1
Graph Energy

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1.1
Introduction

In this Chapter we are concerned with the eigenvalues of graphs and some of their chemical applications. Let G be a (simple) graph, with vertex set $V(G)$ and edge set $E(G)$. The number of vertices of G is n , and its vertices are labelled by $v_1, v_2, \ldots, v_n$. The adjacency matrix $A(G)$ 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 eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the adjacency matrix $A(G)$ are said to be the *eigenvalues of the graph G* and to form its *spectrum*. Details of the spectral theory of graphs can be found in the seminal monograph [1].

The characteristic polynomial of the adjacency matrix, i. e., $\det(\lambda I_n - A(G))$, where 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 $\phi(G, \lambda)$. From linear algebra is known that the graph eigenvalues are just the solutions of the equation $\phi(G, \lambda) = 0$.

One of the most remarkable chemical application of graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of π-electrons in conjugated hydrocarbons. For details, see [2–4]. If G is a molecular graph of a conjugated hydrocarbons with n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then in the so-called Hüchkel molecular orbital (HMO) approximation [3,5], the energy of the i-th molecular orbital is given by

$$E_i = \alpha + \lambda_i \, \beta$$

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where α and β are pertinent constants. In order to simplify the formalism, it is customary to set $\alpha = 0$ and $\beta = 1$ in which case the π-electron orbital energies and the graph eigenvalues coincide.

The total π-electron energy (E) is equal to the sum of the energies of all π-electrons that are present in the respective molecule, i. e., $E = \sum_{i=1}^{n} g_i E_i = \sum_{i=1}^{n} g_i \lambda_i$, where g_i is the number of electrons in the i-th molecular orbital (whose energy is E_i). Because of restrictions coming from the Pauli exclusion principle [5], g_i is 2, 1, or 0. In the majority of chemically relevant cases, $g_i = 2$ whenever $\lambda_i > 0$ and $g_i = 0$ whenever $\lambda_i < 0$, implying $E = 2 \sum_{+} \lambda_i$ with $\sum_{+}$ indicating the summation over positive eigenvalues. Because the sum of all eigenvalues is zero, one immediately arrives at

$$E = E(G) = \sum_{i=0}^{n} |\lambda_i| \,. \tag{1.1}$$

The total π-electron energy and, in particular, the right–hand side of Eq. (1.1) was studied already in the pioneering days of quantum chemistry (see, e. g., [6]). In the 1970s one of the present authors [7] came to the idea to define the *energy of a graph* G as the sum of the absolute values of its eigenvalues. By this, Eq.(1.1) could now be viewed as the definition of a graph invariant (that in the case of some special graphs has a chemical interpretation), but which is applicable to all graphs. This seemingly insignificant change of the approach to $E(G)$ eventually resulted in the development of an entire new *theory of graph energy*. In this Chapter we outline its main results, especially those obtained in the last decade. For earlier mathematical results on graph energy see the review [8] whereas for its chemical aspects [9, 10]

Although put forward already in the 1970s [7], and having much older roots in theoretical chemistry [6], the concept of graph energy has for a long time failed to attract the attention of mathematicians and mathematical chemists. However, around the year 2000, research on graph energy suddenly became a very popular topic, resulting in numerous significant discoveries, and in a remarkable number of publications. Since 2001 over one hundred mathematical papers on E were produced, more than one per month.

This Chapter has six sections, followed by a detailed (yet far from complete) bibliography on graph energy. In the second section numerous upper and lower bounds for graph energy are given, and in many cases the graphs achieving these bounds are characterized. The third section is concerned with hyperenergetic ($E > 2n - 2$) and hypoenergetic ($E < n$) graphs, as well as with pairs of equienergetic graphs ($E(G_1) = E(G_2)$). The fourth section outlines some selected (of very many existing) results on graphs extremal with regard to energy. In the sixth section we briefly state a few results on graph energy, that could not be included in the previous three sections. Concluding remarks are given in the last section.

1.2 Bounds for the energy of graphs

Let G be a graph possessing n vertices and m edges. We say that G is an (n, m)-graphs.

For any (n, m)-graph [1], $\sum_{i=1}^{n} \lambda_i^2 = 2m$.

In what follows we assume that the graph eigenvalues are labelled in a non-increasing manner, i. e., that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \,.$$

If G is connected, then $\lambda_1 > \lambda_2$ [1]. Because $\lambda_1 \geq |\lambda_i|$, $i = 2, \ldots, n$, the eigenvalue λ_1 is referred to as the *spectral radius* of the graph G .

Some simplest and long time known [8] bounds for energy of are the following:

Theorem 1.1 *[11] For an (n, m)-graph G ,*

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

with equality if and only if G is either an empty graph (with $m = 0$, i. e., $G \cong \overline{K_n}$), or a regular graph of degree 1, i. e., $G \cong (n/2)K_2$.

Theorem 1.2 *[12] For a graph G with m edges,*

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

Equality $E(G) = 2\sqrt{m}$ 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 $E(G) = 2m$ holds if and only if G consists of m copies of K_2 and arbitrarily many isolated vertices.

1.2.1 Some upper bounds

Using

$$\sum_{i=2}^{n} \lambda_i^2 = 2m - \lambda_1^2$$

together with the Cauchy–Schwarz inequality, applied to the $(n-1)$-dimensional vectors $(|\lambda_2|, \ldots, |\lambda_n|)$ and $(1, \ldots, 1)$, we obtain the inequality

$$\sum_{i=2}^{n} |\lambda_i| \leq \sqrt{(n-1)(2m-\lambda_1^2)} \, .$$

Thus, we have

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

Since $F(x) := x + \sqrt{(n-1)(2m-x^2)}$ is a decreasing function in the variable x, and the spectral radius obeys the inequality $\lambda_1 \geq 2m/n$ [1], we have:

Theorem 1.3 *[13] Let G be an (n,m)-graph. If $2m \geq n$, then*

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \, . \tag{1.2}$$

Moreover, equality holds in (1.2) if and only if G consists of $n/2$ copies of K_2, or $G \cong K_n$, or G is a non-complete connected strongly regular graph with two non-trivial eigenvalues both having absolute values equal to $\sqrt{(2m-(2m/n)^2)/(n-1)}$.

If $2m \leq n$, then the inequality

$$E(G) \leq 2m \tag{1.3}$$

holds. Moreover, equality holds in (1.3) if and only if G is a disjoint union of edges and isolated vertices.

Recall [1] that a graph G that is neither complete nor empty is said to be *strongly regular* with parameters (n,k,a,c) if it it has n vertices, it is regular of degree k, every pair of its adjacent vertices has a common neighbors, and every pair of its nonadjacent vertices has c common neighbors. A strongly regular graph with parameters (n,k,a,c) has only three distinct eigenvalues and the eigenvalues of G, that are different from k, are the zeros of the quadratic polynomial $x^2-(a-c)x-(k-c)$. Denote these eigenvalues by s and t, and let m_s and m_t be, respectively, their multiplicities. Since k has multiplicity equal to one, and the sum of all the eigenvalues is 0, we have $m_s + m_t = n-1$ and $m_s\, s + m_t\, t = -k$.

