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HYPERENERGETIC AND HYPOENERGETIC GRAPHS

Abstract. The energy $E = E(G)$ of a graph G is the sum of the absolute values of the eigenvalues of G. The motivation for the introduction of this invariant comes from chemistry, where results on E were obtained already in the 1940's. A graph G with n vertices is said to be "hyperenergetic" if $E > 2n-2$, and to be "hypoenergetic" if $E(G) < n$. In this chapter we outline the main hitherto obtained results related to hyperenergetic and hypoenergetic graph.

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

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

CONTENTS

1. Energy of a graph

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

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

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

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

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

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

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

Second, somewhere around the turn of the century mathematicians realized the mathematical value (and, let us say: mathematical beauty) of graph energy, and a vigorous and world-wide mathematical research of E started. The current activities on the mathematical studies of E are remarkable: According to our records, in the year 2006 the number of published papers was 11. In 2007, 2008, and 2009 this number increased to 30, 47, and 59, respectively. In the time of completion of this chapter (August 2010) the author is aware of 54 papers on graph energy published in 2010 or in press. Solely in the 21-th century several hundreds of mathematicians from Australia, Austria, Brazil, Canada, Chile, China, Croatia, Germany, India, Iran, Ireland, Italy, Mexico, Netherlands, Pakistan, Portugal, Rumania, Russia, Serbia, South Africa, South Korea, Spain, Sweden, Turkey, UK, USA, and Venezuela participated or are participating in research on graph energy.

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

2. The chemical connection

Researches related to the energy of a graph can be traced back to the 1940s or even to the 1930s. In the 1930s the German scholar Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called "unsaturated conjugated hydrocarbons". Details of this approach, often referred to as the "Hückel molecular orbital (HMO) theory" can be found in appropriate textbooks [6, 62, 66].

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

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

where Ψ is the so-called wave function of the system considered, $\hat{H}$ the so-called Hamiltonian operator of the system considered, and $\mathcal{E}$ the energy of the system considered. When applied to a particular molecule, the Schrödinger equation enables one to describe the behavior of the electrons in this molecule and to establish their energies. For this one needs to solve Eq. (2), which evidently is an eigenvalue–eigenvector problem of the Hamiltonian operator. In order that the solution of (2) be feasible (yet not completely exact), one needs to express Ψ as a linear combination of a finite number of pertinently chosen basis functions. If so, then Eq. (2) is converted into:

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

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

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

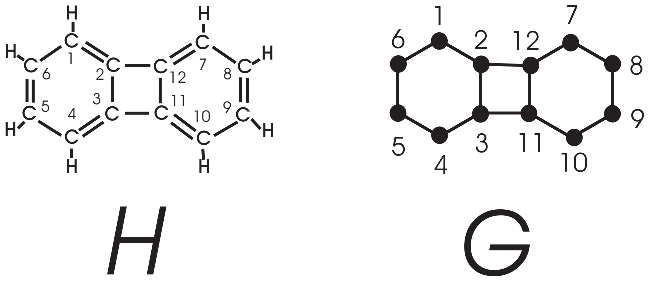

FIGURE 1. Biphenylene H is a typical unsaturated conjugated hydrocarbon. Its carbon–atom skeleton is represented by the molecular graph G. The carbon atoms in the chemical formula H and the vertices of the graph G are labelled by $1, 2, \ldots, 12$ so as to be in harmony with Eqs. (3) and (4).

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

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

The parameters α and β are assumed to be constants, equal for all conjugated molecules. Their physical nature and numerical value are irrelevant for the present considerations; for details see in [6, 62, 66].

