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SELECTED TOPICS FROM THE THEORY OF GRAPH ENERGY: HYPOENERGETIC GRAPHS

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

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1. Introduction: the chemical connection

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

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

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

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

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

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

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

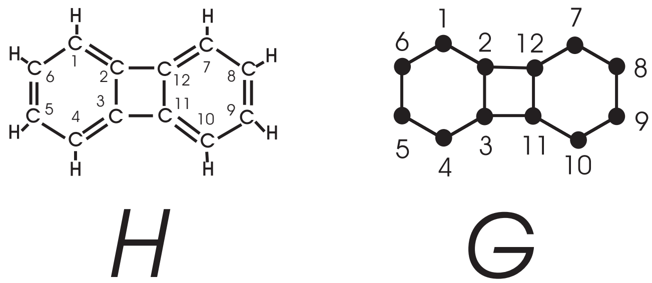

FIGURE 1. Biphenylene H is a typical unsaturated conjugated hydrocarbon. Its carbon–atom skeleton is represented by the molecular graph G. The carbon atoms in the chemical formula H and the vertices of the graph G are labelled by $1, 2, \ldots, 12$ so as to be in harmony with Eqs. (2) and (3).

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

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

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

For instance, the HMO Hamiltonian matrix of biphenylene is:

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

which can be written also as

(3)

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

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

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

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

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

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

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

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

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

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

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

Details on E_π and the way in which the molecular graph G is constructed can be found in the books [5, 6, 7] and reviews [8, 9, 10]. There also more information on the chemical applications of E_π can be found. For what follows, it is only important that because the number of π-electrons in the conjugated hydrocarbon considered is equal to n, it must be $g_1 + g_2 + \cdots + g_n = n$ which immediately implies

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

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

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

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

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

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

whereas for odd n,

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

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

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

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

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

2. The energy of a graph

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

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

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

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

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

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

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

3. Hypoenergetic graphs

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

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

Graphs for which

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

are said to be *non-hypoenergetic*.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

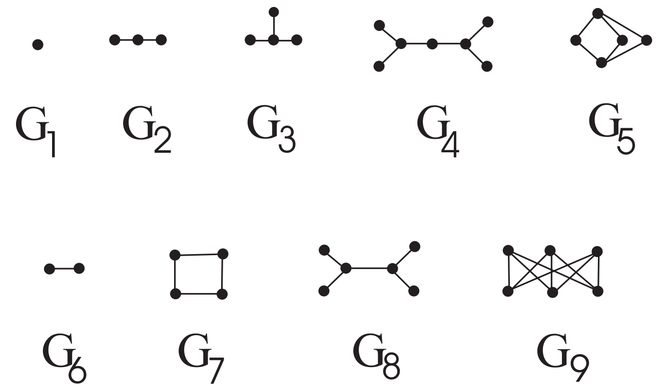

FIGURE 2. G_1, G_2, G_3, G_4 are the only hypoenergetic trees with maximum vertex degree Δ not exceeding 3 [23, 24, 25]. It is conjectured that $G_5 \cong K_{2,3}$ is the only hypoenergetic connected cyclic graph with $\Delta \leqslant 3$. It is also conjectured that G_6, G_7, G_8, G_9 are the only connected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

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

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

4. A lower bound for energy and its applications

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

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

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

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

By another application of the Cauchy–Schwarz inequality,

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

which substituted back into the previous inequality yields

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

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

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

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

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

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

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

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

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

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

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

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

is obeyed, then G is non-hypoenergetic.

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

5. On the energy of biregular graphs

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

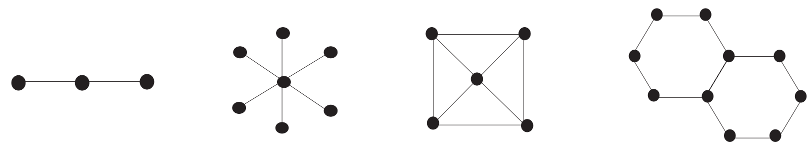

FIGURE 3. Examples of biregular graphs: a (1,2)-biregular tree (the 3-vertex path), a (1,6)-biregular tree (the 7-vertex star), a (3,4)-biregular graph, and a (2,3)-biregular graph (a hexagonal system).

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

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

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

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

and

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

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

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

Further,

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

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

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

and

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

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

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

From (19) we obtain

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

or simplified

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

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

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

and its first derivative

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

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

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

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

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

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

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

and

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

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

Now, the inequality (14) becomes

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

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

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

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

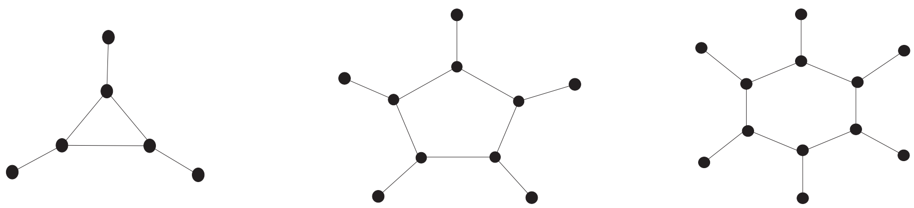

FIGURE 4. Examples of connected quadrangle-free (1,3)-biregular unicyclic graphs.

