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LOWER BOUNDS FOR ENERGY OF QUADRANGLE–FREE GRAPHS

Bo Zhou

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China
e-mail: zhoubo@scnu.edu.cn

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Abstract

The energy $E(G)$ of a graph G is the sum of the absolute values of the eigenvalues of G. For graphs with n vertices and m edges, it is known that $E(G) \leq \sqrt{2mn}$. We prove that for quadrangle-free graphs with n vertices, m edges, minimum vertex degree $\delta \geq 1$ and maximum vertex degree Δ,

$$E(G) > \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}\sqrt{2mn}\,.$$

INTRODUCTION

Let G be a graph without loops and multiple edges. Denote by n and m the number of vertices and edges of G, and by $\lambda_1, \lambda_2, \ldots, \lambda_n$ its eigenvalues. The energy of a graph G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. Obviously, isolated vertices have no influence on the energy of a graph.

In chemistry, the energy of a graph is extensively studied since it can be used to approximate the total π-energy of a molecule (see, e.g., [1–5]).

It is a well-known result [1, 2] that $E(G) \leq \sqrt{2mn}$ holds for all graphs. Gutman [6] has proved that for certain graphs a constant g can be found, such that $g\sqrt{2mn}$ is a lower bound for $E(G)$. Concretely, he proved the following.

Theorem 1. [6] *Let G be a quadrangle-free graph with n vertices, m edges, maximum vertex degree* 2 *and no isolated vertices. Then*

$$E(G) > \frac{4}{5}\sqrt{2mn}\,.$$

Theorem 2. [6] *Let G be a quadrangle-free graph with n vertices, m edges, maximum vertex degree* 3 *and no isolated vertices. Then*

$$E(G) > \frac{2\sqrt{6}}{7}\sqrt{2mn}\,.$$

Gutman [6] pointed out that it would be interesting to extend Theorems 1 and 2 to graphs with maximum vertex degree $\Delta > 3$.

The first Zagreb index M_1 of G is defined as

$$M_1 = M_1(G) = \sum_{\text{vertices}} (d_u)^2$$

where d_u is the degree of vertex u. For details on M_1, see [7, 8].

RESULTS

In this article, we prove that a constant g can be found such that $g\sqrt{2mn}$ is a lower bound for $E(G)$ of a quadrangle-free graph G with minimum vertex degree $\delta \geq 1$ and maximum vertex degree Δ.

Theorem 3. *Let G be a quadrangle-free graph with n vertices, m edges, minimum vertex degree $\delta \geq 1$ and maximum vertex degree Δ. Then*

$$E(G) > \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}\sqrt{2mn}\,.$$

Proof. If $\Delta = 1$, then $G = mK_2$ and the result follows easily.

Suppose that $\Delta > 1$. Let $s_4 = \sum_{i=1}^{n} |\lambda_i|^4$. Then $s_4 = 2M_1 - 2m + 8Q$, where M_1 is the first Zagreb index of G, and Q is the number of quadrangles in G. By [6, 9],

$$E(G) \geq \sqrt{\frac{(2m)^3}{s_4}}$$

with equality if and only if G is the disjoint union of complete bipartite graphs $K_{a_1,b_1}, \ldots, K_{a_k,b_k}$ such that $a_1b_1 = \cdots = a_kb_k$ for some $k \geq 1$.

Recall that

$$M_1 \leq 2m(\delta+\Delta) - n\delta\Delta$$

with equality if and only if all the vertex degrees of G are either δ or Δ, which follows from [10] if $\delta < \Delta$, and is obvious otherwise.

Note that G is a quadrangle-free graph. Therefore

$$E(G) \geq \sqrt{\frac{(2m)^3}{2\,[2m(\delta+\Delta) - n\delta\Delta] - 2m}}$$

with equality if and only if G is the disjoint union of k copies of complete bipartite graph $K_{1,\Delta}$ for some $k \geq 1$.

To find a constant g, such that $E(G) \geq g\sqrt{2mn}$, its sufficient that g satisfies the condition

$$\sqrt{\frac{(2m)^3}{2\,[2m(\delta+\Delta) - n\delta\Delta] - 2m}} \geq g\sqrt{2mn}\,,$$

i.e., we may choose g as

$$g = \min_{G \in \mathcal{G}} \gamma(G)$$

where

$$\gamma(G) = \sqrt{\frac{2m^2}{n\,[2m(\delta+\Delta) - n\delta\Delta] - mn}}\,,$$

and where $\mathcal{G}$ is the set of all quadrangle-free graphs with n vertices, m edges, minimum vertex degree δ and maximum vertex degree Δ.

It is easy to see that when $[2(\delta+\Delta)-1]\,m = 2\delta\Delta n$, $\gamma(G)$ attains its minimal value $\frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}$. But $[2(\delta+\Delta)-1]\,m = 2\delta\Delta n$ becomes $[2(1+\Delta)-1]k\Delta = 2\Delta k(\Delta+1)$, which is obviously impossible if G is the disjoint union of k copies of complete bipartite graph $K_{1,\Delta}$ for $k \geq 1$. Therefore $E(G) > g\sqrt{2mn}$ with $g = \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}$. This proves the theorem. $\square$

Given $\Delta > 1$, it is easy to see that

$$f(\delta) = \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}$$

is an increasing function of δ when $\delta < \Delta$. Hence $f(\delta) \geq \min\{f(1), f(\Delta)\} = f(1) = \frac{2\sqrt{2\Delta}}{2\Delta+1}$. By Theorem 3, we have the following.

Corollary 4. *Let G be a quadrangle-free graph with n vertices, m edges and maximum vertex degree Δ and no isolated vertices. Then*

$$E(G) > \frac{2\sqrt{2\Delta}}{2\Delta+1}\sqrt{2mn}\,.$$

Setting $\Delta = 2, 3$ in Corollary 4, we obtain the results in Theorems 1 and 2, respectively. Recall that a graph is a chemical graph if it is connected and its maximum vertex degree is at most 4. It is easy to see that $\frac{2\sqrt{2\Delta}}{2\Delta+1}$ is a decreasing function of Δ when $\Delta \geq 1$. Setting $\Delta = 4$ in Corollary 4, we have the following.

Corollary 5. *Let G be a chemical quadrangle-free graph with n (> 1) vertices and m edges. Then*

$$E(G) > \frac{4\sqrt{2}}{9}\sqrt{2mn}\,.$$

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