For instance, the HMO Hamiltonian matrix of biphenylene is:

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

which can be written also as

(4)
$$\mathbf{H} = \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0&0&0\\ 0&0&0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&0&0&0&0&1 \end{bmatrix} + \beta \begin{bmatrix} 0&1&0&0&0&1&0&0&0&0&0&0\\ 1&0&1&0&0&0&0&0&0&0&0&1\\ 0&1&0&1&0&0&0&0&0&0&1&0\\ 0&0&1&0&1&0&0&0&0&0&1&0\\ 0&0&0&1&0&1&0&0&0&0&0&0\\ 1&0&0&0&1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&1&0&0&0&1\\ 0&0&0&0&0&0&1&0&1&0&0&0\\ 0&0&0&0&0&0&0&1&0&1&0&0\\ 0&0&0&0&0&0&0&0&1&0&1&0\\ 0&0&1&0&0&0&0&0&0&1&0&1\\ 0&1&0&0&0&0&1&0&0&0&1&0 \end{bmatrix} .$$

The first matrix on the right-hand side of Eq. (4) is just the unit matrix of order $n = 12$, whereas the second matrix can be understood as the adjacency matrix of a graph on $n = 12$ vertices. This graph is also depicted in Fig. 1, and in an evident manner corresponds to the underlying molecule (in our example: to biphenylene).

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

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

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

As a curiosity we mention that neither Hückel himself nor the scientists who did early research in HMO theory were aware of the identity (5), which was first noticed only in 1956 [19]. Much later, not knowing of [19], the same observation was made by the present author (for details see [8, 30]). Anyway, the mere observation of the existence of the connection between HMO theory and spectral graph theory had little impact on theoretical chemistry. Chemists became interested in this connection only after it was shown (to them) how by means of the Sachs theorem some long-time open problems of HMO theory could easily be resolved [18, 27].

As a consequence of (5), the energy levels E_j of the π-electrons are related to the eigenvalues λ_j of the graph G by the simple relation $E_j = \alpha + \beta\, \lambda_j$; $j = 1, 2, \ldots, n$.

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

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

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

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

Details on E_π and the way in which the molecular graph G is constructed can be found in the books [13,17,37] and reviews [28,29]. There also more information on the chemical applications of E_π can be found. For what follows, it is only important that because the number of π-electrons in the conjugated hydrocarbon considered is equal to n, it must be $g_1 + g_2 + \cdots + g_n = n$ which immediately implies

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

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

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

The right-hand side of Eq. (6) is just what in the chemical literature is referred to as "total π-electron energy"; if necessary, then one says "total π-electron energy in β-units".

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

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

whereas for odd n,

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

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

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

If so, then Eq. (6) becomes: $E = E(G) = 2 \sum_+ \lambda_j$ where $\sum_+$ indicates summation over positive eigenvalues. Because for all graphs, the sum of eigenvalues is equal to zero, we can rewrite the above equality as

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

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

3. Hyperenergetic graphs

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

$$E > 2n - 2.$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4. Hypoenergetic graphs

Definition 3. A graph G on n vertices is said to be *hypoenergetic* if

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

Graphs for which

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

are said to be *non-hypoenergetic.*

In the chemical literature it was noticed long time ago that for the vast majority of (molecular) graphs the energy exceeds the number of vertices. In 1973 the theoretical chemists England and Ruedenberg published a paper [14] in which they asked "*why is the delocalization energy negative?*". Translated into the language of graph spectral theory, their question reads: "*why does the graph energy exceed the number of vertices?*", understanding that the graph in question is "molecular".

Recall that in connection with the chemical applications of E, a "molecular graph" means a connected graph in which there are no vertices of degree greater than three [37]. The authors of [14] were, indeed, quite close to the truth. Today we know that only five such graphs violate the relation (9), see below.

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

Theorem 4.1. *If the graph G is non-singular (i.e., no eigenvalue of G is equal to zero), then G is non-hypoenergetic.*

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

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

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

Theorem 4.2. *If G is a graph with n vertices and m edges, and if $m \geqslant n^2/4$, then G is non-hypoenergetic.*

Proof. It is known [4] that for all graphs, $E \geqslant 2\sqrt{m}$. Theorem 4.2 follows from $2\sqrt{m} \geqslant n$. □

Theorem 4.3. [40] *If the graph G is regular of any non-zero degree, then G is non-hypoenergetic.*

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

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

A straightforward consequence of Theorem 3.5 is:

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

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

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

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

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

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

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

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

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

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

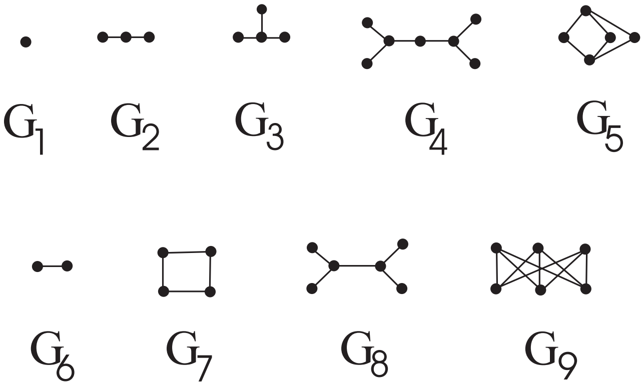

FIGURE 2. Graphs mentioned in Theorems 4.6-4.10

In connection with Theorem 4.7 it must be mentioned that if the maximum vertex degree (Δ) is sufficiently large, then it is not difficult to find hypoenergetic graphs. For instance, the n-vertex star (with $\Delta = n - 1$) is hypoenergetic for all $n \geqslant 3$. In view of this, the recently reported result [67] that there exist hypoenergetic connected unicyclic graphs for all $n \geqslant 7$ and hypoenergetic connected bicyclic graphs for all $n \geqslant 8$ is no surprise whatsoever.

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

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

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

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

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

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

5. Interlude: biregular and triregular graphs

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

Definition 4. Let a and b be integers, $1 \leqslant a < b$. A graph is said to be (a, b)-biregular if the degrees of its vertices assume exactly two different values: a and b.

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

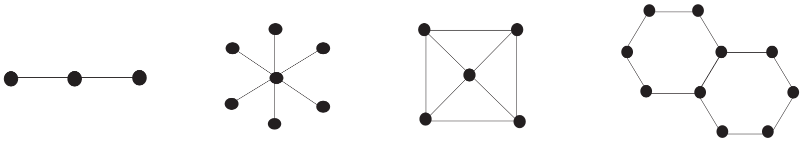

FIGURE 3. Examples of biregular graphs: a (1,2)-biregular tree (the 3-vertex path), a (1,6)-biregular tree (the 7-vertex star), a (3,4)-biregular graph, and a (2,3)-biregular graph (a hexagonal system).

Definition 5. Let x, a, and b be integers, $1 \leqslant x < a < b$. A graph is said to be (x, a, b)-triregular if its vertices assume exactly three different values: x, a, and b.

By Theorem 4.3, the problem considered in this chapter has been completely solved for regular graphs [40]. Hexagonal systems (mentioned in Theorem 4.5) have vertex degrees equal to 2 and 3, and therefore belong to a special class of biregular graphs. From the proof of Theorem 4.5 [31], it can be seen that also other types of biregular graphs have the same property, i.e., satisfy inequality (9). Work along these lines has recently been extended [1, 33, 47, 52, 53]. In what follows we report in due detail our [1, 33] and other colleague's [65] researches on biregular graphs with cyclomatic number $c \leqslant 2$. These considerations may be of particular value for beginners in the field. Namely, these show how by means of relatively elementary graph-theoretic and algebraic reasoning one can obtain not quite trivial results on graph energy. Analogous considerations for triregular graphs can be found in [32, 53] and in the survey [54]. Tricyclic biregular graphs have also been recently examined [52].

6. A lower bound for energy and its applications

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

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

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

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

By another application of the Cauchy–Schwarz inequality,

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

which substituted back into the previous inequality yields

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

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

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

In view of this and the definition of graph energy, Eq. (1), the inequality (10) can be rewritten as

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

The lover bound (11) was independently discovered several times: two times for general graphs [24, 69] and two times for bipartite graphs [12, 58]. Recently a generalized version thereof was obtained [70].

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

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

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

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

Theorem 6.1. *Let G be a graph with n vertices and m edges, possessing q quadrangles, and let $d_1, d_2, \dots, d_n$ be its vertex degrees. If the condition*

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

is obeyed, then G is non-hypoenergetic.

The application of Theorem 6.1 will be the basis for the considerations that follow. Therefore it should be always kept in mind that condition (14) is a *sufficient*, but not a *necessary* condition for the validity of the inequality (9).

