The energy of $C_4$-free graphs of bounded degree

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Abstract
Answering some questions of Gutman, we show that, except for four specific trees, every connected graph $G$ of order $n$, with no cycle of order 4 and with maximum degree at most 3, satisfies

$$|\mu_1| + \cdots + |\mu_n| \geq n,$$

where $\mu_1, \ldots, \mu_n$ are the eigenvalues of $G$.

We give some general results and state two conjectures.

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Our notation follows [1] and [2]; in particular, we write $V(G)$ for the vertex set of a graph $G$ and $|G|$ for $|V(G)|$. Also, $e(G)$ stands for the number of edges of $G$, and $\Delta(G)$ for its maximum degree.

Let $G$ be a graph on $n$ vertices and $\mu_1 \geq \cdots \geq \mu_n$ be the eigenvalues of its adjacency matrix. The value $E(G) = |\mu_1| + \cdots + |\mu_n|$, called the energy of $G$, has been studied intensively - see [3] for a survey.

Motivated by questions in theoretical chemistry, Gutman [4] initiated the study of connected graphs satisfying $E(G) \geq |G|$, raising some problems, whose simplest versions read as:

**Problem 1** Characterize all trees $T$ with $\Delta(T) \leq 3$ satisfying $E(T) < |T|$. 

**Problem 2** Characterize all connected graphs $G$ with $\Delta(G) \leq 3$ satisfying $E(G) < |G|$. 

Here we show that if $G$ is a connected $C_4$-free graph such that $\Delta(G) \leq 3$ and $E(G) < |G|$, then $G$ is one of four exceptional trees. This completely solves the first problem and partially the second one.

Let $d \geq 3$ and $\alpha(d)$ be the largest root of the equation

$$4x^3 - (2d + 1)x + d = 0.$$
Theorem 3 Let $G$ be a $C_4$-free graph with no isolated vertices. If $e(G) \geq \alpha(d)|G|$ and $\Delta(G) \leq d$, then $\mathcal{E}(G) > |G|$.

We note first that Theorem 3 implies Theorem 1 of [4], but the check of this implication is somewhat involved.

To prove Theorem 3 we need three propositions. The first one is known and its proof is omitted.

Proposition 4 Let $G$ be a graph of order $n$, $C$ be the number of its 4-cycles, and $\mu_1, \ldots, \mu_n$ be its eigenvalues. Then
\[
\mu_1^2 + \cdots + \mu_n^2 = 2e(G), \\
\mu_1^4 + \cdots + \mu_n^4 = 2\sum_{u \in V(G)} d_u^2 - 2e(G) + 8C.
\]

Next we give a simple bound on the sum of squares of degrees in graphs.

Proposition 5 Let $G$ be a graph with $n$ vertices and $m$ edges, with no isolated vertices, and let $d_1, \ldots, d_n$ be its degrees. If $\Delta(G) \leq d$, then
\[
d_1^2 + \cdots + d_n^2 \leq (2m + 1)s - dn.
\]

Proof Summing the inequality $(d_i - 1)(d_i - d) \leq 0$ for $i = 1, \ldots, n$, we find that
\[
d_1^2 + \cdots + d_n^2 - d_1 - \cdots - d_n - d(d_1 + \cdots + d_n) + dn \leq 0,
\]
completing the proof. \quad \Box

The following proposition gives more explicit relations between $d$ and $\alpha(d)$.

Proposition 6 If $d = 3$, then $\alpha(d) = 1$. If $d \geq 4$, then
\[
\sqrt{(2d+1)/4} - 1/3 < \alpha(d) < \sqrt{(2d+1)/4}.
\]

Proof If $d = 3$, we have
\[
4x^3 - 7x + 3 = 4(x-1)(x+1) - 3(x-1) = (x-1)(2x-1)(2x+3)
\]
and the first assertion follows.

If $x \geq \sqrt{(2d+1)/4}$, we have
\[
4x^3 - (2d+1)x + d \geq ((2d+1) - (2d+1))x + d > 0,
\]
so the upper bound in (1) follows. On the other hand,
\[
4\left(\sqrt{\frac{2d+1}{4}} - \frac{1}{3}\right)^3 - (2d+1)\left(\sqrt{\frac{2d+1}{4}} - \frac{1}{3}\right) + d < -\frac{19d+11}{3} + \frac{1}{3}\sqrt{8d+4} < 0,
\]
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implying the lower bound in (1) and completing the proof.

\[\frac{(|\mu_1| + \cdots + |\mu_n|)^{2/3}}{\mu_1^4 + \cdots + \mu_n^4} \geq \mu_1^2 + \cdots + \mu_n^2.\]  

(2)

Proof of Theorem 3 As noted by Rada and Tineo [5],

We first show that, in our case, inequality (2) is strict. Indeed, it is a particular case of Hölder’s inequality; hence, if equality holds, the vectors \((|\mu_1|, \ldots, |\mu_n|)\) and \((\mu_4^1, \ldots, \mu_4^n)\) are linearly dependent. That is to say, all nonzero eigenvalues of \(G\) have the same absolute value, and so, \(G\) is a union of complete bipartite graphs. Since \(G\) is \(C_4\)-free, \(G\) must be a forest, contradicting the premise \(e(G) \geq \alpha(d)n \geq n\), and proving the claim.