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

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

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

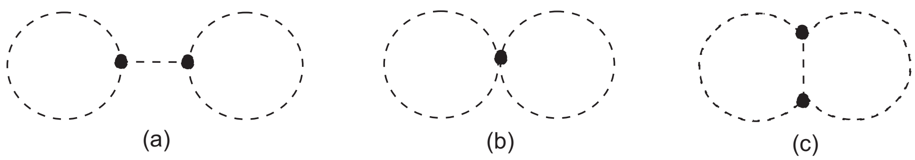

FIGURE 5. Types of bicyclic graphs.

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

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

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

from which

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

For $q = 0$ we obtain

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

or simplified

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

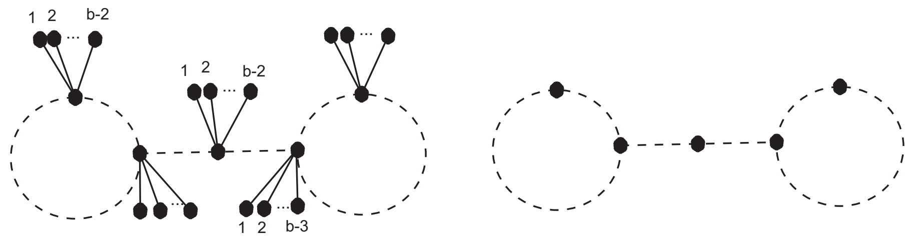

FIGURE 6. Sketches of $(1, b)$-, and $(2, 3)$-biregular bicyclic graphs with disjoint cycles. The vertices that connect cycles in a $(1, b)$-biregular graph ($b \geqslant 3$) are connected also with $b - 3$ pendent vertices, whereas all other vertices in such a graph are connected with $b - 2$ pendent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

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

If we examine the function

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

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

For $q = 1$ we have

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

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

For $q = 2$ we have

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

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

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

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

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

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

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

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

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

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

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

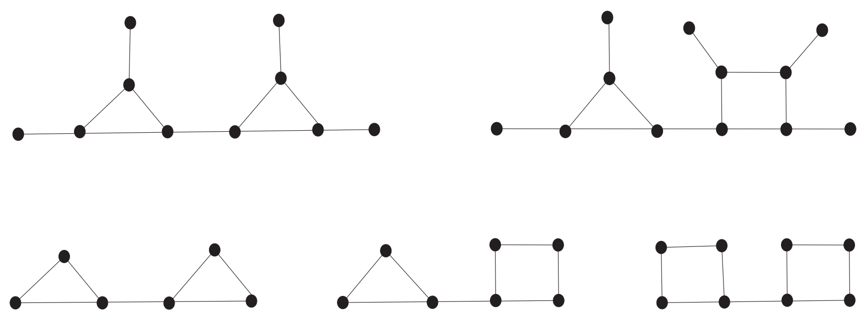

FIGURE 7. Connected bicyclic $(1, 3)$-biregular graphs with disjoint cycles, with $q = 0$ and $q = 1$, and bicyclic $(2, 3)$-biregular graphs with disjoint cycles, with $q = 0$, $q = 1$, $q = 2$. In all these examples the number of vertices is as small as possible.

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

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

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

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

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

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

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

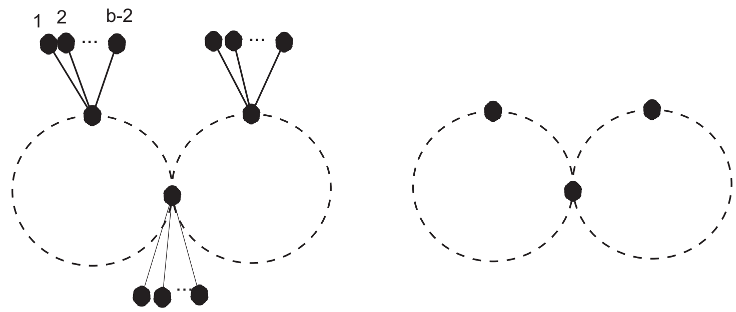

FIGURE 8. Connected bicyclic $(1, b \geqslant 4)$- and $(2, 4)$-biregular graph in which cycles have one common vertex. For the $(1, b)$-biregular graph, $b \geqslant 4$, every vertex except the one belonging to both cycles is connected with $b - 2$ pendent vertices. The vertex belonging to both cycles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

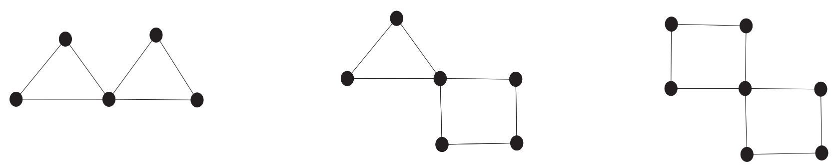

FIGURE 9. Bicyclic $(2, 4)$-biregular graphs in which the cycles have one common vertex, with $q = 0, 1, 2$ quadrangles. In these examples the number of vertices is as small as possible.

