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MORE GRAPHS WHOSE ENERGY EXCEEDS THE NUMBER OF VERTICES

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Abstract. The energy $E(G)$ of a graph G is equal to the sum of the absolute values of the eigenvalues of G. Several classes of graphs are known that satisfy the condition $E(G) > n$, where n is the number of vertices. We now show that the same property holds for (i) biregular graphs of degree a, b, with q quadrangles, if $q \leq abn/4$ and $5 \leq a < b \leq (a-1)^2/2$; (ii) molecular graphs with m edges and k pendent vertices, if $6\,n^3 - (9m+2k)n^2 + 4\,m^3 \geq 0$; (iii) triregular graphs of degree $1, a, b$ that are quadrangle–free, whose average vertex degree exceeds a, that have not more than $12n/13$ pendent vertices, if $5 \leq a < b \leq (a-1)^2/2$.

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1. INTRODUCTION

In this paper we are concerned with a graph invariant defined in terms of graph eigenvalues. Let G be a simple graph and let its vertex set be $V(G) = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix $A(G)$ of the graph G is a square matrix of order n whose (i,j)-entry is equal to unity if the vertices v_i and v_j are adjacent, and is equal to zero otherwise. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $A(G)$ are said to be the eigenvalues of the graph G, and are studied within the Spectral Graph Theory [1]. The *energy* of the graph G is defined as

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

The graph energy is an invariant much studied in the mathematical and mathema-tico–chemical literature; for details see the book [8], the reviews [4, 5], and elsewhere [2, 6, 7, 9, 10, 11, 12, 13, 14]. For the chemical application of E see [5] and the references cited therein.

Recently some classes of graphs satisfying the inequality

$$E(G) > n \tag{1}$$

have been characterized [6, 10]. Among graphs these are

- non-singular graphs, i. e., those for which $\det A(G) \neq 0$ [3];
- regular graphs of degree greater than zero [10];
- hexagonal systems (benzenoid graphs) [6];
- acyclic molecular graphs, with exactly six exceptions [7, 9, 11].

In this paper we point out a few other classes of graphs with the same property. In order to do this we first need some preparations.

2. DEFINITIONS AND PREVIOUS RESULTS

Let, as before, $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the graph G. The p-th spectral moment of G is defined as

$$M_p = \sum_{i=1}^{n} (\lambda_i)^p \ .$$

Recall that

$$M_2 = 2m \qquad \text{and} \qquad M_4 = 2\sum_{i=1}^{n} d_i^2 - 2m + 8q \tag{2}$$

where m and q are, respectively, the number of edges and quadrangles in G.

The following lower bound for the energy is known [12]:

$$E(G) \geq \sqrt{\frac{M_2^3}{M_4}}\ . \tag{3}$$

For generalizations of (3) see [2, 13, 14]

Recall that a graph is said to be regular of degree x if all its vertices have the same degree x.

A graph G is said to be *biregular* of degrees x and y, $(x < y)$, if at least one vertex of G has degree x and at least one vertex has degree y, and if no vertex of G has degree different from x or y. The set of all n-vertex biregular graphs of degrees x and y will be denoted by $\Gamma_n(x, y)$.

For $G \in \Gamma_n(a, b)$, the following special case of the inequality (3) has been recently deduced [6]:

$$E(G) \geq 2m\sqrt{\frac{2m}{(2a+2b-1)2m - 2abn + 8q}}\ . \tag{4}$$

A graph G is said to be *triregular* of degrees x, y, and z, $(x < y < z)$, if at least one vertex of G has degree x, at least one degree y and at least one degree z, and if no vertex of G has degree different from x or y or z. The set of all n-vertex triregular graphs of degrees x, y, and z will be denoted by $\Theta_n(x, y, z)$.

Within the theory of graph energy, in view of its chemical applications [5, 8] a connected graph in which there are no vertices of degree greater than 3 is referred to as a *molecular graph*. Such graphs represent the carbon–atom skeleton of conjugated organic molecules, and play a special role in the Hückel molecular–orbital theory.

3. THE MAIN RESULTS

Theorem 3.1. *Let $G \in \Gamma_n(a, b)$ and let the number of quadrangles (q) of G be less than or equal to $abn/4$. Then the inequality (1) holds if $5 \leq a < b \leq (a-1)^2/2$.*

Proof. We start with the bound (4). If $q \leq abn/4$, then $-2abn + 8q \leq 0$. Combining this with (4) we obtain

$$E(G) \geq 2m\sqrt{\frac{1}{(2a+2b-1)}}$$

i. e.,

$$\frac{E(G)}{n} \geq d\sqrt{\frac{1}{(2a+2b-1)}} > a\sqrt{\frac{1}{(2a+2b-1)}}$$

where $d = 2m/n$ is the average vertex degree of the graph G. But

$$\frac{a}{\sqrt{(2a+2b-1)}} \geq 1$$

if and only if $(a-1)^2/2 \geq b$. Hence $E(G)/n > 1$ if $5 \leq a < b \leq (a-1)^2/2$. □

