On graphs whose energy exceeds the number of vertices

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Abstract

Let \( G \) be a graph on \( n \) vertices, and let \( \lambda_1, \lambda_2, \ldots, \lambda_n \) be the eigenvalues of a \((0, 1)\)-adjacency matrix of \( G \). The energy of \( G \) is \( E = \sum_{i=1}^{n} |\lambda_i| \). We characterize several classes of graphs for which \( E \geq n \).

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1. Introduction

Let \( G \) be a simple graph of order \( n \), and let \( \lambda_1, \lambda_2, \ldots, \lambda_n \) be its eigenvalues (i.e., the eigenvalues of a \((0,1)\)-adjacency matrix \( A(G) \) of \( G \)) \cite{2}. Then the energy of \( G \) is defined as \cite{5}

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

The motivation for this definition comes from chemistry, where the first results on \( E \) were obtained as early as the 1940s \cite{1}; for details on this matter see the recent review \cite{7}. In \cite{6} a survey is given of the basic mathematical results on \( E \), obtained by the end of the 20th century. However, in the last few years research on graph energy has much intensified, resulting in a very large number (over 100) of publications; a regularly updated bibliography can be found at http://www.sgt.pep.ufrj.br.
In this work we are interested in graphs satisfying the condition

\[ E(G) \geq n. \]  (1)

In 1973 the theoretical chemists England and Ruedenberg published a paper [3] 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 [9]. What the authors of [3] failed to observe was that there exist “molecular” graphs violating the condition (1). These include acyclic graphs such as \( K_{1,2} \) and \( K_{1,3} \), with energies \( 2 \sqrt{2} = 2.8284 \ldots \) and \( 2 \sqrt{3} = 3.4641 \ldots \), respectively. A less trivial example is the 7-vertex tree from Fig. 1, whose energy is \( 4 + 2 \sqrt{2} = 6.8284 \ldots \) Among graphs with cycles, the simplest such example is \( K_{2,3} \) for which \( E = 2 \sqrt{6} = 4.898979 \ldots \) whereas \( n = 5 \).

On the other hand, there are large classes of graphs (“molecular” or not) for which condition (1) is satisfied. Here we mention three results of this kind.

**Result 1.** If the graph \( G \) is non-singular (i.e., no eigenvalue of \( G \) is equal to zero), then (1) holds.

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

\[
\frac{1}{n} E(G) \geq \left( \prod_{i=1}^{n} |\lambda_i| \right)^{1/n} = |\det A(G)|^{1/n}.
\]

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

**Result 2.** If \( G \) is a graph with \( n \) vertices and \( m \) edges, and if \( m \geq n^2/4 \), then (1) holds.

**Proof.** It is known [6] that for all graphs, \( E \geq 2 \sqrt{m} \). Result 2 follows from \( 2 \sqrt{m} \geq n \). \( \Box \)

**Result 3** ([10]). If the graph \( G \) is regular of any non-zero degree, then (1) holds.

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

Our initial aim was to demonstrate the validity of (1) for the so-called hexagonal systems, a class of graphs representing benzenoid molecules, thus of great importance in chemical applications [8]. A hexagonal system is defined [12] as a connected plane graph with no cut-vertices in which all interior regions are mutually congruent regular hexagons. For what follows the only relevant property of hexagonal systems is that their vertices are either of degree two or of degree three. In this sense, hexagonal systems are members of the set \( G(2, 3) \) as defined below.

**Definition 1.** Let \( a, b \) be positive integers, \( 1 \leq a < b \). A graph \( G \) is said to be biregular of degree \( a, b \) if its vertices have degree either \( a \) or \( b \), and if it possesses vertices of degree \( a \) and \( b \). The set of all biregular graphs of degree \( a, b \) will be denoted by \( G(a, b) \). If \( G \in G(a, b) \), then the number of vertices of \( G \) of degree \( a \) and \( b \) will be denoted by \( n_a \) and \( n_b \), respectively.
Note that if one requires additionally that vertices of equal degree are not adjacent, then a biregular graph is a semiregular bipartite graph.

