the validity of a slightly more general result of the same kind [394]:

Theorem 10.2. *The energy of a graph cannot be the square root of an odd integer.*

In order to prove Theorem 10.2, we need some preliminaries.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with disjoint vertex sets of orders n_1 and n_2, respectively. The *product* of G_1 and G_2, denoted by $G_1 \times G_2$, is the graph with vertex set $V(G_1) \times V(G_2)$ such that two vertices $(x_1, x_2) \in V(G_1 \times G_2)$ and $(y_1, y_2) \in V(G_1 \times G_2)$ are adjacent if and only if $x_1 y_1 \in E_1$ and $x_2 y_2 \in E_2$. The *sum* of G_1 and G_2, denoted by $G_1 + G_2$, is the graph with vertex set $V(G_1) \times V(G_2)$ such that two vertices $(x_1, x_2) \in V(G_1 + G_2)$ and $(y_1, y_2) \in V(G_1 + G_2)$ are adjacent if and only if either $x_1 y_1 \in E_1$ and $x_2 = y_2$ or $x_2 y_2 \in E_2$ and $x_1 = y_1$.

The above-specified two graph products have the following spectral properties (see [81], p.70). Let $\lambda_i^{(1)}, i = 1, \ldots, n_1$ and $\lambda_j^{(2)}, j = 1, \ldots, n_2$ be, respectively, the eigenvalues of G_1 and G_2.

Lemma 10.1. *The eigenvalues of* $G_1 \times G_2$ *are* $\lambda_i^{(1)} \lambda_j^{(2)}$, $i = 1, \ldots, n_1$, $j = 1, \ldots, n_2$. ■

Lemma 10.2. *The eigenvalues of* $G_1 + G_2$ *are* $\lambda_i^{(1)} + \lambda_j^{(2)}$, $i = 1, \ldots, n_1$, $j = 1, \ldots, n_2$. ■

The eigenvalues of a graph are the zeros of the characteristic polynomial, and the characteristic polynomial is a monic polynomial with integer coefficients. Therefore, we have:

Lemma 10.3. *If an eigenvalue of a graph is a rational number, then it is an integer.* ■

Proof of Theorem 10.2. Consider a graph G, and let $\lambda_1, \lambda_2, \ldots, \lambda_m$ be its positive eigenvalues. Then, as explained above, $\mathscr{E}(G) = 2\sum_{i=1}^{m} \lambda_i$. Denote $\lambda_1 + \lambda_2 + \cdots + \lambda_m$ by λ. By Lemma 10.2, λ is an eigenvalue of some graph H isomorphic to the sum of m disjoint copies of the graph G. By Lemma 10.1, λ^2 is an eigenvalue of the product of two disjoint copies of the graph H.

Suppose that now $\mathscr{E}(G) = \sqrt{q}$, where q is some integer. Then $2\lambda = \sqrt{q}$, i.e., $\lambda^2 = q/4$. If q would be an odd integer, then $q/4$ would be a nonintegral rational number in contradiction to Lemma 10.3.

Therefore, Theorem 10.2 follows. ■

We have an immediate extension of Theorem 10.2:

Observation. The energy of a graph cannot be the square root of the double of an odd integer.

However, this observation is just a special case of a somewhat more general result.

Let H be the same graph as in the preceding section. Thus, λ is an eigenvalue of H. Let H^* be the product of r disjoint copies of H. Then by Lemma 10.1, λ^r is an eigenvalue of H^*. Suppose now that $\mathscr{E}(G) = q^{1/r}$, where q is some integer. Then $2\lambda = q^{1/r}$, i.e., $\lambda^r = q/2^r$. If q would not be divisible by 2^r, then λ^r would be a nonintegral rational number in contradiction to Lemma 10.3. Therefore we have:

Theorem 10.3. *Let r and s be integers such that $r \geq 1$ and $0 \leq s \leq r$ and q be an odd integer. Then $\mathscr{E}(G)$ cannot be of the form $(2^s\,q)^{1/r}$.* ■

For $r = 1$ and $s = 0$, Theorem 10.3 reduces to Theorem 10.1, while for $r = 2$ and $s = 0$, Theorem 10.3 reduces to Theorem 10.2. The The above observation corresponds to $r = 2$ and $s = 1$.