Using routine calculus, it can be shown that the left hand side of inequality (1.2) becomes maximal when $m = (n^2 + n\sqrt{n})/4$. It thus follows:

Theorem 1.4 *[13] Let G be a graph on n vertices. Then*

$$E(G) \leq \frac{n}{2}(\sqrt{n}+1) \tag{1.4}$$

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

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

Obviously, if such a graph with property $E = n(\sqrt{n}+1)/2$ does exist, then n must be a square of a positive integer. Very recently, Haemers [14] conjectured that $n = p^2$ is necessary and sufficient for the existence of such graphs. He also tried to construct such strongly regular graphs, and proved:

Theorem 1.5 *[14] 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) $n = 4^p\,,\ p \geq 1$*; (ii)* $n = 4^p\,q^4\,,\ p,q \geq 1$*; (iii)* $n = 4^{p+1}\,q^2\,,\ p \geq 1$ *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 1.5 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.

Earlier, McCelland [11] showed that $E(G) \leq \sqrt{2mn}$, see Theorem 1.1. It is easy to demonstrate [15] that the inequality (1.2), and therefore also (1.4), improve this bound.

For special classes of graphs one can obtain better bounds.

Theorem 1.6 *[16] Let G be a bipartite graph on* $n > 2$ *vertices. Then*

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n}+\sqrt{2}) \tag{1.5}$$

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

Recall [17] that a *2-(v,k,λ)-design* is a collection of k-subsets or blocks of a set of v points, such that each 2-set of points lies in exactly λ blocks. The incident matrix B of a 2-(v,k,λ)-design is the $v \times b$ matrix defined so that for each point x and block S, $B_{x,s} = 0$ if $x \in S$ and $B_{x,S} = 1$ otherwise.

A graph is said to be *semiregular bipartite* if it is bipartite and each vertex in the same part of bipartition has the same degree.

Among known bounds for λ_1, we need here the following [18]:

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

where $d_1, d_2, \ldots, d_n$ is the degree sequence of the underlying graph G. Equality holds if and only if G is either regular or semiregular bipartite.

Theorem 1.7 *[19] If G is an (n,m)-graph with degree sequence $d_1, d_2, \ldots, d_n$, then*

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

Equality holds if and only if G is either $(n/2)K_2$ (if $m = n/2$), or K_n (if $m = n(n-1)/2$), or a non-complete connected strongly regular graph with two non-trivial eigenvalues both having absolute value $\sqrt{(2m-(2m/n)^2)/(n-1)}$, or $n\,K_1$ (if $m = 0$).

Since

$$4m^2 = \left(\sum_{i=1}^{n} d_i\right)^2 \le n\sum_{i=1}^{n} d_i^2$$

and $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{2m/n} \le x \le \sqrt{2m}$, it follows that the upper bound of Theorem 1.8 is better than that of Theorem 1.6.

Theorem 1.8 *[19] If G is a bipartite (n,m)-graph, $n > 2$, with degree sequence $d_1, d_2, \ldots, d_n$, then*

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

Equality holds if and only if G is either $(n/2)K_2$, or a complete bipartite graph, or the incidence graph of a symmetric 2-(v,k,λ)-design with $k = 2m/n$ and $\lambda = k(k-1)/(v-1)$, $(n = 2v)$, or $n\,K_1$.

An extension of Theorem 1.8, for the case when the number of zero eigenvalues is known, was reported in [20].

For $v_i \in V(G)$, the *2-degree* of v_i, denoted by t_i, is the sum of degrees of the vertices adjacent to v_i. We call $\frac{t_i}{d_i}$ the *average degree* of 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 the vertices adjacent to v_i. A graph G is called *p-pseudo-regular* if there is a constant p, such that each vertex of G has average degree equal to p. A bipartite graph $G = (X, Y)$ is said to be (p_x, p_y)*-pseudo-semiregular* if there are two constants p_x and p_y, such that each vertex in X has average degree p_x and each vertex in Y has average degree p_y.

Theorem 1.9 *[21] Let G be an (n,m)-graph, $m > 0$, with degree sequence $d_1, d_2, \ldots, d_n$, and 2-degree sequence $t_1, t_2, \ldots, t_n$. Let*

$$D_2 = \sum_{i=1}^{n} d_i^2 \qquad \text{and} \qquad T_2 = \sum_{i=1}^{m} t_i^2 \,.$$

Then

$$E(G) \le 2\sqrt{T_2/D_2} + \sqrt{(n-1)(2m - T_2/D_2)} \,.$$

Equality holds if and only if either $G \cong (n/2)K_2$ or $G \cong K_n$ or G is a non-bipartite connected p-pseudo-regular graph with three distinct eigenvalues p, $\sqrt{(2m-p^2)/(n-1)}$, and $-\sqrt{(2m-p^2)/(n-1)}$, provided $p > \sqrt{2m/n}$.

Theorem 1.10 *[21] Let G be a bipartite (n,m)-graph, $m > 0$. Using the same notation as in Theorem 1.9, we have*

$$E(G) \le 2\sqrt{T_2/D_2} + \sqrt{(n-2)(2m - 2\,T_2/D_2)} \,.$$

Equality holds if and only if either $G \cong (n/2)K_2$, or $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1 r_2 = m$, or G is a connected (p_x, p_y)-pseudo-semiregular bipartite graph with four distinct eigenvalues $\sqrt{p_x\, p_y}$, $\sqrt{(2m - 2p_x\, p_y)/(n-2)}$, $-\sqrt{(2m - 2p_x\, p_y)/(n-2)}$, and $-\sqrt{p_x\, p_y}$, provided $p_x\, p_y > \sqrt{2m/n}$.

Theorem 1.11 *[22] Let G be an (n,m)-graphs, $m > 0$ with degree sequence $d_1, d_2, \cdots, d_n$, and 2-degree sequence $t_1, t_2, \cdots, t_n$. Let*

$$S_2 = \sum_{i=1}^{n} \sigma_i^2$$

and let the other symbols be same as in Theorem 1.9. Then

$$E(G) \le 2\sqrt{S_2/T_2} + \sqrt{(n-1)(2m - S_2/T_2)} \,.$$

Equality holds if and only if either $G \cong (n/2)K_2$, or $G \cong K_n$, or G is a non-bipartite connected graph satisfying $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_n/t_n = p$ and has three distinct eigenvalues p, $\sqrt{(2m-p^2)/(n-1)}$, and $-\sqrt{(2m-p^2)/(n-1)}$, provided $p > \sqrt{2m/n}$.