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

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

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

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

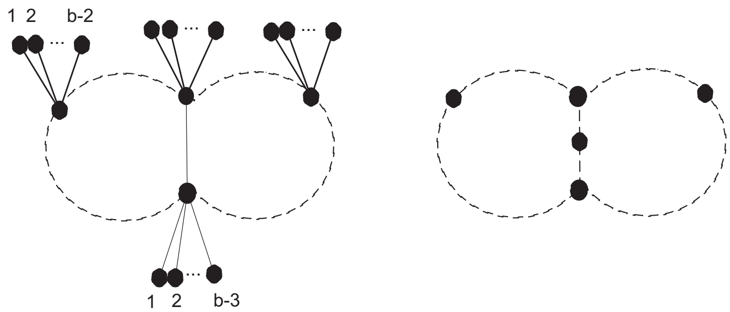

FIGURE 10. Connected bicyclic $(1, b \geqslant 3)$- and $(2, 3)$-biregular graphs in which the cycles have two or more common vertices. Notice that the graphs of first type have only two common vertices, whereas the graphs of the second type can have arbitrarily many common vertices (but more than one,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

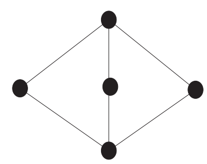

FIGURE 11. The only bicyclic biregular graph in which the number of quadrangles q is 3. For this graph inequality (14) is violated.

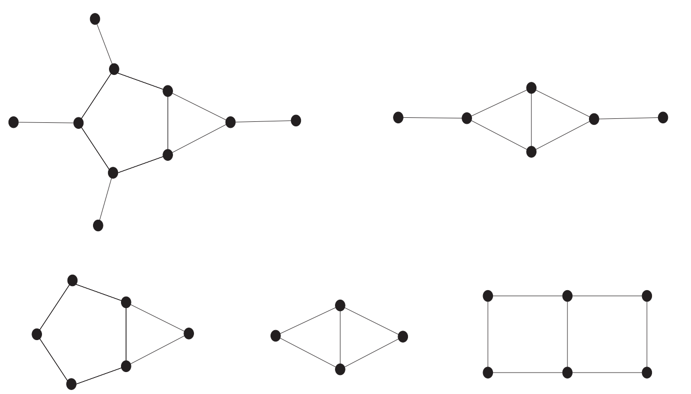

FIGURE 12. Bicyclic $(1, 3)$-biregular graphs in which cycles have two common vertices and $q = 0, 1$, and bicyclic $(2, 3)$-biregular graphs with $q = 0, 1, 2$.

6. On the energy of triregular graphs

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

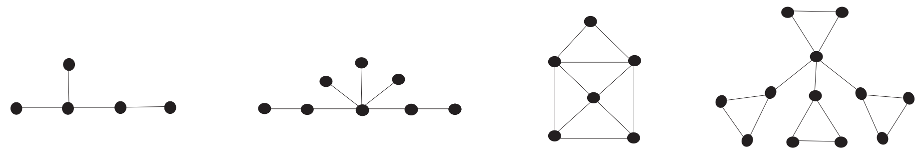

FIGURE 13. (1,2,3)-, (1,2,5)-, (2,3,4)-, and (2,3,5)-triregular graph, respectively.

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

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

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

and

$$x n_x + a n_a + b n_b = 2m \tag{27}$$

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

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

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

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

which combined with Eqs. (28) yields

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

From this,

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

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

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

from which

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

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

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

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

Now, by applying Theorem 1.1 we get

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

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

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

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

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

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

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

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

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

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

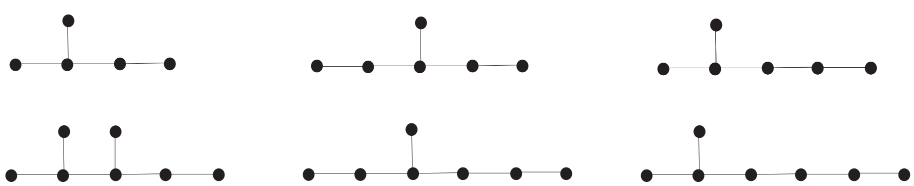

FIGURE 14. $(1,2,3)$-triregular trees not satisfying inequality (14).

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

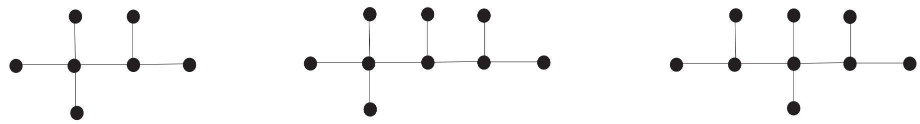

Figure 15. (1, 2, 4)-triregular trees not satisfying inequality (14).

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

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

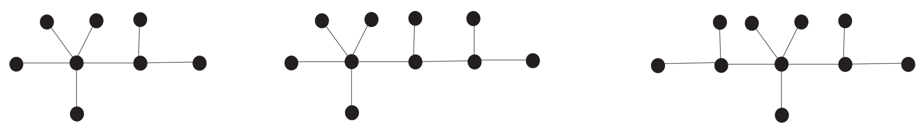

Figure 16. (1, 3, 5)-triregular trees not satisfying inequality (14).