Using the automated conjecture generator GRAFITTI, Fajtlowicz obtained a number of conjectures, of which some pertain to graph energy. Then he proved [107] that $\mathscr{E} > 2\,\mu$, where μ is the maximal cardinality of a matching. Favaron et al. [113] verified the validity of another conjecture by Fajtlowicz, namely, that $\mathscr{E} \geq 2r$, where r is the radius of the graph. More on computer-generated graph conjectures (related to energy) can be found in the survey [20].

Rojo and Medina [423] demonstrated that if G is an arbitrary bipartite graph and k a positive integer, then one can construct a graph G', such that $\mathscr{E}(G') = \sqrt{k}\,\mathscr{E}(G)$.

In [537], the following Nordhaus–Gaddum-type bounds for graph energy were obtained:

$$2(n-1) \leq E(G) + E(\overline{G}) < \sqrt{2}\,n + (n-1)\sqrt{n-1}$$

where $\overline{G}$ is the complement of G. Equality on the left-hand side is attained if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

For a survey on Nordhaus–Gaddum-type relations, see [21].

Akbari and Ghorbani [8] obtained relations between $\mathscr{E}$ and the choice number of a graph, whereas Akbari, Ghorbani, and Zare [11] established relations between $\mathscr{E}$, chromatic number, and the rank of the adjacency matrix. In [257,495], the energy of trees with given domination number is examined. Considerations relevant for graph reconstruction are reported in [455].

One of the present authors together with a Chilean–Portuguese collaboration communicated the first findings on the energy of the line graph [221]; for further results along these lines, see [421,422].

The energy of unitary Cayley graphs was studied in [284,302,411], whereas the energy of circulant graphs in [35,286,428,429,438,453]; the paper [285] considers the distance energy of circulant graphs (cf. the subsequent chapter). In [287], pairs of noncospectral circulant graphs were constructed, having equal energy, Laplacian energy, and distance energy (cf. the subsequent chapter). The works [294,295,357, 420,422,444,504,513] deal with the energies of other special classes of graphs.

A graph is said to be antiregular if all its vertices, except two, have different degrees. Munarini [379] reported results on the spectral properties of antiregular graphs, including those on their energy.

Torgašev [462] determined all graphs with the property $\mathscr{E} \leq 3$. Walikar et al. [479] studied the energies of trees with matching number 3. Neither research was later extended to values greater than 3.

The energy of graphs with weighted edges was not much examined so far. If the weight of an edge increases, the graph energy may either increase or decrease. Cases were determined where the energy is a monotonically increasing function of (positive) edge weights [223]. The simplest such case is when the respective edge is a bridge [435].

Chapter 11
Other Graph Energies

Motivated by the large number of interesting and nontrivial mathematical results that have been obtained for the graph energy, several other energy-like quantities were proposed and studied in the recent mathematical and mathematico–chemical literature. These are listed and briefly outlined in this chapter. Details of the theory of the main alternative graph energies can be found in the references quoted, bearing in mind that research along these lines is currently very active, and new papers/results appear on an almost weekly basis.

11.1 Laplacian Energy

The graph energy 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 [134, 135, 371, 373, 375].

The Laplacian matrix of an (n,m)-graph G is defined as $\mathbf{L}(G) = \triangle(G) - \mathbf{A}(G)$, where $\mathbf{A}$ is the adjacency matrix and $\triangle$ the diagonal matrix whose diagonal elements are the vertex degrees. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of $\mathbf{L}(G)$.

Because $\mu_i \geq 0$ and $\sum_{i=1}^{n} \mu_i = 2m$, it would be trivial to define the Laplacian spectrum version of graph energy as $\sum_{i=1}^{n} |\mu_i|$. Instead, the Laplacian energy was conceived as [250]

$$\mathrm{LE} = \mathrm{LE}(G) := \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| . \tag{11.1}$$

This definition is adjusted so that for regular graphs, $\mathrm{LE}(G) = \mathscr{E}(G)$.