Theorem 1.12 *[22] Let G be a bipartite (n,m)-graph and everything else same as in Theorem 1.11. Then*

$$E(G) \le 2\sqrt{S_2/T_2} + \sqrt{(n-2)(2m - 2\,S_2/T_2)}\,.$$

Equality holds if and only if either $G \cong (n/2)K_2$, or $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1\, r_2 = m$, or 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 $\sigma_1/t_1 = \cdots = \sigma_s/t_s = p_x$ and $\sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n = p_y$, and has four distinct eigenvalues $\sqrt{p_x\, p_y}$, $\sqrt{(2m - 2p_x\, p_y)/(n-2)}$, $-\sqrt{(2m - 2p_x\, p_y)/(n-2)}$,, and $-\sqrt{p_x\, p_y}$, provided $p_x\, p_y > \sqrt{2m/n}$.

For $v \in V(G)$, the *k-degree* $d_k(v)$ of v is the number of walks of length k of G, starting at v.

Theorem 1.13 *[23] Let G be an (n,m)-graph, $m > 0$. Then*

$$E(G) \le \sqrt{\frac{\sum_{v\in V(G)} d_2^2(v)}{\sum_{v\in V(G)} d^2(v)}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v\in V(G)} d_2^2(v)}{\sum_{v\in V(G)} d^2(v)}\right)}\,.$$

Equality holds if and only if either $G \cong (n/2)K_2$, or $G \cong K_n$, or G is a non-bipartite connected p-pseudo-regular graph with three distinct eigenvalues p, $\sqrt{(2m-p^2)/(n-1)}$, and $-\sqrt{(2m-p^2)/(n-1)}$, provided $p > \sqrt{2m/n}$.

Theorem 1.14 *[23] Let G be a connected (n,m)-graph. Then*

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

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

Theorem 1.15 *[23] Let G be a connected (n,m)-graph, $n \ge 2$. Then*

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

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

More upper bounds of the same kind can be found in [24,25].

It is well known [1] that the eigenvalues of a bipartite graph G on $n = 2N$ vertices occur in pairs: $\pm\lambda_1, \pm\lambda_2, \cdots, \pm\lambda_N$, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$. Then the energy of G is given by

$$E(G) = 2(\lambda_1 + \lambda_2 + \cdots + \lambda_N)$$

and

$$\sum_{i=1}^{N} \lambda_i^2 = m .$$

Let $q = \sum_{i=1}^{N} \lambda_i^4$. By the Cauchy–Schwarz inequality, $m^2 \leq Nq$.

Theorem 1.16 *[26] Let G be a bipartite graph on $2N$ vertices. Then the following holds. (i) $m^2 = Nq$ if and only if $G \cong N\,K_2$. (ii) $m^2 = q$ 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 $h + r + s = 2N$. (iii) If $1 < m^2/q < N$, then*

$$E(G) \leq \frac{2}{\sqrt{N}} \left[\left(m - \sqrt{(N-1)Q} \right) + (N-1) \left(m - \sqrt{Q/(N-1)} \right) \right] \quad (1.6)$$

where $Q = Nq - m^2$. Equality holds if G is the graph of a symmetric BIBD. Conversely, if the equality holds and G is regular, then G is the graph of a symmetric BIBD.

Recall [17] that a *balanced incomplete block design* (BIBD) is a family of b blocks of a set of v elements, such that (i) each element is contained in r blocks, (ii) each block contains k elements, and (iii) 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 1.17 *[26] Let G be a bipartite graph on $2N + 1$ vertices. Then the following holds. (i) $Q \geq 0$ and the equality is obeyed if and only if G is the direct sum of an isolated vertex with $N\,K_2$. (ii) Inequality (1.6) remains true if $q < m^2 < Nq$, and the equality holds if G consists of an isolated vertex and a copy of the graph of a symmetric BIBD.*

If $n = 2N$ and $m \geq N$, then the upper bound of Theorem 1.3 is

$$E_*(N, m) = \frac{2m}{N} + 2\sqrt{(N-1)\left[m - \left(\frac{m}{N}\right)^2\right]} .$$

Theorem 1.18 *[26] If $N^3 q \geq m^4$, then $E(G) \leq E_*(N, m)$.*

Therefore, if $N^3 q \leq m^4$, then the bound of Theorem 1.16 improves that of Theorem 1.3.

Ending this subsection we state one of the several bounds for energy obtained by Morales [27–29]. Let G be a bipartite graph on $2N$ vertices. Then

$$E(G) \leq 2\sqrt{m(N-1) + \sqrt{\frac{N(m^2-q)}{N-1}}} .$$

1.2.2 Some lower bounds

In [30] it was shown that for all regular graphs G with degree $k > 0$, the energy is not less than the number of vertices, $E(G) \geq n$. 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 $E \geq n$ holds [31]. Among these are the hexagonal systems (representing benzenoid hydrocarbons [32]).

A lover bound for E was obtained by McClelland [11]. 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,

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

Hence,

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

Theorem 1.19 *[11]* $E(G) \geq \sqrt{2m + n(n-1)|\det A|^{2/n}}$.

If $\det A \neq 0$, which is equivalent to the condition that no graph eigenvalue is equal to zero, then from Theorem 1.19 follows that $E(G) \geq n$.

For bipartite graphs a similar argument yields [33]

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

There are some other lower bounds:

Theorem 1.20 *[26] (i) Let G be a bipartite graph with $2N$ vertices. Then*

$$E(G) \geq 2m\sqrt{\frac{m}{q}}\,. \tag{1.7}$$

Equality holds if and only if either $G = N\,K_2$ 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 inequality 1.7 remains true. Moreover, the equality holds if and 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 $r_1\,s_1 = \cdots = r_j\,s_j$.

Theorem 1.21 *[34] Let G be a bipartite graph with at least one edge and let r, s, t be positive integers, such that $4r = s + t + 2$. Then*

$$E(G) \geq M_r(G)^2[M_s(G)M_t(G)]^{-1/2} \tag{1.8}$$

where $M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k$ is the k-th spectral moment of the graph G.

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

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

Then we have

Theorem 1.22 *[35] Let G be a graph with at least one edge and let r, s, t be non-negative real numbers, such that $4r = s + t + 2$. Then*

$$E(G) \geq M_r^*(G)^2[M_s^*(G)M_t^*(G)]^{-\frac{1}{2}} \tag{1.9}$$

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

From [11] we know that $E(G) \leq \sqrt{2mn}$ holds for all graphs. There exists a constant g such that $g\sqrt{2mn}$ is a lower bound for $E(G)$.

