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TRIREGULAR GRAPHS WHOSE ENERGY EXCEEDS THE NUMBER OF VERTICES

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Abstract

A graph is said to be triregular if its vertex degrees assume exactly three different values. The energy $E(G)$ of a graph G is equal to the sum of the absolute values of the eigenvalues of G. Conditions are established under which the inequality $E(G) > n$ is obeyed for connected n-vertex acyclic, unicyclic, and bicyclic triregular graphs.

INTRODUCTION

In the preceding paper [1] we established necessary and sufficient conditions for the validity of the inequality

$$\sqrt{\frac{M_2(G)^3}{M_4(G)}} \geq n \tag{1}$$

where $M_2(G)$ and $M_4(G)$ are the second and fourth spectral moments, respectively, of the n-vertex graph G. In view of the relation $E(G) \geq \sqrt{M_2(G)^3/M_4(G)}$, whenever (1) is obeyed, the energy $E(G)$ of the graph G exceeds the number of vertices.

Our notation and basic terminology is same as in [1] and will not be described here once again. This, in particular, applies to the graph–energy concept. In [1] a detailed account of the history and current research of the problem of characterizing (molecular) graphs for which $E(G) \geq n$ is given.

In order to avoid any misunderstand, we point our the following: The inequality (1) is a <u>sufficient</u>, but <u>not a necessary</u> condition for the validity of $E(G) \geq n$. In other words, if (1) is satisfied, then the respective graph energy necessarily exceeds the number of vertices. If, however, the inequality (1) is not obeyed, then the relation $E(G) \geq n$ may still hold, but also may be violated.

It is known [2–4] that the equality $E(G) = \sqrt{M_2(G)^3/M_4(G)}$ holds if and only if the components of the graph G are isolated vertices and/or complete bipartite graphs $K_{p_1,q_1}, \ldots, K_{p_k,q_k}$ for some $k \geq 1$, such that $p_1\,q_1 = \cdots = p_k\,q_k$. If G is connected and has at least two vertices, then the above equality holds only if G is a complete bipartite graph. Graphs with such special structure are of no relevance for the present considerations (in particular, the above equality cannot hold for a connected triregular graph). Therefore, whenever the relation (1) is satisfied, the energy of the underlying graph G strictly exceeds the number of vertices, i. e., $E(G) > n$.

In the preceding paper [1] we considered acyclic, unicyclic, and bicyclic biregular graphs. Here we extend our analysis to triregular graphs.

Let G be an n-vertex graph whose vertices have degrees $d_1, d_2, \ldots, d_n$. Let x, a, and b be three positive integers, $1 \leq x < a < b \leq n-1$. Then G is said to be *triregular* if for $i = 1, 2, \ldots, n$, either $d_i = x$ or $d_i = a$ or $d_i = b$, and there exists at least one vertex of degree x, at least one vertex of degree a, and at least one vertex of degree b. If so, then G is a *triregular graph of degrees* x, a, *and* b or, for brevity, an (x, a, b)*-triregular graph*.

Throughout this paper all graphs are understood to be connected.

GENERAL TRIREGULAR GRAPHS

In this section we consider (x, a, b)-triregular graphs, where $1 \leq x < a < b$ and x, a, b are integers. We know that for any graph with n vertices, m edges, q quadrangles, and vertex degrees $d_1, d_2, \ldots, d_n$,

$$\begin{aligned} M_2 &= 2m \\ M_4 &= 2\sum_{i=1}^{n}(d_i)^2 - 2m + 8q \ . \end{aligned}$$

For a triregular graph,

$$n_x + n_a + n_b = n \tag{2}$$

and

$$x\, n_x + a\, n_a + b\, n_b = 2m \tag{3}$$

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 (2) and (3) follows

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

and

$$\begin{aligned} \sum_{i=1}^{n}(d_i)^2 &= x^2 \cdot n_x + a^2 \cdot n_a + b^2 \cdot n_b \\ &= n_x(a-x)(b-x) + 2m(a+b) - abn \ . \end{aligned}$$

From this,

$$M_4 = 2[n_x(a-x)(b-x) + m(2a+2b-1) - abn + 4q] \ . \tag{4}$$

Substituting (4) and $M_2 = 2m$ back into (1) we get

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

from which,

$$n_x \leq \frac{4m^3 + n^2[abn - 4q - m(2a+2b-1)]}{n^2(a-x)(b-x)} \,. \tag{5}$$

Theorem 1. Let G be an (x,a,b)-triregular graph with n vertices, m edges, and q quadrangles. Let n_x be the number of vertices degree x. Then (1) holds if and only if condition (5) is satisfied.