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

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

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

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

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

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

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

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

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

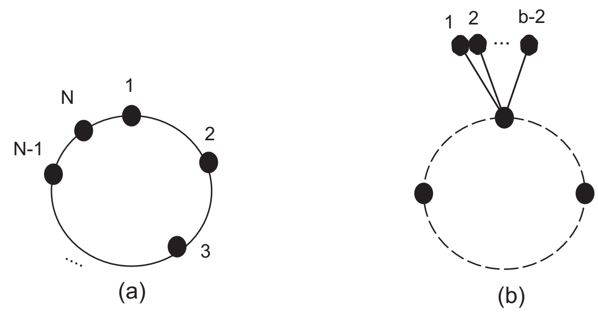

Figure 17. Details related to the proof of Lemma 6.4 for $a = 2$.

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

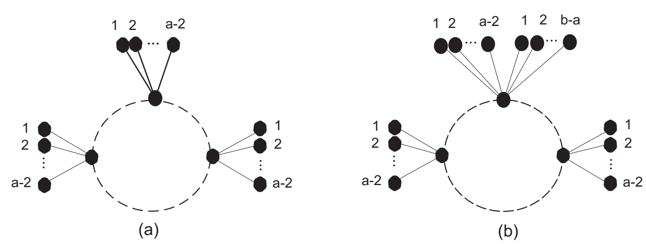

Figure 18. Details related to the proof of Lemma 6.4 for $a > 2$.

For $q = 0$ we have

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

and from Lemma 6.4 it follows

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

that is

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

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

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

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

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

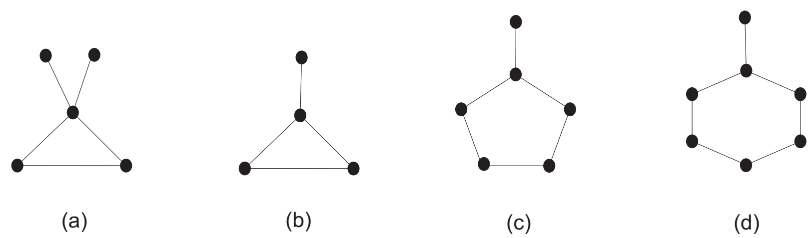

FIGURE 19. Diagram (a) represents the unique unicyclic quadrangle-free $(1, 2, 4)$-triregular graph for which inequality (14) does not hold. Diagrams (b), (c), and (d) pertain to the smallest unicyclic $(1, 2, 3)$-triregular graphs with $N = 3, 5, 6$, respectively.

For $q = 1$ we have

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

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

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

Expressing n in the above inequality we arrive at:

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

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

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

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

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

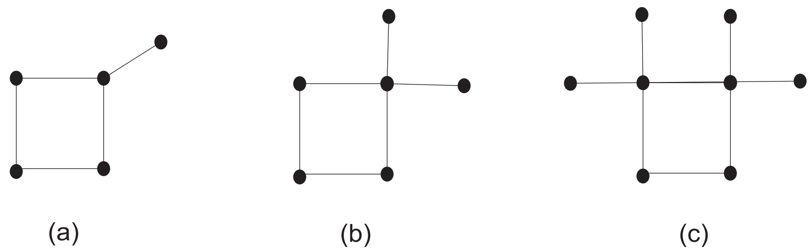

FIGURE 20. Diagram (a) represents the unique unicyclic $(1,2,3)$-triregular graph with $q=1$ for which inequality (14) does not hold. Diagrams (b) and (c) are the unique unicyclic $(1,2,4)$-triregular graphs with $q=1$ and with number of vertices $n=6,8$, respectively for which inequality (14) does not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

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

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

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

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

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

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

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

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

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

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

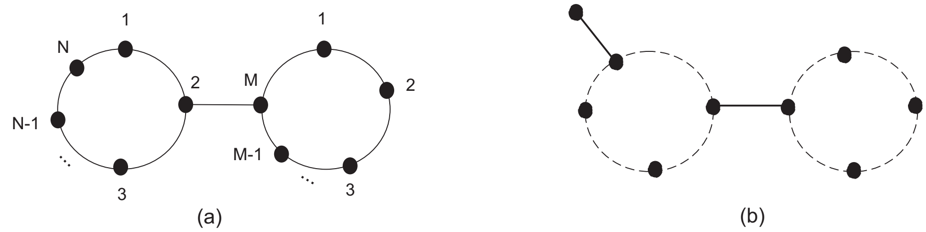

FIGURE 21. Details related to the proof of Lemma 6.10 for $a = 2$, $b = 3$.

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

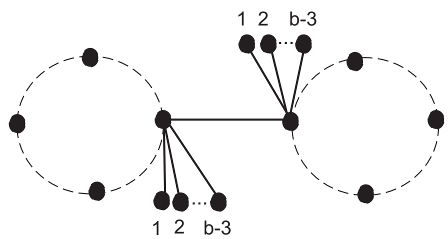

FIGURE 22. Details related to the proof of Lemma 6.10 for $a = 2$, $b > 3$.

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

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

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

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

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

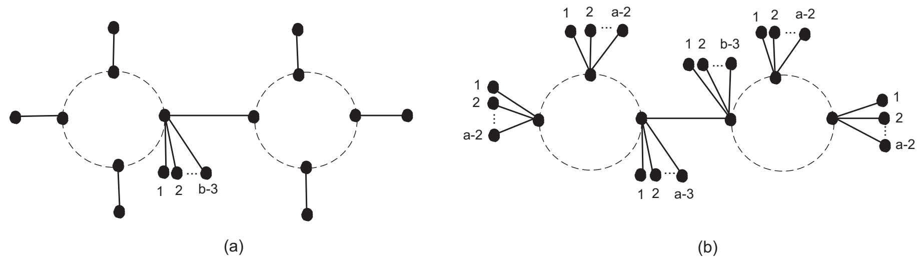

Figure 23. Details related to the proof of Lemma 6.10 for $a > 2$, $b > 3$.