For a quadrangle-free (n,m)-graph G with maximum vertex degree 2, and no isolated vertices, we have [36]

$$E(G) > \frac{4}{5}\sqrt{2mn}\,.$$

If the maximum vertex degree is 3, then [36]

$$E(G) > \frac{2\sqrt{6}}{7}\sqrt{2mn}\,.$$

Some other lower bounds of this type are found in the papers [37–41]. Of these we state here:

Theorem 1.23 *[41] Let G be a quadrangle-free (n,m)-graph with minimum vertex degree $\delta \geq 1$ and maximum vertex degree Δ. Then*

$$E(G) > \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}\sqrt{2mn}\,. \tag{1.10}$$

The authors of [13] 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 $E(G) \geq (1-\varepsilon)(n/2)(\sqrt{n}+1)$. Nikiforov [42, 43] arrived at a stronger statements for sufficiently large n.

Theorem 1.24 *[42] (i) For all sufficiently large n, there exists a graph G of order n with $E(G) \geq \frac{1}{2}n^{3/2} - n^{11/10}$. (ii) For almost all graphs*

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

1.3 Hyperenergetic, hypoenergetic and equienergetic graphs

1.3.1 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 $E(G) > 2(n-1)$. From Nikiforov's Theorem 1.24 we see that almost all graphs are hyperenergetic. Therefore any search for hyperenergetic graphs appears nowadays are a futile task. Yet, before Theorem 1.24 was discovered, a number of such results were obtained. We outline here some of them.

In [7] it was conjectured that the complete graph K_n has greatest energy among all n-vertex graphs. This conjecture was soon shown to be false [44].

The first systematic construction of hyperenergetic graphs was proposed by Walikar et al. [45], who showed that the line graphs of K_n , $n \geq 5$, and of $K_{n/2,n/2}$, $n \geq 8$, are hyperenergetic. These results were eventually extended to other graphs with large number of edges [46,47].

Hou et al. [48] 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 [49–51] as well as Kneser graphs and their complements [52] are hyperenergetic. In fact, almost all circulant graphs are hyperenergetic [49].

Graphs on n vertices with fewer than $2n-1$ edges are not hyperenergetic [53, 54]. This, in particular, implies that Hückel graphs (graphs representing conjugated molecules [2–4], in which the vertex degrees do not exceed 3) cannot be hyperenergetic.

1.3.2 Hypoenergetic graphs

A graph on n vertices, whose energy is less than n is said to be *hypoenergetic*. In what follows, for obvious reasons we assume that the graphs considered have no isolated vertices.

Studies of hypoenergetic graphs started only quite recently [31,55], and until now very few results on such graphs are known.

There are reasons to believe (cf. Theorem 1.24) that there are few hypoenergetic graphs.

Theorem 1.25 *[56] (i) There exist hypoenergetic trees of order n with maximum vertex degree $\Delta \leq 3$ only for $n = 1,3,4,7$ (a single such tree for each value of n , see Fig. 1.1); (ii) If $\Delta = 4$, then there exist hypoenergetic trees for all $n \geq 5$, such that $n \equiv k \pmod 4$ $k = 0,1,3$; (iii) If $\Delta \geq 5$, then there exist hypoenergetic trees for all $n \geq \Delta + 1$.*

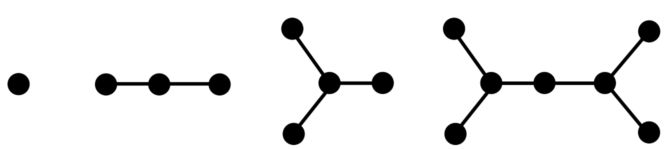

Fig. 1.1 The only four hypoenergetic trees with maximum vertex degree not exceeding 3.

Independently of the paper [56], and almost in the same time, Nikiforov [57] arrived at results essentially same as Theorem 1.25, (i).

Computer search indicates that there exist hypoenergetic trees with $\Delta = 4$ also for $n \equiv 2 \ (mod\ 4)$. The existence of these kind of trees is still under our consideration.

1.3.3
Equienergetic graphs

Two non-isomorphic 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 [1]. In a trivial manner such graphs are equienergetic.

Therefore, in what follows we will be interested only in non-cospectral 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 non-trivial equienergetic graphs (all having $E = 4$) is shown in Fig. 1.2. The smallest pair of equienergetic non-cospectral connected graphs with equal number of vertices is shown in Fig. 1.3. These examples indicate that there exist many (non-trivial) 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. [58] and Balakrishnan [59]. Since 2004 a plethora of papers was published on equienergetic graphs [60–72]. In what follows we state some of the results obtained along these lines.

Let G be a graph on n vertices and let $V(G) = \{v_1, v_2, \ldots, v_n\}$. Take another set of vertices $U = \{u_1, u_2, \ldots, u_n\}$. Define a graph DG whose vertex set is $V(HDG) = V(G) \cup U$ and whose edge set consists only of the edges joining

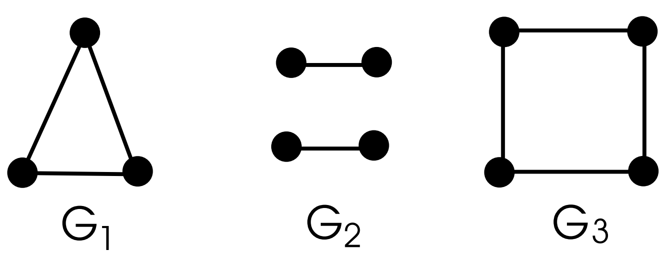

Fig. 1.2 Three non-cospectral equienergetic graphs with $E = 4$. Note that $Sp(G_1) = \{2, -1, -1\}$, $Sp(G_2) = \{1, 1, -1, -1\}$, and $Sp(G_3) = \{2, 0, 0, -2\}$.

u_i to the neighbors of v_i in G, for $i = 1, 2, \dots, n$. The resulting graph DG is called the identity duplication graph of G [64,73].

With the same notation as above, and let $u_1, u_2, \dots, u_n$ be vertices of another copy of G. Make u_i adjacent to the neighbors of v_i in G, for $i = 1, 2, \dots, n$. The resulting graph [64] is denoted by D_2G.

The adjacency matrix of DH is

$$A(DG) = \begin{bmatrix} 0 & A(G) \\ A(G) & 0 \end{bmatrix} = A \bigotimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} .$$

Thus if $spec(G) = \{\lambda_i\,,\ i = 1, \dots, n\}$, then $spec(DH) = \{\lambda_i, \lambda_i\,,\ i = 1, \dots, n\}$. The adjacency matrix of D_2H is

$$A(D_2G) = \begin{bmatrix} A(G), & A(G) \\ A(G), & A(G) \end{bmatrix} = A \bigotimes \begin{bmatrix} 1, & 1 \\ 1, & 1 \end{bmatrix} .$$

and therefore $spec(D_2G) = \{2\lambda_1, 2\lambda_2 \dots, 2\lambda_n, 0, 0, \dots, 0\}$. We thus have:

Theorem 1.26 *[64] DG and D_2G are a pair of equienergetic graphs.*

Let G be an r-regular graph on n vertices, and $V(G) = \{v_1, \dots, v_n\}$. Introduce a set of n isolated vertices $\{u_1, u_2, \dots, u_n\}$ 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.