TRIREGULAR TREES

Let T be a triregular n-vertex tree with vertex degrees 1, a, and b, $1 < a < b \leq n-2$. The number of its edges is $m = n-1$. For such a tree, $n \geq 5$. By applying Theorem 1 we get

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

where n_1 is the number of pendent vertices.

Since for every triregular tree, $n_1 \geq a+b-2$, the right–hand side of the latter inequality must be greater than $a+b-2$. Thus, we require

$$\frac{(5+ab-2a-2b)n^3 + (2a+2b-13)n^2 + 12n - 4}{n^2(a-1)(b-1)} \geq a+b-2 \,. \tag{6}$$

For a $(1,2,3)$-triregular tree the relation (6) yields $(n^3 - 3n^2 + 12n - 4)/(2n^2) \geq 3$, which implies $n^3 - 9n^2 + 12n - 4 \geq 0$. This latter inequality holds for every $n \geq 8$.

Theorem 2.1. Let T be a $(1,a,b)$-triregular tree, $1 < a < b$, and let n be the number of its vertices. Then (1) holds if and only if relation (6) is satisfied.

Corollary 2.2. Let T be a $(1,2,3)$-triregular tree and let n be the number of its vertices. Then (1) holds if and only if $n \geq 8$.

Recall that $(1,2,3)$-triregular graphs are of particular importance in chemical applications, since these are molecular graphs of conjugated π-electron systems [5–7].

Another noteworthy special case of Theorem 2.1 is for $(1,3,4)$-triregular trees, for which (6) reduces to $3n^3 - 29n^2 + 12n - 4 \geq 0$. This inequality holds for $n \geq 10$. Since the smallest such tree has exactly 7 vertices, we conclude that (1) is not true for such trees with $n = 7, 9, 11$. In the same way for a $(1, 3, 5)$-triregular tree we have $4n^3 - 45n^2 + 12n - 4 \geq 0$ and this is true for $n \geq 11$. Again, we conclude that (1) is violated for such trees with $n = 8, 10$.

Inequality (1) holds for $(1, 4, 5)$–, $(1, 4, 6)$–, $(1, 4, 7)$–, and $(1, 5, 6)$-triregular trees for $n \geq 12$, $n \geq 13$, $n \geq 14$, and $n \geq 14$, respectively.

UNICYCLIC TRIREGULAR GRAPHS

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

Inequality (5) together with the conditions $m = n$ and $x = 1$ yields

$$n_1 \leq \frac{n(5 + ab - 2a - 2b) - 4q}{(a-1)(b-1)} . \tag{7}$$

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

Lemma 3.1. Let G be a unicyclic $(1, a, b)$-triregular graph with n vertices and n_1 pendent vertices. Then

$$n_1 \geq b - a + N(a-2)$$

where N is the 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.

Proof. Consider first the case $a = 2$, $b \geq 3$. We construct such a graph with minimal number of pendent vertices. Start with the N-vertex cycle, in which each vertex is of degree 2. Choose only one vertex in the cycle and connect it with $b - 2$ vertices, each of degree 1. 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 the cycle we must add another $a - 2$ pendent vertices, so at the moment we have $N(a-2)$ pendent vertices and each vertex in the cycle is of degree a. Then, we choose only one vertex in the cycle and connect it with additional $b - a$ pendent vertices. This vertex is of degree b and any other vertex in the cycle is of degree a. By this we constructed a graph with minimal number of pendent vertices, equal to $b-a+N(a-2)$. ■

If $q=0$, then (7) becomes

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

and by Lemma 3.1,

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

that is

$$n \geq [b-a+N(a-2)]\frac{(a-1)(b-1)}{(5+ab-2a-2b)} \ . \tag{8}$$

Theorem 3.2. Let G be an n-vertex unicyclic $(1,a,b)$-triregular graph, $2 \leq a < b$. Let G be quadrangle–free and its cycle be of size N , $N \neq 4$. Then (1) holds if and only if condition (8) is satisfied.