Various properties of the Laplacian energy were established in the papers [13, 44, 57, 96, 109, 110, 119, 184, 250, 322, 351, 353, 401, 417–419, 441, 446, 454, 463, 481, 531–533, 536, 537, 539]. Of these, we mention the conjecture [184] that for all graphs, $\mathrm{LE} \geq \mathscr{E}$. This conjecture was corroborated by numerous examples [184, 401] but was eventually, by means of counterexamples, shown to be false in

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2_11,

the general case [351, 454]. Finally, it was proven [418, 441] that $\mathrm{LE}(G) \geq \mathcal{E}(G)$ holds for all bipartite graphs. Du et al. [104] proved that the conjecture is true for almost all graphs (see also [103]).

The fact that for a (disconnected) graph G consisting of (disjoint) components G_1 and G_2, the equality

$$\mathrm{LE}(G) = \mathrm{LE}(G_1) + \mathrm{LE}(G_2) \tag{11.2}$$

is not generally valid, may be considered as a serious drawback of the Laplacian-energy concept [250]. An attempt to overcome this problem is outlined in Sect. 11.4.

The Nordhaus–Gaddum-type bounds [21] for LE read [537]

$$2(n-1) \leq \mathrm{LE}(G) + \mathrm{LE}(\overline{G}) < n\sqrt{n^2-1}$$

with equality on the left-hand side if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

In [401], it was found that the energy and the Laplacian energy behave very differently for trees, namely, that the energy and the Laplacian energy of a tree are nearly inversely proportional. It was conjectured [401] that

$$\mathrm{LE}(P_n) < \mathrm{LE}(T) < \mathrm{LE}(S_n)$$

holds for any tree T on n vertices, different from the path (P_n) and the star (S_n). Trevisan et al. [463] have shown that the conjecture is true for trees of diameter 3. Furthermore, the authors of [119] proved that the right-hand side of the above conjecture is generally true.

In [1, 441], also the analogue of LE, obtained from the signless Laplacian matrix $\mathbf{L}^+(G) = \triangle(G) + \mathbf{A}(G)$, was considered. Details of the theory of spectra of the signless Laplacian matrix are found in the review [88]. Let $\mu_1^+, \mu_2^+, \ldots, \mu_n^+$ be the eigenvalues of $\mathbf{L}^+(G)$. Then, in analogy to Eq. (11.1), we define

$$\mathrm{LE}^+ = \mathrm{LE}^+(G) := \sum_{i=1}^{n} \left| \mu_i^+ - \frac{2m}{n} \right| .$$

Also in this case, for regular graphs, $\mathrm{LE}^+(G) = \mathcal{E}(G)$.

For bipartite graph $\mathrm{LE}^+ = \mathrm{LE}$. For nonbipartite graphs, the relation between LE^+ and LE is not known but seems to be not simple. More on LE^+ is found in Sect. 11.4.

11.2 Distance Energy

Let G be a connected graph on n vertices, whose vertices are $v_1, v_2, \ldots, v_n$. The distance matrix $\mathbf{D}(G)$ of G is the matrix whose (i, j)-entry is the distance (= length of the shortest path) between the vertices v_i and v_j. The spectrum of the distance matrix was studied [80, 370] but to a much lesser extent than the spectra of the adjacency and Laplacian matrices.

Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of $\mathbf{D}(G)$. Since the sum of these eigenvalues is zero, there is no obstacle to define the distance energy as [291, 402]

$$\mathrm{DE} = \mathrm{DE}(G) := \sum_{i=1}^{n} |\rho_i| \,.$$

Until now, only some elementary (and not very exciting) properties of the distance energy were established: bounds [45,103,137,289,291,405,541], examples of distance equienergetic graphs [290,355,402,406], and formulas for DE of special types of graphs [52, 285, 406, 452]. For a generalization of the distance–energy concept, see [323].

11.3 Energy of Matrices

Nikiforov [383, 384, 387] proposed a significant extension and generalization of the graph–energy concept. Let $\mathbf{M}$ be a $p \times q$ matrix with real-valued elements, and let $s_1, s_2, \ldots, s_p$ be its singular values. Then the energy of $\mathbf{M}$ is defined as [383]

$$\mathscr{E}(\mathbf{M}) := \sum_{i=1}^{p} s_i \,. \tag{11.3}$$

Recall that the singular values of the (real) matrix $\mathbf{M}$ are equal to the (positive) square roots of the eigenvalues of $\mathbf{M}\mathbf{M}^t$. The definition of the energy of a matrix is just the trace or nuclear norm of the matrix, and this norm is widely studied in matrix theory and functional analysis. We refer the readers to [31] (p. 35) and [386].

