MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 499-508

ISSN 0340 - 6253

BIREGULAR GRAPHS WHOSE ENERGY EXCEEDS THE NUMBER OF VERTICES

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(Received July 19, 2008)

Abstract

A graph is said to be biregular if its vertex degrees assume exactly two 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 biregular graphs.

INTRODUCTION

In their seminal paper [1] England and Ruedenberg posed the question "*Why is the delocalization energy negative?*". Translated into the language of contemporary chemical graph theory [2–4], this question reads "*Why is the total π-electron energy* (as computed within the Hückel molecular orbital approximation and expressed in the units of the carbon–carbon resonance integral β) *greater than the number of vertices of the underlying molecular graph?*". In view of the recently very popular concept of graph energy E (see the reviews [5–7] and the references cited therein) one may reformulate the same question as "*Why is the energy of an n-vertex graph greater than n ?*".

By asking "*why*" England and Ruedenberg were aiming at some physical (quantum chemical) explanation of this phenomenon, which they indeed were able to offer [1]. From a mathematical point of view it is better to consider the problem *which* (molecular) graphs have the mentioned property. Namely, simple examples show [8] that the condition $E > n$ is not always obeyed.

The graph energy is defined as follows [5–7]: Let G be an n-vertex graph and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues [9]. Then the energy of G is

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

Recall [4] that in the vast majority of cases $E(G)$ coincides with the HMO total π-electron energy of the conjugated system whose molecular graph is G.

In this work we are concerned with finding conditions under which the inequality

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

is satisfied for certain, below specified, classes of (molecular) graphs.

The main earlier results along these lines are the following:

- Inequality (1) is satisfied by graphs whose all eigenvalues are non-zero [10].
- Inequality (1) is satisfied by all r-regular graphs, $r > 0$, [11].
- Inequality (1) is satisfied by all benzenoid graphs [12].

- For almost all graphs $E(G) = [4/(3\pi) + O(1)]\; n^{3/2}$ and therefore almost all graphs satisfy (1) [13].
- Additional results can be found in the papers [12, 14].

A closely analogous problem was also studied, namely the characterization of graphs for which $E < n$, the so-called hypoenergetic graphs [8,15–17].

PRELIMINARIES

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the graph G, then the k-th spectral moment of G is

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

For what follows we need the well known expressions:

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

where m is the number of edges, q the number of quadrangles, and d_i the degree of the i-th vertex, $i = 1, 2, \ldots, n$.

It is known [18–20] that the energy of any graph is bounded from below as

$$E(G) \geq \sqrt{\frac{(M_2)^3}{M_4}} \ . \tag{2}$$

In view of this, whenever the condition

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

is satisfied, also the inequality (1) will be satisfied.

In what follows we will examine the expression $\sqrt{(M_2)^3/M_4}$ and search for necessary and sufficient conditions under which the inequality (3) holds.

* * * * *

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

An alternative name for a biregular graph is "bidegreed graph" [21].

* * * * *

Throughout this paper all graphs are understood to be connected.

BIREGULAR TREES

Trees necessarily possess vertices of degree 1 (pendent vertices). Therefore for biregular trees it must be $a = 1$.

Let b be an integer, $1 < b \leq n-1$. Let T be a $(1,b)$-biregular tree with $n \geq 3$ vertices, and let k be the number of its pendent vertices. This tree has $m = n-1$ edges.

We begin with the equalities

$$k + n_b = n \tag{4}$$

and

$$1 \cdot k + b \cdot n_b = 2m = 2(n-1) \tag{5}$$

where n_b is the number of vertices of T of degree b. From (4) and (5) we have

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

Let d_i denote the degree of the i-th vertex in T. Then

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

For the considered biregular tree T we have

$$M_2 = 2(n-1) \tag{6}$$

and

$$\begin{aligned} M_4 &= 2\sum_{i=1}^{n}(d_i)^2 - 2(n-1) = 2n(b+2) - 4(b+1) - 2(n-1) \\ &= 2b(n-2) + 2(n-1) \ . \end{aligned} \tag{7}$$

Substituting the identities (6) and (7) back into (3) we get

$$\sqrt{\frac{4(n-1)^3}{b(n-2)+(n-1)}} \geq n \ . \tag{8}$$

From (8) we obtain

$$b \leq \frac{3n^2 - 5n + 2}{n^2} \ . \tag{9}$$

Bearing in mind that $b \geq 2$, the right–hand side of the inequality (9) must be at least 2, so $n \geq 5$. If we examine the function

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

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

The inequality (9) holds if and only if $b = 2$ and $n \geq 5$. We thus arrive at:

Theorem 1. Let T be a $(1, b)$-biregular tree with n vertices. Then (3) holds if and only if $b = 2$ and $n \geq 5$. Consequently, (1) holds if $b = 2$ and $n \geq 5$.