If $a=2$, then (8) reduces to $n \geq (b-2)(b-1)$.

Corollary 3.3. Let G be an n-vertex unicyclic $(1,2,b)$-triregular graph, $b \geq 3$. Let G be quadrangle–free and its cycle be of size N , $N \neq 4$. Then (1) holds if and only if $n \geq (b-1)(b-2)$.

For example, for the (unique) unicyclic $(1,2,4)$-triregular graph with $n=5$ the inequality stated in Corollary 3.3 does not hold, but it is obeyed by every unicyclic quadrangle–free $(1,2,3)$-triregular graph.

For $q=1$ from (7) it follows

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

We have $N=4$ and, by Lemma 3.1, $n_1 \geq 3a+b-8$. Thus the right–hand side of the above inequality must be at least $3a+b-8$. In view of this,

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

resulting in

$$n \geq \frac{(a-1)(b-1)(3a+b-8)+4}{(a-1)(b-1)+4-(a+b)} \ . \tag{9}$$

Theorem 3.4. Let G be an n-vertex unicyclic $(1,a,b)$-triregular graph, $2 \leq a < b$, whose cycle is of size 4. Then (1) holds if and only if condition (9) is satisfied.

If $a = 2$ then (9) is simplified as $n \geq (b-1)(b-2)+4$, leading to

Corollary 3.5. Let G be an n-vertex unicyclic $(1,2,b)$-triregular graph, $b \geq 3$, whose cycle is of size 4. Then (1) holds if and only if $n \geq (b-1)(b-2)+4$.

Corollary 3.6. Let G be an n-vertex unicyclic $(1,2,3)$-triregular graph, whose cycle is of size 4. Then (1) holds for every $n \geq 6$.

BICYCLIC TRIREGULAR GRAPHS

In the case of bicyclic (x,a,b)-triregular graphs it must be $x = 1$. Then the inequality (5), together with the condition $m = n+1$, yields

$$n_1 \leq \frac{(5+ab-2a-2b)n^3+(13-2a-2b-4q)n^2+12n+4}{n^2(a-1)(b-1)} \,. \tag{10}$$

Note that here q may assume the values 0, 1, 2, or 3.

As outlined already in [1], there are three types of bicyclic graphs:

(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.

Each of these types will be considered separately. In cases (a) and (b), $q \in \{0,1,2\}$ whereas in case (c), $q \in \{0,1,2,3\}$.

Case (a): Bicyclic triregular graphs with disjoint cycles

Lemma 4.1. Let G be a bicyclic $(1,a,b)$-triregular graph, $2 \leq a < b$, with disjoint cycles and with n_1 pendent vertices. Then

$$n_1 \geq \begin{cases} 1 & \text{if } a=2\,,\ b=3 \\ 2(b-3) & \text{if } a=2\,,\ b>3 \\ (a-2)(N_1+N_2-2)+(b-3)+(a-3) & \text{otherwise} \end{cases}$$

where N_i is the number of vertices of the i-th cycle of G, $i = 1,2$.

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

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

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.

For $2 < a < b$ we have to connect each vertex of degree 2 with $a - 2$ pendent vertices. There are $N_1 + N_2 - 2$ vertices of degree 2 so we arrive at $(a-2)(N_1 + N_2 - 2)$ 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 $b > 3$. If $a > 3$, again, 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. In this way we obtain the $(1, a, b)$-triregular graph with minimal number of pendent vertices, equal to $(a - 2)(N_1 + N_2 - 2) + (b - 3) + (a - 3)$. ■

Consider first $(1, 2, 3)$-triregular graphs. From (10) it follows that

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

By Lemma 4.1, the right–hand side of this inequality must be at least 1. Therefore,

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

i. e., $n^3 + (1 - 4q)n^2 + 12n + 4 \geq 0$. For $q = 0, 1, 2$ this yields

$$\begin{aligned} n^3 + n^2 + 12n + 4 &\geq 0 \\ n^3 - 3n^2 + 12n + 4 &\geq 0 \\ n^3 - 7n^2 + 12n + 4 &\geq 0 \end{aligned}$$

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

Theorem 4.2. Inequality (1) is obeyed by all bicyclic $(1, 2, 3)$-triregular graphs with disjoint cycles.