By direct computation it follows that

$$E(H) = \sqrt{5}\left[E(G) + \sqrt{r^2 + \frac{4}{5}n\,k} - r\right] .$$

Combining this and Theorem 1.26 one arrives at:

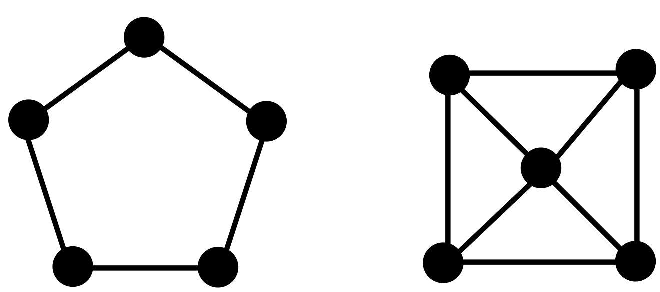

Fig. 1.3 The smallest pair of connected equienergetic graphs with equal number of vertices.

Theorem 1.27 *[64] There exists a pair of n-vertex non-cospectral equienergetic graphs for* $n = 6, 14, 18$ *and* $n \geq 20$.

Ramane and Walikar [65] recently obtained a stronger result.:

Theorem 1.28 *[65] There exists a pair of connected non-cospectral equienergetic n-vertex graphs for all* $n \geq 9$.

If G is a graph and $L(G) = L^1(G)$ its line graph, then $L^k(G), k = 2, 3, \ldots,$ defined recursively via $L^k(G) = L(L^{k-1}(G))$, are the iterated line graphs of G .

If G is an r-regular graph with n vertices and m edges, then the characteristic polynomials of G and $L(G)$ are related as [1]

$$\phi(L(G), x) = (x+2)^{m-n} \phi(G, x - r + 2) .$$

If $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$, then $spec(L(G)) = \{r + r - 2, \lambda_2 + r - 2, \ldots, \lambda_n + r - 2, -2, \ldots, -2\}$ and $spec(L^2(G)) = \{2r - 6, \ldots, 2r - 6, r + 3r - 6, \lambda_2 + 3r - 6, \ldots, \lambda_n + 3r - 6, -2, \ldots, -2\}$. Now, because 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,

$$E(L^2(G)) = 2 \times 2 \times \frac{nr(r-2)}{2} = 2nr(r-2) .$$

In a similar manner, also $E(L^k(G))$, $k > 2$, depends solely on n and r .

Theorem 1.29 *[62] Let* G_1 *and* G_2 *be two non-cospectral regular graphs of the same order and of 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 non-cospectral equienergetic graphs of equal order and with the same number of edges. 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 , from [61] we know that $\overline{L^2(G_1)}$ and $\overline{L^2(G_2)}$ are also equienergetic, and $E(\overline{L^2(G_1)}) = E(\overline{L^2(G_2)}) = (nr-4)(2r-3) - 2$, 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_i are adjacent if and only if G is connected, and G^* is regular of degree $r + 1$ if and only if G is regular of degree r . Then we have:

Theorem 1.30 *[66] Let G_1, G_2 be two r-regular graphs of order n . Then*

(i) $(L^2(G_1))^*$ *and* $(L^2(G_2))^*$ *are equienergetic bipartite graphs, and*

$$E((L^2(G_1))^*) = E((L^2(G_2))^*) = nr(3r-5) \,.$$

(ii) $(\overline{L^2(G_1)})^*$ *and* $(\overline{L^2(G_2)})^*$ *are equienergetic bipartite graphs, and*

$$E((\overline{L^2(G_1)})^*) = E((\overline{L^2(G_2)})^*) = (5nr-16)(r-2)+nr-8 \,.$$

(iii) $\overline{(L^2(G_1))^*}$ *and* $\overline{(L^2(G_2))^*}$ *are equienergetic bipartite graphs, and*

$$E(\overline{(L^2(G_1))^*}) = E(\overline{(L^2(G_2))^*}) = (2nr-4)(2r-3)-2 \,.$$

By means of a computer search it was shown that there are numerous pairs of non-cospectral equienergetic trees [58]. Some of these are depicted in Fig. 1.4.

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. 1.4. Using standard recursive methods [1, 4],one can compute their characteristic poly-

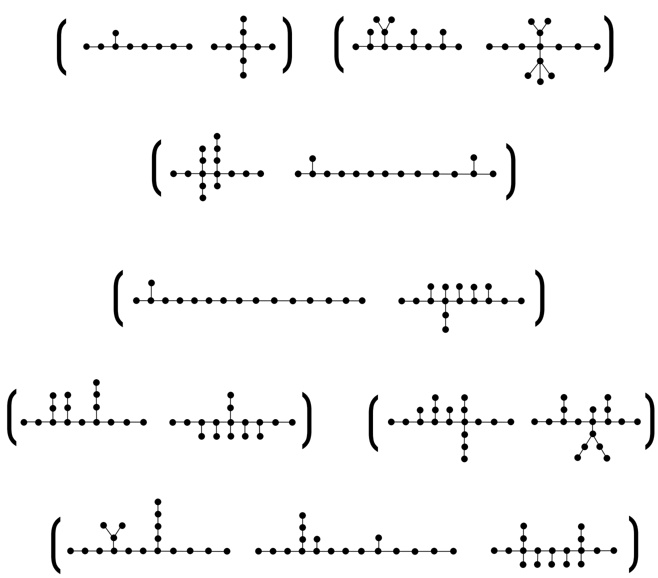

Fig. 1.4 Equienergetic trees [58]. Of the three 18-vertex trees at the bottom of this figure, the first two are cospectral, but not cospectral with the third tree.

nomials as:

$$\begin{aligned}\phi(T_A,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 117\,\lambda^{14} - 421\,\lambda^{12} + 853\,\lambda^{10}\\ &- 973\,\lambda^{8} + 588\,\lambda^{6} - 164\,\lambda^{4} + 16\,\lambda^{2}\end{aligned}$$

$$\begin{aligned}\phi(T_B,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 117\,\lambda^{14} - 421\,\lambda^{12} + 853\,\lambda^{10}\\ &- 973\,\lambda^{8} + 588\,\lambda^{6} - 164\,\lambda^{4} + 16\,\lambda^{2}\end{aligned}$$

$$\begin{aligned}\phi(T_C,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 111\,\lambda^{14} - 359\,\lambda^{12} + 632\,\lambda^{10}\\ &- 632\,\lambda^{8} + 359\,\lambda^{6} - 111\,\lambda^{4} + 17\,\lambda^{2} - 1\,.\end{aligned}$$

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:

$$\phi(T_A,\lambda) = \lambda^2\,(\lambda^2-1)(\lambda^2-2)^2\,(\lambda^2-4)(\lambda^4-3\,\lambda^2+1)(\lambda^4-5\,\lambda^2+1)$$

$$\phi(T_C,\lambda) = (\lambda^2-1)^3\,(\lambda^4-3\,\lambda^2+1)(\lambda^4-5\,\lambda^2+1)(\lambda^4-6\,\lambda^2+1)\,.$$

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 moment 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.