Corollary 3.2. *Let $G \in \Gamma_n(a,b)$ quadrangle–free. Then (1) holds if $5 \leq a < b \leq (a-1)^2/2$.*

Consider now triregular graphs. If $G \in \Theta_n(1,a,b)$ and if G has m edges, then

$$k + n_a + n_b = n \tag{5}$$

and

$$1 \cdot k + a\, n_a + b\, n_b = 2m \tag{6}$$

where k is the number of vertices of degree 1, whereas n_a and n_b are the number of vertices of degree a and b, respectively. From Eqs. (5) and (6) we get

$$n_a = \frac{b(n-k)-(2m-k)}{b-a} \qquad , \qquad n_b = \frac{(2m-k)-a(n-k)}{b-a} \ .$$

If d_i is the degree of the i-th vertex, then

$$\begin{aligned}
\sum_{i=1}^{n} d_i^2 &= 1^2\, k + a^2\, n_a + b^2\, n_b \\
&= k + a^2 \left[\frac{b(n-k)-(2m-k)}{b-a}\right] + b^2 \left[\frac{(2m-k)-a(n-k)}{b-a}\right] \\
&= k + (2m-k)(b+a) - (n-k)ab \ . \qquad (7)
\end{aligned}$$

Using Eq. (7), and bearing in mind (2), we obtain

$$\begin{aligned}
M_4 &= 2k + 2(2m-k)(b+a) - 2(n-k)ab - 2m + 8q \\
&= (2b+2a-1)(2m-k) - 2ab(n-k) + k + 8q \ .
\end{aligned}$$

Thus the inequality (3) can be rewritten as

$$E(G) \geq 2m \sqrt{\frac{2m}{(2b+2a-1)(2m-k)-2ab(n-k)+k+8q}} \ . \tag{8}$$

If $G \in \Theta_n(1,2,3)$ is a quadrangle–free molecular graph, then $q=0$, $a=2$, and $b=3$. From (8) we then have

$$E(G) \geq 2m \sqrt{\frac{2m}{9(2m-k)-12(n-k)+k}} \ .$$

i. e.,

$$\frac{E(G)}{n} \geq \frac{2m}{n} \sqrt{\frac{m}{9m - 6n + 2k}} \, .$$

But

$$\frac{2m}{n} \sqrt{\frac{m}{9m - 6n + 2k}} \geq 1$$

if and only if $6\,n^3 - (9m + 2k)n^2 + 4\,m^3 \geq 0$. Thus we have the following:

Theorem 3.3. *Let G be quadrangle–free molecular graph with n vertices, m edges and k pendent vertices. If $6\,n^3 - (9m+2k)n^2 + 4\,m^3 \geq 0$, then the relation (1) is satisfied.* □

Corollary 3.4. *Let G be quadrangle–free molecular graph with n vertices and m edges. If $4(n^3 + m^3) \geq 9mn^2$, then the relation (1) is satisfied.*

Proof. We have $k \leq n$ where k is the number of pendent vertices. If

$$9mn^2 \leq 4(n^3 + m^3)$$

then

$$\begin{aligned} 0 &\leq 4n^3 - 9mn^2 + 4\,m^3 = 6\,n^3 - (9m + 2n)n^2 + 4\,m^3 \\ &\leq 6\,n^3 - (9m + 2k)n^2 + 4\,m^3 \, . \end{aligned}$$

Corollary 2 follows now from the Theorem 2. □

In connection with Theorem 2 and its Corollary 2.1 one should note that the case $m = n - 1$, i. e., the case when the molecular graph G is a tree was studied in [7, 9, 11]. It was shown there that all acyclic molecular graphs, with exactly six exceptions satisfy the relation (1). All acyclic molecular graphs with $n \geq 8$ vertices satisfy the relation (1).

Theorem 3.5. *Let the graph $G \in \Theta_n(1, a, b)$ be quadrangle–free and let it has not more than $12n/13$ pendent vertices. If $5 \leq a < b \leq (a-1)^2/2$ and if the average vertex degree of G exceeds a, then the relation (1) is satisfied.*

Proof. Since G is quadrangle–free, from (8), we have

$$\begin{aligned} \frac{E(G)}{n} &\geq \frac{2m}{n} \sqrt{\frac{2m}{(2b + 2a - 1)(2m - k) - 2ab(n - k) + k}} \\ &\geq \frac{2m}{n} \sqrt{\frac{2m - k}{(2b + 2a - 1)(2m - k) - 2ab(n - k) + k}} \, . \qquad (9) \end{aligned}$$

Note that $k \leq 12n/13$ implies $k \leq 12(n-k) \leq 2ab(n-k)$, i. e., $-2ab(n-k)+k \leq 0$.

Using this in the inequality (9), we obtain

$$\frac{E(G)}{n} \geq d\sqrt{\frac{1}{(2b+2a-1)}} > \frac{a}{\sqrt{2b+2a-1}}$$

where, as before, $d = 2m/n$ and, as required in the statement of Theorem 3, $d > a$. Now,

$$\frac{a}{\sqrt{2b+2a-1}} \geq 1$$

holds if and only if $(a-1)^2/2 \geq b$. Thus $E(G) > n$. □

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