Formula (11.3) is in full harmony with the ordinary graph–energy concept. As easily seen, $\mathscr{E}(G) = \mathscr{E}(\mathbf{A}(G))$. Also,

$$\mathrm{LE}(G) = \mathscr{E}\left(\mathbf{L}(G) - \frac{2m}{n}\mathbf{I}\right) \qquad \text{and} \qquad \mathrm{LE}^+(G) = \mathscr{E}\left(\mathbf{L}^+(G) - \frac{2m}{n}\mathbf{I}\right) .$$

Viewing at graph energy as the sum of the singular values of the adjacency matrix enabled one to use a theorem earlier discovered by Fan [108], by means of which several new results on $\mathscr{E}$ could be deduced [10, 55, 94, 95, 418, 441].

By means of formula (11.3), an infinite number of "energies" can be imagined. Until now, only the energy of the incidence matrix (see Sect. 11.4) and the energy of an arbitrary (square) (0, 1)-matrix [301] were studied. Let us hope that no graph/matrix–energy deluge will happen in the future, but see [5, 15, 22, 32, 44, 46, 78, 92, 122, 138, 303, 304, 366, 381, 424, 436, 460, 545].

11.4 LEL and Incidence Energy

In order to find a Laplacian-eigenvalue-based energy, in which a formula of the type (11.2) would be generally valid, Liu and Liu [350] proposed a "Laplacian-energy-like" invariant, defined as

$$\mathrm{LEL} = \mathrm{LEL}(G) := \sum_{i=1}^{n} \sqrt{\mu_i} \tag{11.4}$$

where the notation is same as in Sect. 11.1. As a direct consequence of this definition, the relation

$$\mathrm{LEL}(G) = \mathrm{LEL}(G_1) + \mathrm{LEL}(G_2)$$

is satisfied by any graph G whose components are G_1 and G_2. On the other hand, if G is a regular graph, then $\mathrm{LEL}(G) = \mathscr{E}(G)$ does not hold.

Formula (11.4) does not have the form of an "energy" and therefore was initially viewed as a dead end of the research on graph energies. Only a few results on LEL were reported [54,103,288,345,354,356,445,450,451,456,461,546]. It was pointed out [251] that in spite of its dependence on Laplacian eigenvalues, LEL is more similar to $\mathscr{E}$ than to LE.

The Laplacian eigenvalues $\mu_1, \mu_2, \dots, \mu_n$ are the zeros of the Laplacian characteristic polynomial $\psi(G,\lambda)$. Therefore, the numbers $\pm\sqrt{\mu_i}$, $i = 1, 2, \dots, n$ are the zeros of the polynomial $\psi(G,\lambda^2)$. Consequently, $\mathrm{LEL}(G)$ is equal to half of the sum of the absolute values of all zeros of $\psi(G,\lambda^2)$ which makes it possible to apply the Coulson integral technique, cf. Chap. 3. In particular, since

$$\psi(G,\lambda) = \sum_{k\geq 0} (-1)^k \, c_k(G)\, \lambda^{n-k}$$

with $c_k(G) \geq 0$ for all $k \geq 0$ (see [81]), in analogy to Eq. (3.12), we get [195]

$$\mathrm{LEL}(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{\mathrm{d}x}{x^2} \ln \left[\sum_{k\geq 0} c_k(G)\, x^{2k} \right] . \tag{11.5}$$

From formula (11.5), we see that $\mathrm{LEL}(G)$ is a monotonically increasing function of each of the coefficients $c_k(G)$.

For any n-vertex tree T, it has been shown [538] that for all $k \geq 0$,

$$c_k(S_n) \leq c_k(T) \leq c_k(P_n) \tag{11.6}$$

and that equality for all values of k occurs if and only if $T \cong S_n$ and $T \cong P_n$, respectively. Combining (11.5) and (11.6), we immediately obtain

$$\mathrm{LEL}(S_n) \leq \mathrm{LEL}(T) \leq \mathrm{LEL}(P_n)$$

with equality if and only if $T \cong S_n$ and $T \cong P_n$, respectively.