1.4
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 E-values. The first such result was obtained for trees [74], when it was demonstrated that the star has minimum and the path maximum energy. In the meantime, a remarkably large number of papers were published on such extremal problems: for general graphs [13, 14, 16, 75–78], trees and chemical trees [79–93], unicyclic [94–107], bicyclic [108–114], tricyclic [115, 116], and tetracyclic graphs [117], as well as for benzenoid and related polycyclic systems [118–122].

In this section we state a few of these results, selecting those that can be formulated in a simple manner.

We first mention to elementary results.

The n-vertex graph with minimum energy is $\overline{K_n}$, the graph consisting of isolated vertices. Its energy is zero.

The minimum–energy n-vertex graph without isolated vertices is the complete bipartite graph $K_{n-1,1}$, also known as the star [12]. Its energy is equal to $2\sqrt{n-1}$, cf. Theorem 1.2.

Finding the maximum–energy n-vertex graph(s) is a much more difficult task, and a complete solution of this problem is not known. For some results along these lines see Theorem 1.5.

Let G be a graph on n vertices and $A(G)$ its adjacency matrix. As before, let the characteristic polynomial of G be

$$\phi(G,\lambda) = \det(\lambda I_n - A(G)) = \sum_{k=0}^{n} a_k \, \lambda^{n-k} \, .$$

A classical result of the theory of graph energy is [6,8] that $E(G)$ can be computed from the characteristic polynomial of G, by by means of

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{ix\, \phi'(G,ix)}{\phi(G,ix)} \right] dx$$

where $\phi'(G,\lambda)$ denotes the first derivative of $\phi(G,\lambda)$, and where $i = \sqrt{-1}$. More on the Coulson integral formula can be found elsewhere [4,123,124].

Another way to write the Coulson integral formula is [74]

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{k \geq 0} (-1)^k \, a_{2k} \, x^{2k} \right)^2 + \left(\sum_{k \geq 0} (-1)^k \, a_{2k+1} \, x^{2k+1} \right)^2 \right] dx \, . \tag{1.11}$$

If the graph G is bipartite, then its characteristic polynomial is of the form

$$\phi(G,\lambda) = \sum_{k \geq 0} (-1)^k \, b_k \, \lambda^{n-2k}$$

and $b_k \geq 0$. Then the Coulson integral formula is simplified as:

$$E(G) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k \geq 1} b_k \, x^{2k} \right] dx.$$

If G is a tree (or, more generally, a forest), then

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

and

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k \geq 1} m(G,k)\, x^{2k} \right] dx \tag{1.12}$$

where $m(G,k)$ is the number of matchings of size k of G, i. e., the number of selections of k independent edges in G.

Consider now Eq. (1.11) and let G_1 and G_2 be two graphs. If the inequalities

$$\begin{aligned} (-1)^k\, a_{2k}(G_1) &\leq (-1)^k\, a_{2k}(G_2) \\ (-1)^k\, a_{2k+1}(G_1) &\leq (-1)^k\, a_{2k+1}(G_2) \end{aligned} \tag{1.13}$$

are satisfied by all values of k, then from Eq. (1.11) follows that $E(G_1) \leq E(G_2)$. If, in addition, at least one of these inequalities is strict, then $E(G_1) < E(G_2)$.

Bearing this in mind we define a partial order $\prec$ and write $G_1 \preceq G_2$ or $G_2 \succeq G_1$ if the conditions (1.13) are obeyed by all k. If, moreover, at least one of the inequalities in (1.13)is strict, then we write $G_1 \prec G_2$ or $G_2 \succ G_1$. Thus we have:

$$G_1 \preceq G_2 \quad \Rightarrow \quad E(G_1) \leq E(G_2)$$

$$G_1 \prec G_2 \quad \Rightarrow \quad E(G_1) < E(G_2)\,.$$

As a special case of the above, if G_1 and G_2 are a bipartite graphs, then [125]

$$G_1 \prec G_2 \Leftrightarrow (\forall k)\; b_k(G_1) \leq b_k(G_2)$$

whereas if G_1 and G_2 are trees (or, more generally, forests), then

$$G_1 \prec G_2 \Leftrightarrow (\forall k)\; m(G_1,k) \leq m(G_2,k)\,.$$

If for some $k' \neq k''$,

$$\begin{aligned} (-1)^{k'}\, a_{2k'}(G_1) &< (-1)^{k'}\, a_{2k'}(G_2) \\ (-1)^{k''}\, a_{2k''}(G_1) &> (-1)^{k''}\, a_{2k''}(G_2) \end{aligned}$$

or

$$\begin{aligned} (-1)^{k'}\, a_{2k'+1}(G_1) &< (-1)^{k'}\, a_{2k'+1}(G_2) \\ (-1)^{k''}\, a_{2k''+1}(G_1) &> (-1)^{k''}\, a_{2k''+1}(G_2) \end{aligned}$$

then the graphs G_1 and G_2 cannot be compared by means of the relation $\prec$. Then their energies cannot be compared by using the Coulson integral formula.

Practically all (above quoted) results on graphs that are extremal with regard to energy were obtained by establishing the existence of the relation $\prec$ between the elements of some class of graphs.

Theorem 1.31 *[74] If T_n is a tree on n vertices, then*

$$E(S_n) \le E(G) \le E(P_n)$$

where S_n and P_n denote, respectively, the star and the path with n vertices. Equality holds only if $G \cong S_n$ or $G \cong P_n$.

Eventually, the first few minimum– and maximum–energies n-vertex trees were determined [88,89]. For instance, let P_n^* be the tree obtained by attaching a P_3 to the third vertex of P_{n-2} . Then P_n^* is the tree with second–maximum energy [74].

Denote by Φ_n the class of trees on n vertices having a perfect matching, and by Ψ_n the subclass of Φ_n consisting of trees whose vertex degrees do not exceed 3. Let F_n be obtained by adding a pendent edge to each vertex of the star $K_{1,(n/2)-1}$, B_n be the graph obtained from F_{n-1} by attaching a P_3 to the 2-degree vertex of a pendent edge. Let G_n be obtained by adding a pendent edge to each vertex of the path $P_{n/2}$, D_n be the tree obtained from G_{n+2} by deleting the third and the fourth pendent edges.