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

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

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

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

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

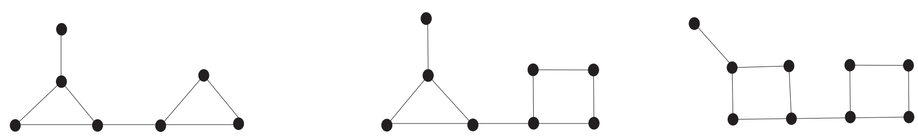

Figure 24. Bicyclic $(1, 2, 3)$-triregular graphs with disjoint cycles, with $q = 0, 1, 2$, and with minimal number of vertices.

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

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

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

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

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

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

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

respectively, resulting in:

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

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

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

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

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

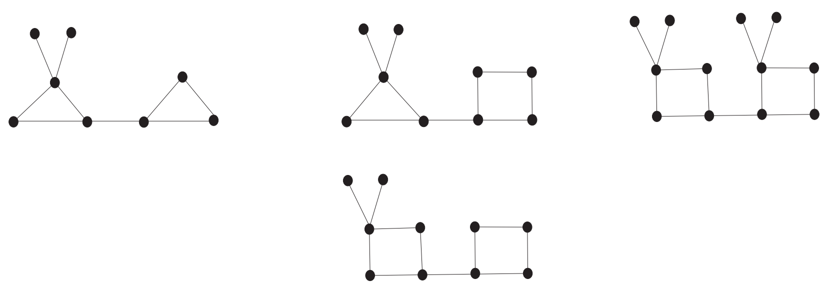

FIGURE 25. Examples of bicyclic $(1,2,4)$-triregular graphs with disjoint cycles. Only the graph with $q = 2$ and $n = 10$ violates inequality (14).

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

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

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

(32)

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

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

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

For $q = 2$ we obtain

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

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

Consider now some special cases of Theorem 6.13.

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

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

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

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

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

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

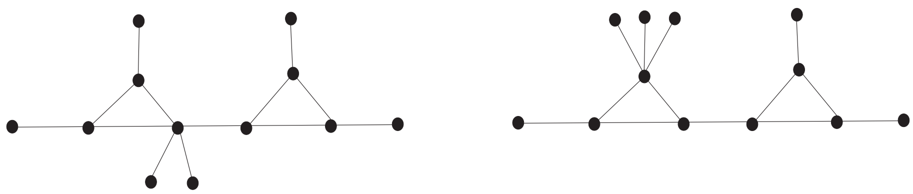

Figure 26. The only bicyclic $(1,3,5)$-triregular graphs with two disjoint cycles of size 3, which do not satisfy condition (14).

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

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

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

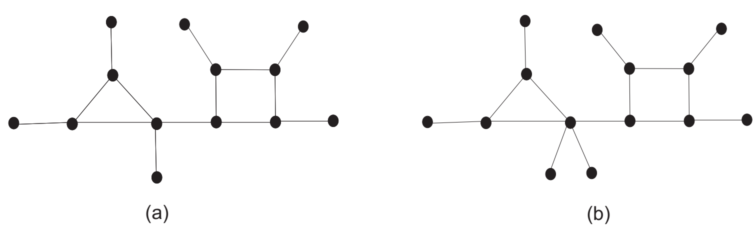

Figure 27. Some bicyclic triregular graphs violating condition (14).

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

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

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

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

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

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

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

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

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

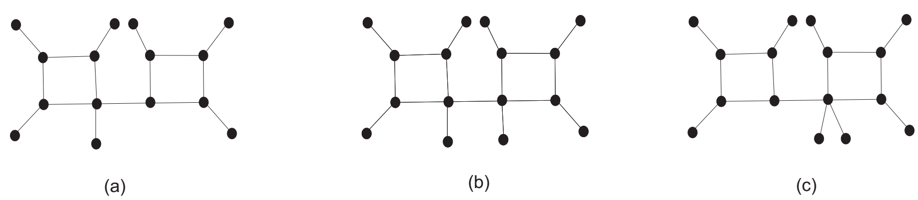

FIGURE 28. Some further bicyclic triregular graphs violating condition (14).

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

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

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

where N and M are the sizes of the cycles.

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

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

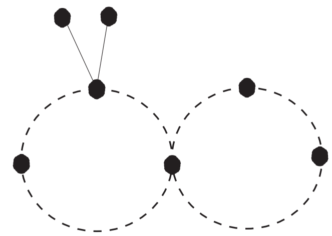

FIGURE 29. Details related to the proof of Lemma 6.14 for $a = 2$, $b = 4$.

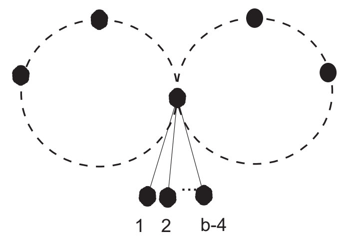

FIGURE 30. Details related to the proof of Lemma 6.14 for $a = 2$, $b > 4$.