7. On the energy of biregular graphs

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

7.1. Biregular trees. Let T be an (a, b)-biregular tree. Since trees necessarily possess vertices of degree 1 (pendent vertices), it must be $a = 1$ and $1 < b \leqslant n-1$, where n is the number of vertices. This tree has at least 3 vertices and $m = n-1$ edges. The number of pendent vertices will be denoted by k.

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

For trees, of course, $q = 0$.

We begin with the equalities

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

and

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

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

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

Further,

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

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

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

and

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

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

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

From (19) we obtain

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

or simplified

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

Bearing in mind that $b \geqslant 2$, the right-hand side of the latter inequality must be at least 2, implying $n \geqslant 5$. By examining the function

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

and its first derivative

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

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

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

Theorem 7.1. *Let T be a $(1, b)$-biregular tree with n vertices. Then* (14) *holds if and only if $b = 2$ and $n \geqslant 5$.*

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

7.2. Unicyclic biregular graphs. For connected unicyclic (a, b)-biregular graphs we have $m = n$, $a = 1$, and $b \geqslant 3$. Further, $M_2 = 2n$ whereas M_4 we obtain in the following way.

We have $k + n_b = n$ and $1 \cdot k + b \cdot n_b = 2n$, from which

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

and

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

Therefore,

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

Now, the inequality (14) becomes

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

and we obtain $b \leqslant 3 - 4q/n$. Because the graph G is unicyclic, the number of quadrangles q can be either 0 or 1. For $q = 0$ we obtain $b \leqslant 3$, and with condition $b \geqslant 3$ we conclude that $b = 3$.

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

Theorem 7.2. *Let G be a connected unicyclic (a, b)-biregular graph with n vertices. Then* (14) *holds if and only if $a = 1$, $b = 3$, and $q = 0$.*

A few examples of biregular graphs that satisfy Theorem 7.2 are shown in Fig. 4. From these examples the general structure of such graphs should be evident:

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

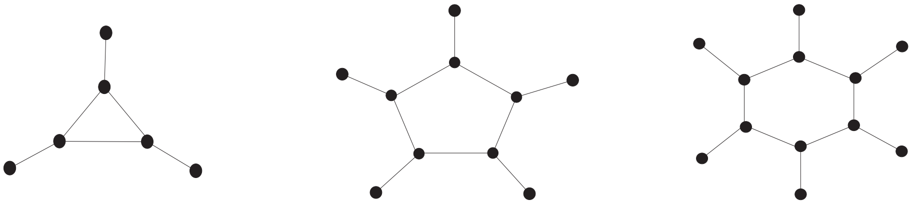

FIGURE 4. Examples of connected quadrangle-free (1,3)-biregular unicyclic graphs.

7.3. Bicyclic biregular graphs.

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

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

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

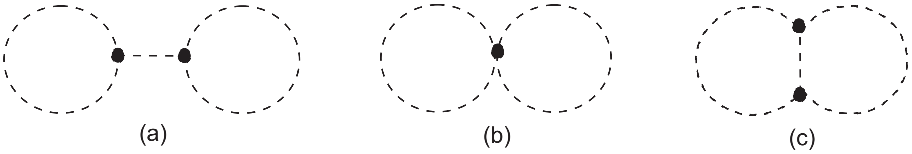

FIGURE 5. Types of bicyclic graphs.

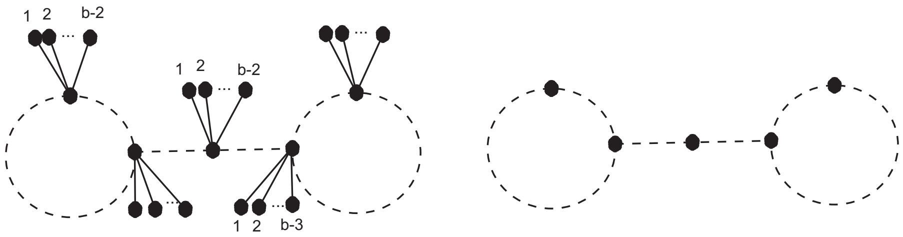

Figure 6. Sketches of $(1, b)$-, and $(2, 3)$-biregular bicyclic graphs with disjoint cycles. The vertices that connect cycles in a $(1, b)$-biregular graph ($b \geqslant 3$) are connected also with $b-3$ pendent vertices, whereas all other vertices in such a graph are connected with $b-2$ pendent vertices.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