Theorem 1.32 *[79] (i) F_n and B_n are, respectively, the unique tree with minimum and second–minimum energy in Φ_n .*

(ii) G_n and D_n are, respectively, the unique tree with minimum and second–minimum energy in Ψ_n .

Eventually, Zhang and Li [80] determined the first four trees with maximum energy in Φ_n .

Let $B_{n,d}$ be obtained from the path P_d with d vertices by attaching $n-d$ pendent edges to an end vertex of P_d .

Theorem 1.33 *[82] Among n-vertex trees with diameter at least d , $B_{n,d}$ is the unique tree with minimum energy (see Fig. 1.5).*

Theorem 1.34 *[86, 87] Among n-vertex trees having exactly k pendent vertices, $B_{n,n-k+1}$ is the unique tree with minimum energy (see Fig. 1.5).*

Let $S(n,m,r)$ be obtained by attaching one pendent vertex to each of the m pendent vertices of the star $K_{1,m+r}$. Let $Y(n,m,r)$ be obtained by attaching m P_2's to one end vertex of P_{r+1} . Let $D(n,p,q)$ be obtained from P_2 by adding p

and q pendent vertices to the vertices of P_2. Let $T^2_{r,s,t}$ be the tree obtained from P_3 by adding r, s, t pendent vertices to its first, second, and third vertex. Lin et al. [84] determined the trees of given maximum degree Δ, having minimum and maximum energies.

Theorem 1.35 *[84] Let T be an n-vertex tree, $n \geq 4$. Let*

$$T_1^*(n,\Delta) \cong \begin{cases} S(n, n-\Delta-1, 2\Delta-n+1) & \text{if } 3 \leq \lfloor \frac{n}{2} \rfloor \leq \Delta(T) \geq n-2 \\ Y(n, \Delta-1, 2\Delta-n+1) & \text{if } 3 \leq \Delta(T) \leq \lfloor \frac{n}{2} \rfloor \\ P_n & \text{if } \Delta(T) = 2 \end{cases} .$$

Then $E(T) \leq E(T_1^*(n,\Delta))$, with equality if and only if $T \cong T_1^*(n,\Delta)$.

Theorem 1.36 *[84] Let T be an n-vertex tree, $n \geq 7$. Let*

$$T_2^*(n,\Delta) \cong \begin{cases} D(n, \Delta-1, n-\Delta-1) & \text{if } \lceil \frac{n}{2} \rceil \leq \Delta(T) \leq n-2 \\ T^2_{\Delta-1,\Delta-1,n-2\Delta-1} & \text{if } \lceil \frac{n}{2} \rceil \leq \Delta(T) \leq \lceil \frac{n}{2} \rceil - 1 \end{cases} .$$

If $\lceil (n+1)/3 \rceil \leq \Delta(T) \leq n-2$, then $E(T) \leq E(T_2^*(n,\Delta))$, with equality if and only if $T \cong T_2^*(n,\Delta)$.

In the above, the trees with a given maximum vertex degree Δ and maximum E happen to be trees with a single vertex of degree Δ. Recently, we [93] offered a simple proof of this result and, in addition, characterized the maximum energy trees having two vertices of maximum degree Δ.

Let $D(p,q)$ be a double star obtained by joining the centers of two stars S_p and S_q by an edge, and $F(p,q)$ be the tree obtained from $D(p-1,q)$ by attaching a pendent edge to one of the vertices of degree one which joins the vertex of degree q in $D(p-1,q)$.

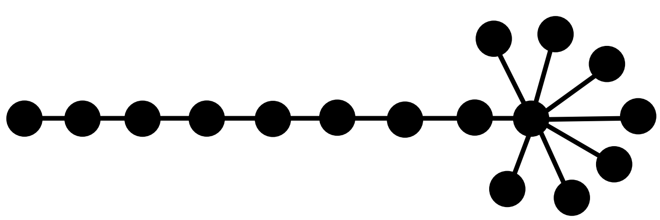

Fig. 1.5 The minimal–energy tree with prescribed diameter [82]. This is also the minimal–energy tree with prescribed number of pendent vertices [86, 87].

Theorem 1.37 *[81] Let T be a tree with a (p,q)-bipartition $(p,q \geq 1, p+q \geq 3)$. Then*

$$E(T) \geq \sqrt{2(p+q-1)+2\sqrt{(p+q-1)^2-4(p-1)(q-1)}} + \sqrt{2(p+q-1)-2\sqrt{(p+q-1)^2-4(p-1)(q-1)}}$$

with equality if and only if $T \cong D(p,q)$.

Furthermore, if $q \geq p \geq 2$ and $T \ncong D(p,q)$, then $E(T) \geq E(F(p,q))$, with equality if and only if $T \cong F(p,q)$.

Let $B(p,q)$ be the graph formed by attaching $p-2$ and $q-2$ vertices to two adjacent vertices of a quadrangle, respectively, and $H(3,q)$ be the graph formed by attaching $q-2$ vertices to the pendent vertex of $B(2,3)$.

Theorem 1.38 *[97] In the class of bipartite unicyclic graphs with a (p,q)-bipartition, $(q \geq p \geq 2)$, the graph $B(p,q)$ has minimum energy if $p \geq 4$ or $p=2$, whereas $B(3,q)$ or $H(3,q)$ have minimum energy if $p=3$.*

Let S_n^3 be the graph obtained from the star graph with n vertices by adding an edge. Hou [94] showed that S_n^3 is the graph with minimum energy among all unicyclic graphs, see Fig. 1.6.

Let $\mathcal{U}(n,d)$ be the class of connected unicyclic graphs with n vertices and diameter d, where $2 \leq d \leq n-2$. Let $U(n,d)$ be the graph obtained by attaching a path of length $d-3$ at a vertex of C_4 and $n-d-1$ pendent edges at another vertex, such that these two vertices are not adjacent, see Fig. 1.7.

Theorem 1.39 *[106] Let $G \in \mathcal{U}(n,d)$ with $d \geq 3$ and $G \neq U(n,d)$. Then $E(G) > E(U_{n,d})$.*

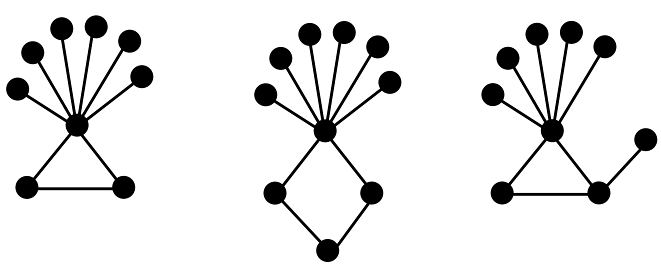

Fig. 1.6 Unicyclic graphs with minimal [94], second–minimal, and third–minimal energy [98].