If $G \in \mathcal{G}(a, b)$, and if $G$ has $n$ vertices and $m$ edges, then evidently,

$$n_a + n_b = n,$$  \hspace{1cm} (2)

$$a n_a + b n_b = 2m.$$  \hspace{1cm} (3)

In this paper we determine conditions under which biregular graphs satisfy condition (1).

2. An auxiliary upper bound for graph energy

Let $M_k$ denote the $k$th spectral moment of the graph $G$,

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

and note that for even $k$,

$$M_k := \sum_{i=1}^{n} |\lambda_i|^k.$$  

Our starting point is the inequality

$$E(G) \geq \sqrt{(M_2)^3 \over M_4},$$  \hspace{1cm} (4)

that seems to be first given by Rada and Tineo [11], and has recently been utilized also in [13].

As is well known [2],

$$M_2 = 2m.$$  \hspace{1cm} (5)

By easy combinatorial reasoning (using the fact that $M_k$ is equal to the number of closed walks of length $k$), it can be shown that

$$M_4 = 2 \sum_{i=1}^{n} (d_i)^2 - 2m + 8q,$$  \hspace{1cm} (6)

where $d_i$ is the degree of the $i$th vertex, and $q$ the number of quadrangles. Substituting identities (5) and (6) back into (4) we get

$$E(G) \geq 2m \sqrt{2m \over 2 \sum_{i=1}^{n} (d_i)^2 - 2m + 8q}.$$  \hspace{1cm} (7)

If $G \in \mathcal{G}(a, b)$, then the inequality (7) becomes

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

In order to obtain (8) note that for a graph $G \in \mathcal{G}(a, b)$,

$$\sum_{i=1}^{n} (d_i)^2 = a^2 n_a + b^2 n_b.$$  \hspace{1cm} (9)
From (2) and (3),
\[ n_a = \frac{bn - 2m}{b - a} \quad \text{and} \quad n_b = \frac{2m - an}{b - a} \]
which combined with (9) yields.
\[ \sum_{i=1}^{n} (d_i)^2 = 2(a + b)m - abn. \]

Then
\[ M_4 = 4(a + b - 2)m - 2abn + 8q \]
and (8) follows.

3. On the energy of quadrangle-free biregular graphs

In this section we consider quadrangle-free biregular graphs, that is graphs \( G \in \mathcal{G}(a, b) \) for which \( q = 0 \). Then the inequality (8) can be written in the form
\[ \frac{E(G)}{n} \geq d \sqrt{\frac{d}{(2a + 2b - 1)d - 2ab}}, \tag{10} \]
where \( d = 2m/n \) is the average vertex degree of the graph \( G \). Therefore \( a < d < b \).

From (10) it can be seen that in order to find the conditions under which (1) holds, we need to examine the function
\[ f(x) := x \sqrt{\frac{x}{(2a + 2b - 1)x - 2ab}} \]
for \( x \in (a, b) \) and find when it is greater than unity.

By direct calculation we obtain that
\[ f(a) = \frac{a}{\sqrt{2a - 1}} \quad \text{and} \quad f(b) = \frac{a}{\sqrt{2b - 1}} \]
and that \( f(a) < f(b) \).

Let \( \alpha(x) := (2a + 2b - 1)x - 2ab \). Because \( \alpha(a) = 2a^2 - a > 0 \) and \( \alpha(b) = 2b^2 - b > 0 \), it is \( \alpha(x) > 0 \) for all \( x \in (a, b) \).

The first derivative of \( f(x) \) is of the form \( x\alpha(x)^{-3/2} f_0(x) \) where
\[ f_0(x) := (2a + 2b - 1)x - 3ab. \]
Because \( x\alpha(x)^{-3/2} \) is always positive, the function \( f(x) \) will increase monotonically in the interval \((a, b)\) if \( f_0(x) > 0 \) for \( x \in (a, b) \).

Because \( f_0(b) = b(2b - a - 1) \) is evidently positive-valued, we only need to find conditions for \( f_0(a) \geq 0 \). Since \( f_0(a) = a(2a - b - 1) \), we see that the latter condition will be obeyed if \( 2a \geq b + 1 \).