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

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

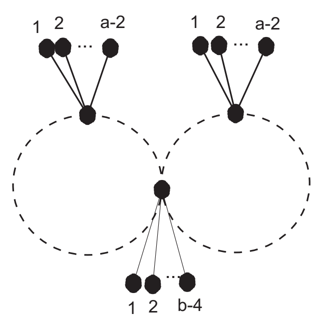

FIGURE 31. Details related to the proof of Lemma 6.14 for $a > 2$, $b > 3$.

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

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

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

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

For $q = 0$ we have

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

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

For $q = 1$ we have

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

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

For $q = 2$ we have

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

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

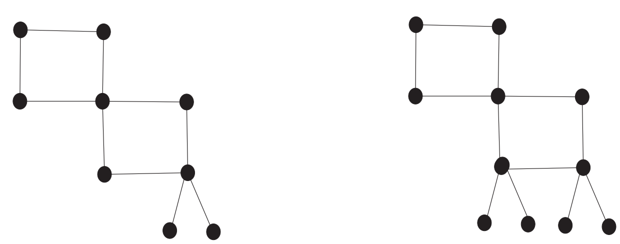

FIGURE 32. Bicyclic (1,2,4)-triregular graphs on 9 and 11 vertices. These violate inequality (14).

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

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

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

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

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

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

and from Lemma 6.14 it follows that

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

where $N, M \neq 4$.

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

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

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

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

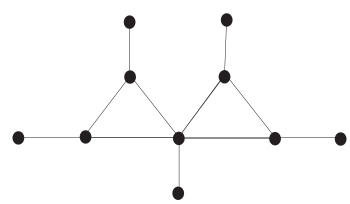

FIGURE 33. A 10-vertex graph for which condition (14) does not hold.

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

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

and from Lemma 6.14 it follows that

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

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

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

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

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

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

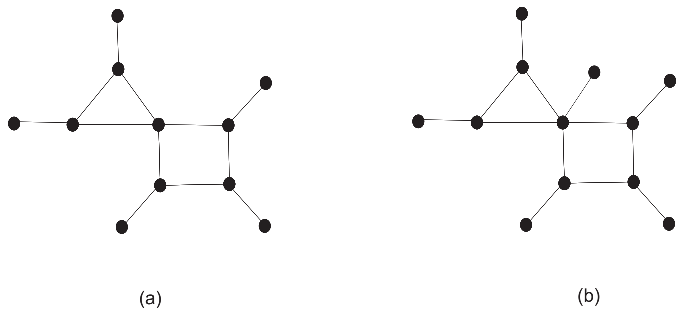

FIGURE 34. A bicyclic (1,3,4)-triregular graph on 11 vertices and a bicyclic (1,3,5)-triregular graph on 12 vertices for which condition (14) does not hold.

For $q = 2$ inequality (31) becomes

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

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

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

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

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

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

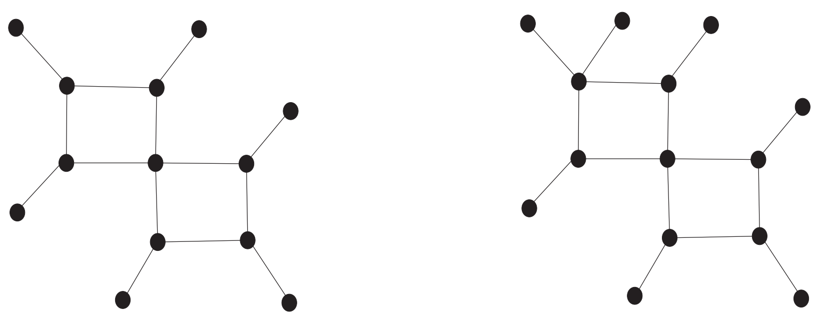

FIGURE 35. A 13- and a 14-vertex bicyclic (1,3,4)-triregular graph for which condition (14) does not hold.

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

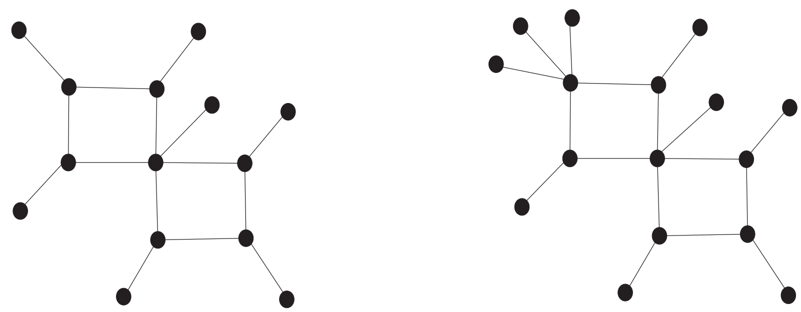

FIGURE 36. A 14- and a 16-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

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

$$\frac{(5+ab-2a-2b)n^3+(13-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant (a-2)(N+M)-2a+b$$
$$\frac{(5+ab-2a-2b)n^3+(9-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant (a-2)(4+M)-2a+b$$
$$\frac{(5+ab-2a-2b)n^3+(5-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geqslant 6a+b-16$$

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

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

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

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

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

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

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

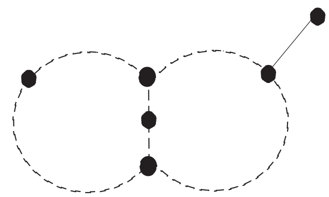

FIGURE 37. Details related to the proof of Lemma 6.17 for $a = 2$, $b = 3$.