Of course, the tree specified in Theorem 1 is just the n-vertex path.

UNICYCLIC BIREGULAR GRAPHS

For unicyclic graphs we have $m = n$. If a unicyclic graph is biregular, then $a = 1$ and $b \geq 3$. Further, $M_2 = 2n$ whereas M_4 we obtain in the following way. We have

$$k + n_b = n \qquad \text{and} \qquad 1 \cdot k + b \cdot n_b = 2n \ .$$

Therefrom,

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

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 (3) becomes

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

and we obtain $b \leq 3 - 4q/n$.

Because the graph considered is unicyclic, the number of quadrangles q can be either 0 or 1. For $q = 0$ we obtain $b \leq 3$, and with condition $b \geq 3$ we conclude that $b = 3$. For $q = 1$ we obtain $b \leq 3 - 4/n$. Bearing in mind that $n \geq 8$ (since 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 (3) holds.

Theorem 2. Let G be a connected unicyclic (a,b)-biregular graph. Then (3) holds if and only if $a = 1$, $b = 3$, and $q = 0$. Consequently, (1) holds if $a = 1$, $b = 3$, and $q = 0$.

BICYCLIC BIREGULAR GRAPHS

For bicyclic (a,b)-biregular graphs we have $m = n+1$, and the inequality (3) becomes

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

There are three possible cases:

(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.

Case (a): Bicyclic biregular 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 $a=1$, $b\geq 3$ and with $a=2$, $b=3$.

If $a=1$, $b\geq 3$ then inequality (3) becomes

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

from which

$$b\leq \frac{3n^3+(11-4q)n^2+12n+4}{n^3+2n^2}\ . \tag{10}$$

For $q=0$ we obtain

$$b\leq \frac{3n^2+5n+2}{n^2}\ . \tag{11}$$

With $b\geq 3$, the right–hand side of the inequality (11) must be at least 3. Another condition is $n\geq 10$, since the smallest bicyclic $(1,b)$-biregular graph with disjoint cycles has exactly 10 vertices.

If we examine the function

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

we get $f'(x)<0\quad \forall x\in[10,+\infty>$. Thus f is a monotonically decreasing function. The lower bound for f is 3 because $\lim\limits_{x\to+\infty} f(x)=3$, 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

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

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

For $q=2$ we have

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

For $n\geq 14$ the right–hand side of the inequality (13) is less than 3 and thus there is no bicyclic $(1,b)$-biregular graph with $q=2$, such that the inequality (3) holds.

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

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

which implies $n^3 + (3 - 4q)n^2 + 12n + 4 \geq 0$. For $q = 0, 1, 2$ we have

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

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

Theorem 3.1. Let G be a connected bicyclic (a, b)-biregular graph with disjoint cycles. Then (3) holds if and only if $a = 1$, $b = 3$, and $q = 0, 1$, or if $a = 2$, $b = 3$, and $q = 0, 1, 2$. Consequently, (1) holds if $a = 1$, $b = 3$ and $q = 0, 1$, or if $a = 2$, $b = 3$, and $q = 0, 1, 2$.

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

If in a bicyclic (a, b)-biregular graph the cycles have a single common vertex, then we have two types of such graphs: with $a = 1$, $b \geq 4$ and with $a = 2$, $b = 4$.

For the graphs of the first type the inequalities (11), (12), and (13) hold. These, in view of the condition $b \geq 4$, are not satisfied by any value of n.

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

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

which is equivalent to $n^3 + (1 - 4q)n^2 + 12n + 4 \geq 0$. Setting $q = 0, 1, 2$ we arrive at inequalities which are fulfilled for arbitrary $n \in \mathbb{N}$.

Theorem 3.2. Let G be a connected bicyclic (a, b)-biregular graph in which the cycles share a single common vertex. Then (3) holds if and only if $a = 2$ and $b = 4$. Consequently, (1) holds if $a = 2$ and $b = 4$.

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

If in a bicyclic (a, b)-biregular graph the cycles possess two or more common vertices, then we have two types of such graphs: with $a = 1$, $b \geq 3$ and with $a = 2$, $b = 3$. For these we obtain the same result as for bicyclic graphs with disjoint cycles.

Theorem 3.3. Let G be a connected bicyclic (a,b)-biregular graph with cycles sharing two or more vertices. Then (3) holds if and only if $a = 1$, $b = 3$, and $q = 0, 1$, or if $a = 2$, $b = 3$, and $q = 0, 1, 2$. Consequently, (1) holds if $a = 1$, $b = 3$ and $q = 0, 1$, or if $a = 2$, $b = 3$, and $q = 0, 1, 2$.

Acknowledgements: One author (I.G.) thanks the Serbian Ministry of Science for partial support of this work, through Grant no. 144015G.

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