This implies that the function \( f(x) \) increases monotonically in the interval \((a, b)\) if, and only if, \( 2a \geq b + 1 \). Then, from (10) it follows that \( E(G)/n > f(a) \), i.e.,
\[ E(G) > \frac{a}{\sqrt{2a - 1}}n \tag{11} \]
and this inequality holds for \( a < b \leq 2a - 1 \), that is for \( a = 2, b = 3; a = 3, b = 4; a = 3, b = 5; a = 4, b = 5; a = 4, b = 6; a = 4, b = 7, \) etc. Inequality (11) is strict, because the parameter \( d \) in (10) is strictly greater than \( a \).
We thus proved the following:

**Theorem 1.** Let $G$ be an $n$-vertex quadrangle-free biregular graph of degree $a, b$. Then for $2 \leq a < b \leq 2a - 1$, the inequality (11) holds.

In view of the fact that $a/\sqrt{2a - 1} > 1$ whenever $a > 1$, we have

**Corollary 1.1.** Quadrangle-free biregular graphs of degree $a, b$, such that $2 \leq a < b \leq 2a - 1$, satisfy condition (1).

**Corollary 1.2.** All hexagonal systems satisfy condition (1). Moreover, for these graphs, $E > \sqrt{4/3}n$.

Recall that $\sqrt{4/3} = 1.25470 \ldots$

### 4. On the energy of biregular graphs with disjoint quadrangles

In this section we consider biregular graphs that may possess quadrangles, but we require that all such quadrangles be disjoint (i.e., no two of them have a common vertex). If all quadrangles of an $n$-vertex graph are disjoint, then $q \leq n/4$. Therefore, by substituting $n/4$ instead of $q$, the inequality (8) yields

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

(12)

which should be compared with (10). In a same manner as in the preceding section, the relation (1) will hold if the function

$$g(x) := x \sqrt{\frac{x}{(2a + 2b - 1)x - 2(ab - 1)}}$$

is greater than unity for $x \in (a, b)$.

An analysis that is essentially same as in the preceding section for $f(x)$, leads to the conclusion that the function $g(x)$ increases monotonically in the interval $(a, b)$ if, and only if, $2a^2 - a + 3 \geq ab$, i.e., $b \leq 2a - 1 + 3/a$. Then, from (12) it follows that $E(G)/n > g(a)$, i.e.,

$$E(G) > \frac{a\sqrt{a}}{\sqrt{2a^2 - a + 2}}n$$

(13)

and this inequality holds for $a < b \leq 2a - 1 + 3/a$, that is for $a = 1, b = 2, 3, 4; a = 2, b = 3, 4; a = 3, b = 4, 5, 6; a = 4, b = 5, 6, 7$, etc. Inequality (13) is strict, because the parameter $d$ in (12) is strictly greater than $a$. We thus arrive at

**Theorem 2.** Let $G$ be an $n$-vertex biregular graph of degree $a, b$ in which all quadrangles (if any) are mutually disjoint. Then for $1 \leq a < b \leq 2a - 1 + 3/a$, the inequality (13) holds.

For $a = 1$ the term $g(a) = 1/\sqrt{3}$ is less than unity. For $a = 2$ the term $g(a)$ is equal to unity whereas for $a > 2$ this term is greater than unity. Bearing this in mind we have:
Corollary 2.1. Biregular graphs of degree 2, 3 and 2, 4, in which all quadrangles (if any) are mutually disjoint, satisfy condition (1).

Corollary 2.2. Biregular graphs of degree $a, b$ in which all quadrangles (if any) are mutually disjoint, such that $3 \leq a < b \leq 2a - 1 + 3/a$, satisfy conditions stronger than (1), namely $E > \sqrt{27/17}$ for $a = 3$, $E > \sqrt{32/15}$ for $a = 4$, etc.

Recall that $\sqrt{27/17} = 1.26025\ldots$ and $\sqrt{32/15} = 1.46059\ldots$

Remark 1. For $a = 1, b \geq 2$, there exist graphs $G \in \mathcal{G}(a, b)$, such that $E < n$. The simplest example is the $n$-vertex star, for which $E = 2\sqrt{n-1}$. The graph $K_{2,3}$ mentioned earlier is an example of a biregular graph with non-disjoint quadrangles, for which $E < n$.