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

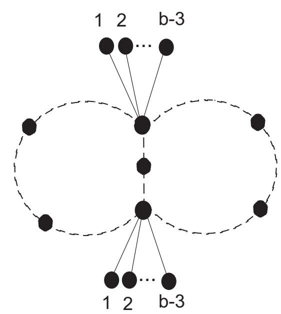

FIGURE 38. Details related to the proof of Lemma 6.17 for $a = 2$, $b > 3$.

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

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

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

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

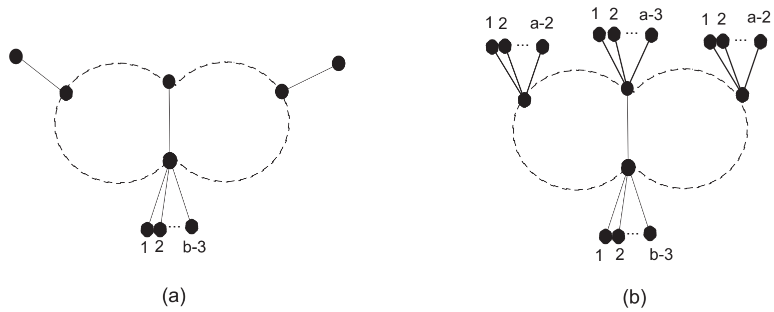

FIGURE 39. Details related to the proof of Lemma 6.17 for $a > 2$, $b > 3$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

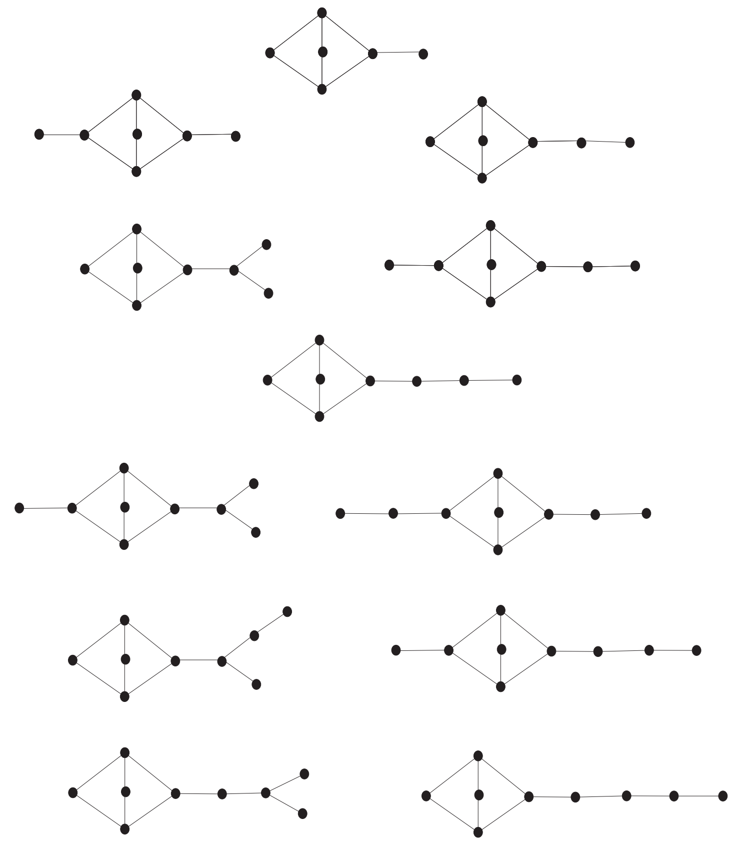

FIGURE 40. All bicyclic (1,2,3)-triregular graphs with $q = 3$, for which condition (14) does not hold. These have 6, 7, 8, and 9 vertices.

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

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

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

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

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

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

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

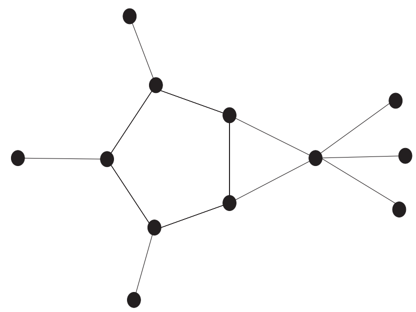

FIGURE 41. A 12-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

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

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

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

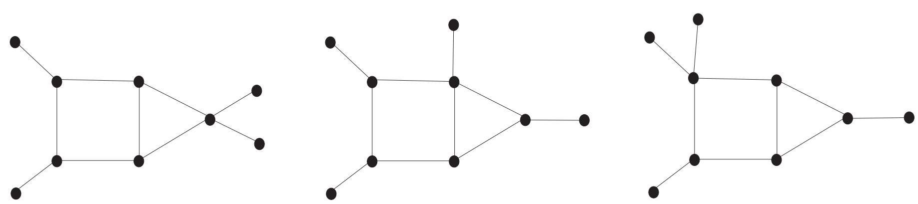

FIGURE 42. Bicyclic (1,3,4)-triregular graphs on 9 vertices for which condition (14) does not hold.