Next we consider the case $a = 2$, $b \geq 4$. From (10) it follows that

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

From Lemma 4.1 we get that the right–hand side of the above inequality must be at least $2(b-3)$, which implies

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

i. e., $n^3 + (3 + 6b - 2b^2 - 4q)n^2 + 12n + 4 \geq 0$. For $q = 0, 1, 2$ we then obtain

$$2b^2 - 6b - 3 \leq \frac{n^3 + 12n + 4}{n^2} \tag{11}$$

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

$$2b^2 - 6b + 5 \leq \frac{n^3 + 12n + 4}{n^2} \tag{13}$$

respectively, which results in:

Theorem 4.3. Let G be a bicyclic $(1, 2, b)$-triregular graph with disjoint cycles, $b \geq 4$. Let n be the number of its vertices and q the number of its quadrangles. Then (1) holds if and only if for $q = 0$, $q = 1$, and $q = 2$, the inequalities (11), (12), and (13), respectively, are satisfied.

For example, for any bicyclic $(1, 2, 4)$-triregular graph, (11) and (12) hold for all values of n (for which such graphs exist), whereas (13) is not true only for $n = 10$.

In the case $2 < a < b$, from (10) and Lemma 4.1 it follows that

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b - 4q)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geq (a-2)(N_1 + N_2) + b - a - 2$$

which for $q = 0$ (that is, $N_1, N_2 \neq 4$), for $q = 1$ (that is, $N_1 = 4$, $N_2 \neq 4$), and for $q = 2$ (that is, $N_1 = N_2 = 4$) gives

$$\frac{(5+ab-2a-2b)n^3+(13-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geq (a-2)(N_1+N_2)+b-a-2 \tag{14}$$

$$\frac{(5+ab-2a-2b)n^3+(9-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geq (a-2)(4+N_2)+b-a-2 \tag{15}$$

$$\frac{(5+ab-2a-2b)n^3+(5-2a-2b)n^2+12n+4}{n^2(a-1)(b-1)} \geq 7a+b-18 \tag{16}$$

respectively.

Theorem 4.4. Let G be a bicyclic $(1,a,b)$-triregular graph with disjoint cycles, $2 < a < b$. Let n be the number of its vertices, and N_1, N_2 the size of its cycles, of which q cycles are quadrangles. Then (1) holds if and only if for $q=0$, $q=1$, and $q=2$, the inequalities (14), (15), and (16), respectively, are satisfied.

Consider now two special cases of Theorem 4.4, that may be of interest in chemical applications.

If $a=3$, $b=4$, and $N_1=N_2=3$, then

$$\frac{3n^3-n^2+12n+4}{6n^2} \geq 5$$

that is $3n^3-31n^2+12n+4 \geq 0$. This condition holds for $n \geq 10$. On the other hand, the smallest such graphs have 14 vertices, implying that (1) is satisfied for all such graphs.

If $a=3$, $b=4$, and $N_1=N_2=4$, then

$$\frac{3n^3-9n^2+12n+4}{6n^2} \geq 7$$

that is $3n^3-51n^2+12n+4 \geq 0$. This condition holds for $n \geq 17$ whereas the smallest such graph has 16 vertices. Thus (1) is violated for the (unique) such graph with $n=16$.

Case (b): Bicyclic triregular graphs with cycles sharing a single vertex

In analogy to Lemma 4.1 we can prove:

Lemma 4.5. Let G be a bicyclic $(1, a, b)$-triregular graph, $2 \leq a < b$, in which the cycles share a single vertex. Let n_1 be the number of its pendent vertices. Then

$$n_1 \geq \begin{cases} 2 & \text{if } a = 2\,,\ b = 4 \\ (a-2)(N_1 + N_2 - 2) + b - 4 & \text{otherwise} \end{cases}$$

where N_i is the number of vertices in the i-th cycle, $i = 1, 2$.