5. Beyond biregular graphs

It is a well known empirical fact (cf. [3]) that many graphs, including some molecular graphs that are not biregular, have the property (1). This especially applies to graphs with many edges (cf. Result 2). Therefore, as far as the validity of Eq. (1) is concerned, the study of connected graphs with a small number of edges may be most interesting.

From the point of view of chemical applications it would be interesting to find the $n$-vertex molecular graph(s) with minimum energy and to see if Eq. (1) holds for them. This, however, appears to be a rather difficult task.

One referee of this paper expressed the opinion that all quadrangle–free molecular graphs obey Eq. (1). This, however, is not true, as seen from the examples shown in Fig. 1 (see below).

It is plausible to expect that a minimum–energy $n$-vertex molecular graph is a tree, although a proof of such a seemingly obvious fact is not known. For $n \leq 22$ the minimum-energy trees with maximum vertex degree $\Delta \leq 3$ have been found by a systematic computer search, and are displayed in Fig. 1. For the case $\Delta = 4$ the analogous trees are established in an earlier work [4]. In [4] by means of a systematic computer search the trees with $\Delta = 4$ and minimal energy were identified for $n \leq 22$. The conclusion in [4] was that for $n > 22$, these results are insufficient for formulating a conjecture about the structure of the $n$-vertex trees with $\Delta = 4$ and minimal energy.

Even by a careful examination of the trees shown in Fig. 1 no regularity in their structure could be envisaged. In particular, knowing the trees from Fig. 1 it does not seem possible to forecast which tree will arise with $n = 23, n = 24$, etc. The same conclusion was reached in the case $\Delta \leq 4$ and we are confident that the more general problem, namely the characterization of trees with $\Delta \leq k$, whose energy is minimal, is a prohibitively difficult task.

Without knowing the structure of the minimum-energy chemical trees (or, more generally, of the trees with $\Delta \leq k$), it is not easy to arrive at any generally valid result concerning their $E$-value. Therefore, a question raised by one of the referees, namely “What is the minimum energy of trees of order $n$ with maximum degree $\Delta \leq k$?” is at the moment without answer, with little hope that it will be answered in a foreseen future. Even more difficult would be to find an answer to the referee’s second question: “What is the minimum energy of connected quadrangle-free graphs of order $n$ with maximum degree $\Delta \leq k$?”

Numerical calculations show that for the trees from Fig. 1, Eq. (1) is violated for $n = 3, 4, 7$, and is obeyed for $n = 5, 6$ and $8 \leq n \leq 22$. Based on these results it is straightforward to conjecture that all acyclic molecular graphs (i.e., trees with $\Delta \leq 3$) with $n \geq 8$ vertices obey condition (1).
Then we may further conjecture that all molecular graphs with $n \geq 8$ vertices obey condition (1). If so, then the number of molecular graphs (with $\Delta \leq 3$) that violate condition (1) is finite.

It may well be that the difficulties encountered in connection with Eq. (1) could be settled more easily by revising our point of view and by seeking the solution of the following

**Problem 1.** Characterize the connected graphs for which Eq. (1) is not obeyed.

Somewhat easier special cases of the above task would be

**Problem 2.** Characterize the connected graphs with $\Delta \leq k$ for which Eq. (1) is not obeyed, for $k = 3, 4, 5, \ldots$ Or, at least, do this for $k = 3$.

**Problem 3.** Characterize the trees with $\Delta \leq k$ for which Eq. (1) is not obeyed, for $k = 3, 4, 5, \ldots$ Or, at least, do this for $k = 3$.

In fact, it seems that there exist exactly four $n$-vertex trees with $\Delta \leq 3$ with energy less than $n : K_1, K_{1,2}, K_{1,3}$, and the 7-vertex tree in Fig. 1. However, in order to prove this we would need to demonstrate that there is no tree with $\Delta \leq 3$ and $n \geq 8$ (or, if we trust in computers, with $n > 22$) that violates condition (1). This brings us back to the earlier difficulties.

Thus, Problems 1, 2, and 3 remain a challenge for colleagues.
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