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

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

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

from which

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

For $q = 0$ we obtain

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

or simplified

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

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

If we examine the function

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

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

For $q = 1$ we have

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

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

For $q = 2$ we have

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

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

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

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

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

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

$$\begin{aligned} n^3 + 3n^2 + 12n + 4 &\geqslant 0 \\ n^3 - n^2 + 12n + 4 &\geqslant 0 \\ n^3 - 5n^2 + 12n + 4 &\geqslant 0 \end{aligned}$$

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

Theorem 7.4. *Let G be a connected bicyclic (a, b)-biregular graph with disjoint cycles and let n be the number of its vertices. Then the inequality* (14) *holds if and only if either $a = 1$, $b = 3$, $q = 0$ or $a = 1$, $b = 3$, $q = 1$ or $a = 2$, $b = 3$.*

Some of the graphs satisfying the Theorem 7.4 are depicted in Fig. 7.

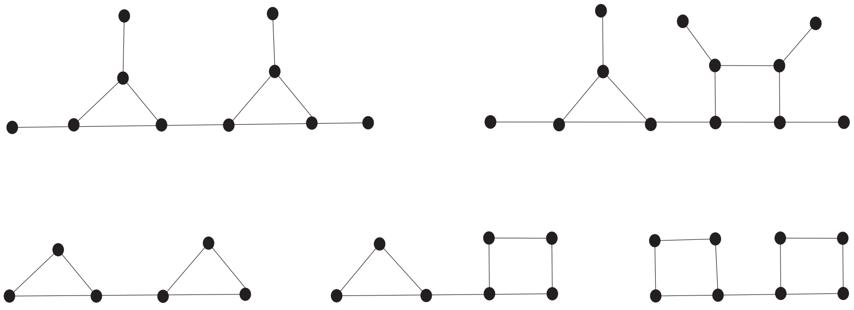

FIGURE 7. Connected bicyclic $(1, 3)$-biregular graphs with disjoint cycles, with $q = 0$ and $q = 1$, and bicyclic $(2, 3)$-biregular graphs with disjoint cycles, with $q = 0$, $q = 1$, $q = 2$. In all these examples the number of vertices is as small as possible.

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

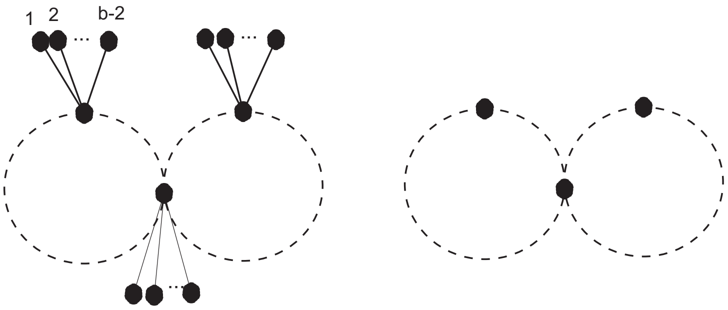

FIGURE 8. Connected bicyclic $(1, b \geqslant 4)$- and $(2, 4)$-biregular graph in which cycles have one common vertex. For the $(1, b)$-biregular graph, $b \geqslant 4$, every vertex except the one belonging to both cycles is connected with $b - 2$ pendent vertices. The vertex belonging to both cycles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

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

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

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

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

Theorem 7.5. *Let G be a connected bicyclic (a, b)-biregular graph with n vertices in which the cycles share a single common vertex. Then condition* (14) *is obeyed if and only if $a = 2$ and $b = 4$.*

A few examples graphs specified in Theorem 7.5 are shown in Fig. 9.