For the (n, m)-graphs with minimum energy we have the following conjecture:

Conjecture 1. [12] If $m \leq n + \lfloor (n-7)/2 \rfloor$, then the connected (n, m)-graph, $n \geq 6$ and $n - 1 \leq m \leq 2(n-2)$, has minimum energy if it is obtained from the star, by adding to it $m - n + 1$ additional edges all incident to the same vertex. If $m > n + \lfloor (n-7)/2 \rfloor$, the minimum–energy graph is the bipartite graph with two vertices in one class, one of which is connected to all vertices on the other class.

This conjecture is true for $m = n - 1, n$ (cf. Theorem 1.31). The conjecture was proved to be true for $m = n - 1,\ 2(n-2)$ in [12] by Caporosi et al., and for $m = n$ by Hou [94]. Recently, Li, Zhang and Wang [78] obtained a positive solution to the second part of the conjecture for bipartite graphs, and furthermore, determined the graph with the second–minimal energy among connected bipartite (n, m)-graphs, $n \leq m \leq 2n - 5$.

Let $S_n^{3,3}$ be the graph formed by joining $n - 4$ pendent vertices to a vertex of degree three of $K_4 - e$, and $P_n^{6,6}$ be the graph obtained from two C_6's by joining them by a path of length $n - 10$. Let $G(n)$ be the class of bicyclic graphs G on n vertices containing no disjoint odd cycles of lengths k and ℓ with $k + \ell \equiv 2 \pmod 4$. Then $S_n^{3,3}$ is the graph with minimum energy in $G(n)$ [110].

Let P_n^6 be obtained by connecting a vertex of the cycle C_6 with a terminal vertex of the path P_{n-6}.

Theorem 1.40 *[96] Among n-vertex bipartite unicyclic graphs either P_n^6 or C_n have maximal energy. Thus, if n is odd, then P_n^6 is the maximal–energy unicyclic n-vertex graph.*

Computer–aided calculation shows that C_n is the maximal–energy unicyclic graph only for $n = 10$ [95]. However, the proof of the seemingly very simple inequality $E(C_n) < E(P_n^6)$ has not been accomplished so far. The reason for

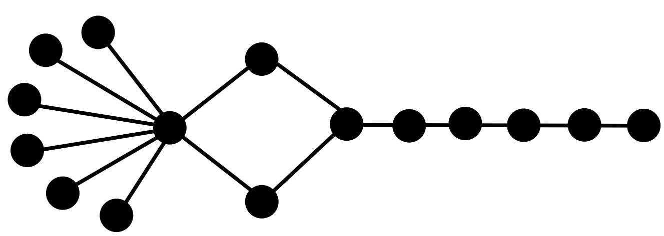

Fig. 1.7 The minimal–energy unicyclic graph with prescribed diameter [106].

this lies in the fact that the graphs C_n and P_n^6 are not comparable by the relation $\prec$.

For the bicyclic graphs with maximum energy, the following conjecture was stated, based on computer–aided numerical experiments [75]:

Conjecture 2. If $n = 14$ and $n \geq 16$ the maximum-energy bicyclic molecular graph is $P_n^{6,6}$, obtained by attaching six-membered cycles to the end vertices of the path P_{n-12}.

Recently a partial proof of this conjecture was obtained [111].

Theorem 1.41 *[111] Let $\mathcal{A}(n)$ be the subset consisting of graphs obtained from two cycles C_a and C_b $(a, b \geq 10$ and $a \equiv b \equiv 2$ (mod 4)), by joining them by an edge. Let $\mathcal{B}_n$ denote the set of all other bipartite bicyclic graphs on n vertices. Then $P_n^{6,6}$ has maximum energy in $\mathcal{B}_n$.*

1.5 Miscellaneous

We state here a few noteworthy results on graph energy, that did not fit into the previous sections.

$E(G) \geq 4$ holds for all connected graphs, except for K_1, K_2, $K_{2,1}$, and $K_{3,1}$ [126].

The rank ρ of a graph is the rank of its adjacency matrix. For a connected bipartite graph G of rank ρ, [126]

$$E(G) \geq \sqrt{(\rho+1)^2 - 5}\,.$$

For any graph, $E \geq \rho$.

Let $\chi(G)$ be the chromatic number of the graph G. For any n-vertex graph G, $E(G) \geq 2(n - \chi(\overline{G}))$ [126].

The inequality $E(G) + E(\overline{G}) \geq 2n$ is satisfied by all n-vertex graphs, $n \geq 5$, except by K_n and $K_n - e$ [126].

As an immediate special case of the Koolen–Moulton upper bound (1.2), for an n-vertex regular graph of degree r, we have $E(G) \leq E_0$, where

$$E_0 := r + \sqrt{r(n-1)(n-r)}\,.$$

Balakrishnan [59] showed that for any $\varepsilon > 0$, there exist infinitely many n, for which there are n-vertex regular graphs of degree r, $r < n-1$, such that $E(G)/E_0 < \varepsilon$.

No answer is known to the question if there exist n-vertex regular graphs of degree r for which $E(G)/E_0 > 1-\varepsilon$ [59].

A direct consequence of Eq. (1.12) is that by deleting an edge e from a tree (or forest) T, the energy necessarily decreases, $E(T) - E(T-e) > 0$. In the general case the difference $E(G) - E(G-e)$ may be smaller than, greater, than, or equal to zero, and the complete solution of this problem is not known. Some partial results along these lines are recently obtained [127].

The energy of a graph is never an odd integer [128]. The energy of a graph is never the square root of an odd integer [129].

The way in which the energy depends on various structural features of the underlying (molecular) graph was much studied in the chemical literature, in most cases empirically [9, 10]. Scores of approximate formulas for E were put forward, in particular formulas that relate the E-value of an (n, m)-graph with n and m [9, 10, 130]. Of these we call the readers' attention to a recent empirical finding that $E(G)$ is an almost perfectly linear (decreasing) function of the number of zeros in the spectrum of G [131, 132].

1.6 Concluding remarks

At this moment the most significant open problem in the theory of graph energy seems to be the characterization of n-vertex graphs with greatest energy. Although quite recently much progress in this direction has been achieved (cf. Theorem 1.5), the problem is still far from being completely solved. An additional difficulty that recently emerged [14] is the fact that for some values of n, there exist numerous maximum–energy n-vertex graphs.

There have been several recent attempts to extend the graph–energy concept to eigenvalues of matrices other than the adjacency matrix. Especially much work was done on the so-called "*Laplacian graph energy*", based on the spectrum of the Laplacian matrix, and on "*distance graph energy*", based on the spectrum of the distance matrix. The "energy" has been re-defined so that it could be associated with any matrix, including non-square matrices. The discussion of such energy–like quantities goes, however, beyond the ambit of the present survey.

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