Bearing in mind that for any triregular graph considered in this section it must be $b \geq 4$, the simplest case will be the bicyclic $(1, 2, 4)$-triregular graphs. For such graphs relation (10) reduces to

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

By Lemma 4.5, its right–hand side must be at least 2, and so we have

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

from which $n^3 - (5+4q)n^2 + 12n + 4 \geq 0$. Then, an analysis analogous to what was used for obtaining Theorems 4.3 and 4.4 results in:

Theorem 4.6a. 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_1, N_2 the size of its cycles, of which q cycles are quadrangles. Then (1) holds if and only if , the inequalities

$$n^3 - 5n^2 + 12n + 4 \ \geq\ 0 \tag{17}$$

$$n^3 - 9n^2 + 12n + 4 \ \geq\ 0 \tag{18}$$

$$n^3 - 13n^2 + 12n + 4 \ \geq\ 0 \tag{19}$$

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

Inequalities (17) and (18) hold for all bicyclic $(1, 2, 4)$-triregular graphs with $q = 0$ and $q = 1$. Inequality (19) is satisfied for $n \geq 12$, whereas there exists bicyclic $(1, 2, 4)$-triregular graphs with $q = 2$ and $n = 9$ and $n = 11$. In view of this, we have:

Theorem 4.6b. Relation (1) holds for all graphs specified in Theorem 4.6a, for which $q = 0$ and $q = 1$, and for all graphs with $q = 2$ and $n \geq 13$. In case $q = 2$ it is violated for graphs with $n = 9$ and $n = 11$.

If the graph G is bicyclic $(1, a, b)$-triregular, $2 < a < b$, an analogous reasoning leads to:

Theorem 4.7. 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_1, N_2 the size of its cycles, of which q cycles are quadrangles. Then (1) holds if and only if the inequalities

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a - 1)(b - 1)} \geq (a - 2)(N_1 + N_2) - 2a + b \tag{20}$$

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a - 1)(b - 1)} \geq (a - 2)(4 + N_2) - 2a + b \tag{21}$$

$$\frac{(5 + ab - 2a - 2b)n^3 + (5 - 2a - 2b)n^2 + 12n + 4}{n^2(a - 1)(b - 1)} \geq 6a + b - 16 \tag{22}$$

are satisfied for $q = 0$, $q = 1$, and $q = 2$, respectively. In (20) $N_1, N_2 \neq 4$; in (21) $N_2 \neq 4$.

We elaborate now a few special cases of Theorem 4.7.

If $a = 3$, $b = 4$, and $N_1 = N_2 = 3$, then $q = 0$ and we have

$$\frac{3n^3 - n^2 + 12n + 4}{6n^2} \geq 4$$

that is $3n^3 - 25n^2 + 12n + 4 \geq 0$ and this holds for $n \geq 8$. Since the smallest such graph has 9 vertices, the above relation is satisfied for all such graphs, and therefore (1) holds for all such graphs.

If $a = 3$, $b = 5$, and $N_1 = N_2 = 3$, then $4n^3 - 43n^2 + 12n + 4 \geq 0$, and this holds for $n \geq 11$. Thus this condition is not obeyed by the unique such graph with 10 vertices.

If $q = 1$, $a = 3$, $b = 4$, and $N_2 = 3$, then

$$\frac{3n^3 - 5n^2 + 12n + 4}{6n^2} \geq 5$$

i. e., $3n^3 - 35n^2 + 12n + 4 \geq 0$, which holds for $n \geq 12$. The unique such graph with 11 vertices violates the condition.

For $q = 1$, $a = 3$, $b = 5$, and $N_2 = 3$ the condition (21) reduces to $4n^3 - 55n^2 + 12n + 4 \geq 0$, which holds for $n \geq 14$. The unique such graph with $n = 12$ does not obey this requirement, and therefore (1) is violated by only a single such graph.

If $q = 2$, $a = 3$, and $b = 4$, relation (22) gives $3n^3 - 45n^2 + 12n + 4 \geq 0$, implying that it must be $n \geq 15$. The graphs with $n = 13, 14$ fail to satisfy (22) and thus for them (1) does not hold.

If $q = 2$, $a = 3$, and $b = 5$, then $4n^3 - 67n^2 + 12n + 4 \geq 0$, from which $n \geq 17$. The graphs with $n = 14$ and $n = 16$ provide exceptions for which (1) is not satisfied.

Case (c): Bicyclic triregular graphs with cycles sharing two or more vertices

In this case, in analogy to Lemma 4.1 we have:

Lemma 4.8. Let G be a bicyclic $(1, a, b)$-triregular graph, $2 \leq a < b$, in which the cycles have two or more common vertices. Let n_1 be the number of its pendent vertices. Then

$$n_1 \geq \begin{cases} 1 & \text{if } a = 2\,,\ b = 3 \\ 2(b-3) & \text{if } a = 2\,,\ b \geq 4 \\ (a-2)(N_1 + N_2 - 4) + (b-3) + (a-3) & \text{otherwise} \end{cases}$$

where N_i is the number of vertices in the i-th cycle, $i = 1, 2$.