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

For the graphs depicted in Fig. 10 we obtain the same results as for bicyclic graphs with disjoint cycles, but we must add the case when $q = 3$ because there exists a unique bicyclic biregular graph in which the number of quadrangles is exactly 3. This is the complete bipartite graph on $2 + 3$ vertices, $K_{2,3}$, shown in

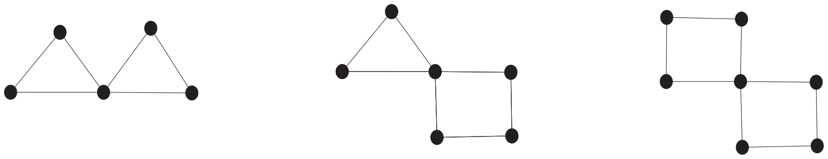

FIGURE 9. Bicyclic $(2, 4)$-biregular graphs in which the cycles have one common vertex, with $q = 0, 1, 2$ quadrangles. In these examples the number of vertices is as small as possible.

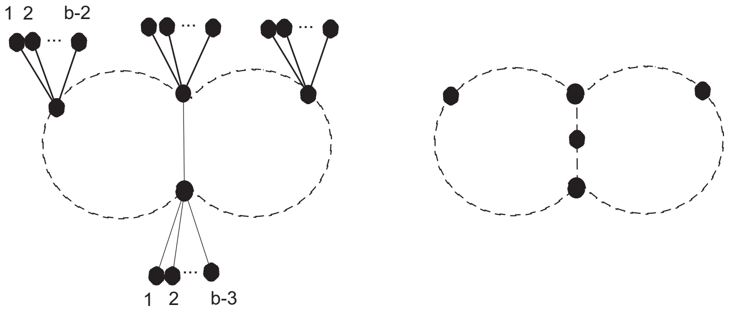

FIGURE 10. Connected bicyclic $(1, b \geqslant 3)$- and $(2, 3)$-biregular graphs in which the cycles have two or more common vertices. Notice that the cycles of the graphs of the first type have only two common vertices, whereas the cycles of the graphs of the second type may have arbitrarily many common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

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

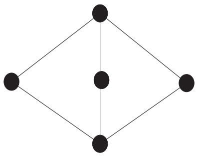

FIGURE 11. The only bicyclic biregular graph in which the number of quadrangles q is 3. For this graph inequality (14) is violated. Recall that according to Theorem 4.9 this graph is hypoenergetic.

Theorem 7.6. *Let G be a connected bicyclic (a, b)-biregular graph with n vertices, whose cycles have two or more common vertices. Then inequality* (14) *holds if and only if* $a = 1$, $b = 3$, $q = 0, 1$ *or* $a = 2$, $b = 3$, $q = 0, 1, 2$.

Examples of graphs for which Theorem 7.6 holds are shown in Fig. 12.

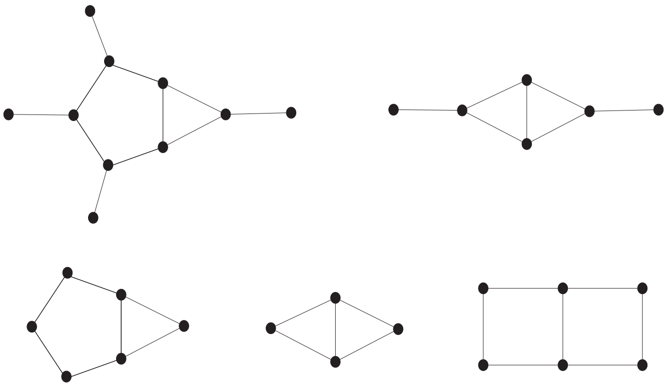

FIGURE 12. Bicyclic $(1,3)$-biregular graphs in which cycles have two common vertices and $q = 0,1$, and bicyclic $(2,3)$-biregular graphs with $q = 0,1,2$.

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

Theorem 6.1.bis. *If the graph G satisfies the inequality* (14)*, then the energy of G is greater than (or, exceptionally, equal to) the number of vertices of G, i.e., inequality (9) holds. Therefore G is necessarily not hypoenergetic. If, however, the graph G does not satisfy the inequality* (14)*, then it may be hypoenergetic, but need not. Anyway, the search for hypoenergetic graphs must be done among those that violate inequality* (14)*.*

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