From (2), by Propositions 4 and 5, we obtain

\[E^2(G) > \frac{\mu_1^2 + \cdots + \mu_n^2}{\mu_1^4 + \cdots + \mu_n^4} = \frac{8m^3}{2 \sum_{u \in V(G)} d^2(u) - 2m} = \frac{4m^3}{(2d + 1)m - dn} = \frac{n^2}{2} \frac{4m^3}{(2d + 1)(m/n) - d} \]

Using calculus, we find that the expression

\[\frac{4x^3}{(2d + 1)x - d}\]

increases with \(x\). Hence, the premise \(m/n \geq \alpha(d)\) implies that

\[E^2(G) > n^2 \frac{4\alpha^3}{(2d + 1)\alpha - d} = n^2,\]

completing the proof.

As a corollary we obtain the following

**Theorem 7** Let \(G\) be a graph of order \(n\) with at least \(n\) edges and with no isolated vertices. If \(G\) is \(C_4\)-free and \(\Delta(G) \leq 3\), then \(E(G) > n\).

It is reasonable to conjecture that \(E(G) \geq |G|\) holds for all connected \(C_4\)-free graphs with \(\Delta(G) \leq 3\). In view of Theorem 3, this assertion can fail only if \(G\) is a tree, and indeed, as pointed out by Gutman, there are four trees for which the assertion fails.

**Fact 8 (Gutman [4])** The trees \(K_1, K_{1,2}, K_{1,3}\), and the balanced binary tree on 7 vertices are the only trees of order up to 22 with \(\Delta(T) \leq 3\) and \(E(T) < |T|\).

However, it turns out that these trees are the only exceptions, and the following theorem holds.

**Theorem 9** Let \(T\) be a tree different from the four trees listed in Fact 8. If \(\Delta(T) \leq 3\), then \(E(T) \geq |T|\).
Proof In view of Fact 8, we shall assume that \( n \geq 23 \). Let \( \mu_1, \ldots, \mu_n \) be the eigenvalues of \( T \). Set \( \mu = \mu_1 \) and note that, since \( T \) is bipartite, we also have \( |\mu_n| = \mu \). Hölder’s inequality implies that

\[
(|\mu_2| + \cdots + |\mu_{n-1}|)^{2/3} (\mu_2^4 + \cdots + \mu_{n-1}^4)^{1/3} \geq \mu_2^2 + \cdots + \mu_{n-1}^2.
\]

Hence Propositions 4 and 5 give

\[
(\mathcal{E} (G) - 2\mu)^2 \geq \frac{\mu_2^2 + \cdots + \mu_{n-1}^2}{\mu_2^4 + \cdots + \mu_{n-1}^4} = \frac{(2m - 2\mu^2)^3}{\sum_{u \in V(G)} d^2(u) - 2m - 2\mu^4} \geq \frac{4(n - 1 - \mu^2)^3}{4n - 7 - \mu^4}.
\]  

(3)

First we show that if \( \mu \geq \sqrt{7} \), then

\[
\frac{4(n - (\mu^2 + 1))^3}{4n - 7 - \mu^4} > (n - 2\mu)^2.
\]  

(4)

We shall make use of the fact \( \mu < \Delta (T) \leq 3 \). After some algebra we see that (4) is equivalent to

\[
(\mu^4 - 12\mu^2 + 16\mu - 5)n^2 + 4(-\mu^5 + 3\mu^4 + 2\mu^2 - 7\mu + 3)n + 4(-3\mu^4 + 4\mu^2 - 1) > 0.
\]

We have, in view of \( \sqrt{7} \leq \mu \leq 3 \),

\[
(\mu^4 - 12\mu^2 + 16\mu - 5)n^2 + 4(-\mu^5 + 3\mu^4 + 2\mu^2 - 7\mu + 3)n + 4(-3\mu^4 + 4\mu^2 - 1) > \left(7(7 - 12) + 16\sqrt{7} - 5\right)n^2 + 4(2\mu^2 - 7\mu + 3)n + 4(-243 + 27)
\]

\[
> 2n^2 + 4\left(14 - 7\sqrt{7} + 3\right)n - 4 \cdot 216 \geq 2n^2 - 8n - 4 \cdot 216
\]

\[
\geq 46 \cdot 19 - 4 \cdot 216 = 10 > 0.
\]

Combining (3) and (4), we complete the proof if \( \mu \geq \sqrt{7} \).

Assume now that \( \mu < \sqrt{7} \). Hofmeister’s inequality implies that

\[
\sum_{u \in V(G)} d^2(u) \leq n\mu^2 < 7n,
\]

and, as in the proof of Theorem 3, we obtain

\[
\mathcal{E}^2 (G) \geq \frac{8(n - 1)^3}{2 \sum_{u \in V(G)} d^2(u) - 2(n - 1)} \geq \frac{8(n - 1)^3}{14n - 2(n - 1)} = \frac{8(n - 1)^3}{12n + 2} > n^2,
\]

completing the proof. \( \square \)
Concluding remarks

Some of the above results can be strengthened. Here we formulate two plausible conjectures.

Let the tree $B_n$ be constructed by taking three disjoint copies of the balanced binary tree of order $2^{n+1} - 1$ and joining an additional vertex to their roots.

**Conjecture 10** The limit

$$c = \lim_{n \to \infty} \frac{\mathcal{E}(B_n)}{3 \cdot 2^{n+1} - 2}$$

exists and $c > 1$.

**Conjecture 11** Let $\varepsilon > 0$. If $T$ is a sufficiently large tree with $\Delta(T) \leq 3$, then $\mathcal{E}(T) \geq (c - \varepsilon) |T|$.

The empirical data given in [4] seem to corroborate these conjectures, but apparently new techniques are necessary to prove or disprove them.

References

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