The analysis of the graphs encountered in Case (c) is analogous as in the previous two cases, and proceeds by pertinently combining inequality (10) and Lemma 4.8. Its details are skipped. The main difference is that in Case (c) the graphs contain three cycles (of which, of course, only two are independent). As a consequence, the number q of quadrangles may assume also the value 3.

Any two of the three cycles of the graphs considered in Case (c) may be chosen as independent. We will always choose those having the smallest size. These cycle sizes will be denoted by N_1 and N_2.

From a chemical point of view Case (c) is the least interesting one because there are hardly any molecular graphs of this kind.

For $(1,2,3)-$, (1,2,b)$-$, and (1,a,b)-triregular graphs, $2 < a < b \geq 4$, we get analogous results as in Cases (a) and (b), except that we must consider also the possibility $q = 3$.

Theorem 4.9. Inequality (1) is obeyed by all bicyclic $(1,2,3)$-triregular graphs having cycles that share two or more vertices.

Theorem 4.10. Let G be an n-vertex bicyclic $(1,2,b)$-triregular graph with cycles sharing two or more vertices, $b \geq 4$. Let q be the number of its quadrangles. Then (1) holds if and only if the inequalities

$$\begin{aligned}
2b^2 - 6b - 3 &\leq \frac{n^3 + 12n + 4}{n^2} \\
2b^2 - 6b + 1 &\leq \frac{n^3 + 12n + 4}{n^2} \\
2b^2 - 6b + 5 &\leq \frac{n^3 + 12n + 4}{n^2} \\
2b^2 - 6b + 9 &\leq \frac{n^3 + 12n + 4}{n^2}
\end{aligned}$$

are satisfied for $q = 0$, $q = 1$, $q = 2$, and $q = 3$, respectively.

Theorem 4.11. Let G be an n-vertex bicyclic $(1,a,b)$-triregular graph with cycles sharing two or more vertices, $2 < a < b$. Let N_1 and N_2 be the sizes of its two cycles. Let q be the number of its quadrangles. Then (1) holds if and only if

$$\frac{(5 + ab - 2a - 2b)n^3 + (13 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geq (a-2)(N_1 + N_2) + b - 3a + 2$$

for $q = 0$ and $N_1, N_2 \neq 4$,

$$\frac{(5 + ab - 2a - 2b)n^3 + (9 - 2a - 2b)n^2 + 12n + 4}{n^2(a-1)(b-1)} \geq (a-2)(4 + N_2) + b - 3a + 2$$

for $q = 1$, $N_1 = 4$, and $N_2 \neq 4$,

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

for $q = 1$ and $N_1 = N_2 = 3$,

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

for $q = 2$ and $N_1 = N_2 = 4$, and

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

for $q = 3$ and $N_1 = N_2 = 4$.

CONCLUDING REMARKS

In this and the preceding paper [1] we have completed the research of the domain of validity of the inequality (1) for acyclic, unicyclic, and bicyclic biregular and triregular graphs. Researches of this kind were first done in [4] (by solving the problem for general regular graphs), whereas some incomplete results were communicated in [8] (for acyclic and unicyclic biregular graphs), and in [9] (for acyclic and unicyclic triregular graphs).

The obvious question at this point is if the considerations can be extended to tetraregular, pentaregular, etc. graphs. In principle, this would be possible, although the difficulties anticipated would be significant. Namely, if one knows only the number of vertices (n) and edges (m), then only two “book–keeping” equations, such as (2) and (3), can be established. These suffice for biregular graphs and (as shown in this paper) with some pertinent tricks can be used also for triregular graphs. In graphs with four, five, etc. different vertex degrees, two equations would not be enough for any reasonable analysis.

The other way of extending our considerations would be towards tricyclic, tetracyclic, etc. graphs. Here the difficulties are seen in the prohibitively large number of cases and subcases, that need to be taken into account and separately examined.

For these reasons we do not intend to continue our studies in either of these directions. However, some other colleagues may try and may succeed.

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