Independently of the research on LEL, Jooyandeh et al. [299] introduced the "incidence energy" IE as the energy of the incidence matrix of a graph, cf. Eq. (11.3).

If G is a graph with vertices $v_1, v_2, \ldots, v_n$ and edges $e_1, e_2, \ldots, e_m$, then its vertex-edge incidence matrix is an $n \times m$ matrix whose (i, j)-entry is equal to 1 if v_i is an end vertex of the edge e_j and is zero otherwise.

It could be shown that [195]

$$\mathrm{IE}(G) = \sum_{i=1}^{n} \sqrt{\mu_i^+}$$

which, in turn, implies that for bipartite graphs, the incidence energy is same as LEL. This finding gave a new rationale to the study of both LEL and IE. A few results obtained along these lines can be found in the papers [9,196,251,456,457,534,542]. For a review on both LEL and IE, see [346]. For generalizations of incidence energy, see [323, 448, 449].

11.5 Other Energies

In the general case, the eigenvalues of a digraph are complex numbers. In view of this, the definition of graph energy via Eq. (1.2) cannot be straightforwardly extended to digraphs. According to Rada [23, 136, 392, 396–398], the energy of a digraph D with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ can be defined as

$$\mathscr{E}(D) := \sum_{i=1}^{n} |Re(\lambda_i)|$$

where $Re(z)$ stands for the real part of the complex number z. If so, then the Coulson integral formula is applicable to $\mathscr{E}(D)$.

Another approach to the energy of digraphs is the previously mentioned work by Kharaghani and Tayfeh-Rezaie [301], utilizing the singular values of the adjacency matrix of D.

When speaking of the energy of a digraph, one must not forget that the existence of a directed cycle is a necessary condition for the existence of a nonzero eigenvalue. In other words, the energy of a digraph without directed cycles (e.g., of any directed tree) is equal to zero.

A third approach to digraphs was put forward by Adiga, Balakrishnan, and So [2]. They and some other authors [126, 460] studied the *skew energy* defined as the sum of the absolute values of the eigenvalues of the skew-adjacency matrix. (Recall that the (i, j)-entry of the skew-adjacency matrix is $+1$ if an edge is directed from the i-th vertex to the j-th vertex, in which case the (j, i)-entry is -1. If there is no directed edge between the vertices i and j, then the respective matrix element is zero.) The skew Laplacian energy of a digraph was considered in [4].

The energy of signed graphs was also examined [122].

Without being aware of the Laplacian and distance energy, Consonni and Todeschini [71] introduced a whole class of matrix-based quantities, defined as

$$\sum_{i=1}^{n} |x_i - \overline{x}| \tag{11.7}$$

where $x_1, x_2, \ldots, x_n$ are the eigenvalues of the respective matrix, and $\overline{x}$ is their arithmetic mean. Evidently, if the underlying matrix is the adjacency, Laplacian, or distance matrix, then the quantity defined via (11.7) is just the ordinary graph energy, Laplacian energy, and distance energy, respectively. Consonni and Todeschini used the invariants defined via (11.7) for constructing mathematical models capable to predict various physicochemical properties of organic molecules. Therefore, their article [71] is valuable for documenting the applicability of various "energies" in natural sciences (in particular, in chemistry).

Motivated by formula (11.7), in the paper [193], its "ultimate" extension was proposed. Namely, $x_1, x_2, \ldots, x_n$ may be arbitrary real numbers without any need to be associated with some graph or matrix. Even then, some general properties of this "ultimate energy," in particular lower and upper bounds, could be established [193]:

$$\sqrt{n\,\mathrm{Var}(x) + n(n-1)\,P(\overline{x})^{2/n}} \leq \sum_{i=1}^{n} |x_i - \overline{x}| \leq n\,\mathrm{Var}(x)$$

where $\mathrm{Var}(x)$ is the variance of the numbers $x_1, x_2, \ldots, x_n$ and $P(x) = \prod_{i=1}^{n} (x - x_i)$. Earlier reported lower and upper bounds for energy, Laplacian energy, and distance energy happen to be special cases of the above bounds for the "ultimate energy."

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Index

X. Li et al., *Graph Energy*, DOI 10.1007/978-1-4614-4220-2,