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

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

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

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

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

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

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

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

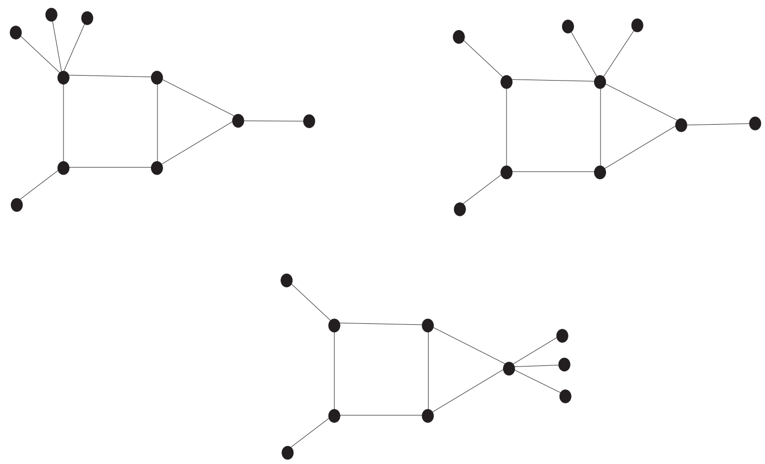

FIGURE 43. Bicyclic (1,3,5)-triregular graphs on 10 vertices for which condition (14) does not hold.

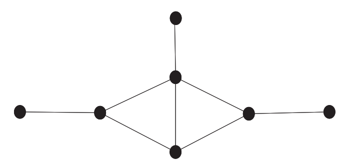

FIGURE 44. A 7-vertex bicyclic (1,3,4)-triregular graph for which condition (14) does not hold.

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

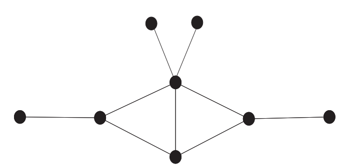

FIGURE 45. An 8-vertex bicyclic (1,3,5)-triregular graph for which condition (14) does not hold.

For $q = 2$ we obtain

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

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

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

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

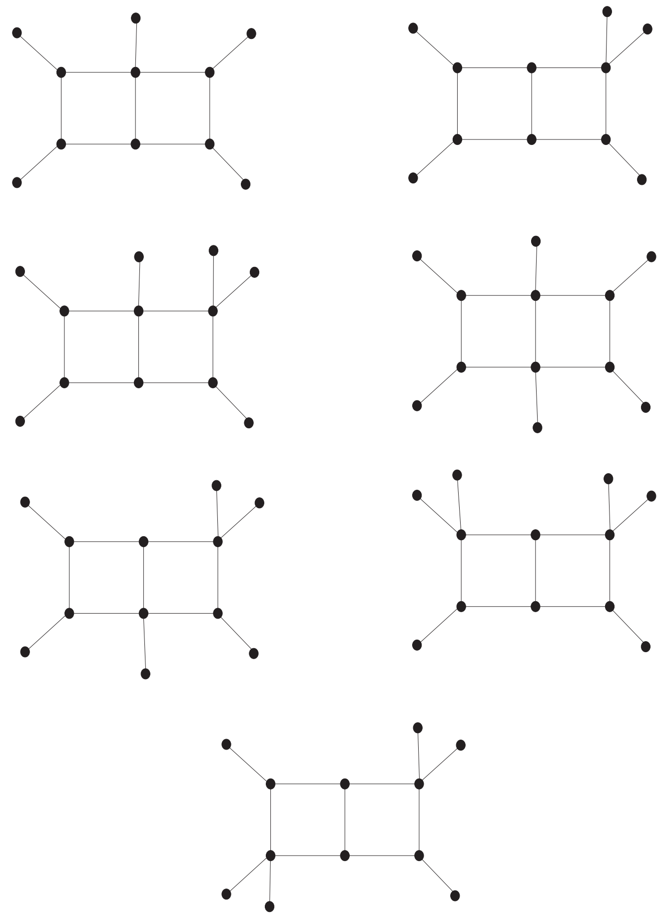

FIGURE 46. Bicyclic (1,3,4)-triregular graphs on 11 and 12 vertices, with $q = 2$, for which condition (14) does not hold.

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

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

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

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

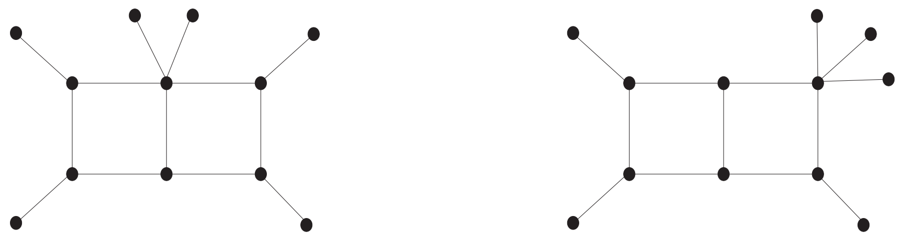

FIGURE 47. Two 12-vertex bicyclic (1,3,5)-triregular graphs with $q = 2$ for which condition (14) does not hold.

(a) $q = 0$ *and*

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

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

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

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

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

(d) $q = 2$ *and*

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

7. Epilogue

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

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

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