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The energy of C_4-free graphs of bounded degree

V. Nikiforov*

Department of Mathematical Sciences, University of Memphis, Memphis, TN 38152, USA

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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

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

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

We give some general results and state two conjectures.

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1. Introduction

Our notation follows [1,2]; 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 $\mu_1 \geqslant \cdots \geqslant \mu_n$ be the eigenvalues of its adjacency matrix. The value $\mathscr{E}(G) = |\mu_1| + \cdots + |\mu_n|$, 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 $\mathscr{E}(G) \geqslant |G|$; in particular, he raised several problems, whose simplest versions read as:

* Tel.: +1 901 678 3133; fax: +1 901 678 2416.
E-mail address: vnikifrv@memphis.edu

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Problem 1. Characterize all trees T with $\Delta(T) \leqslant 3$ satisfying $\mathscr{E}(T) < |T|$.

Problem 2. Characterize all connected graphs G with $\Delta(G) \leqslant 3$ satisfying $\mathscr{E}(G) < |G|$.

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

Let $d \geqslant 3$ and let $\alpha(d)$ 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 $e(G) \geqslant \alpha(d)|G|$ and $\Delta(G) \leqslant d$, then $\mathscr{E}(G) > |G|$.*

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 $\Delta(G) \leqslant d$, then*

$$d_1^2 + \cdots + d_n^2 \leqslant (2m+1)s - dn.$$

Proof. Summing the inequality $(d_i - 1)(d_i - d) \leqslant 0$ for $i = 1, \ldots, n$, we find that

$$d_1^2 + \cdots + d_n^2 - d_1 - \cdots - d_n - d(d_1 + \cdots + d_n) + dn \leqslant 0,$$

completing the proof. □

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

Proposition 6. *If $d = 3$, then $\alpha(d) = 1$. If $d \geqslant 4$, then*

$$\sqrt{(2d+1)/4} - 1/3 < \alpha(d) < \sqrt{(2d+1)/4}. \tag{1}$$

Proof. If $d = 3$, we have

$$4x^3 - 7x + 3 = 4x(x-1)(x+1) - 3(x-1) = (x-1)(2x-1)(2x+3)$$

and the first assertion follows.

If $x \geqslant \sqrt{(2d+1)/4}$, we have

$$4x^3 - (2d+1)x + d \geqslant ((2d+1) - (2d+1))x + d > 0,$$