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Some new upper bounds for the energy of graphs

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Abstract: Let $G = (V,E)$ be a graph of order n and size m. The energy of a graph is defined as $E(G) = \sum_{I=1}^{n} |\lambda_i|$, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are eigenvalues of the adjacency matrix of G. Some new upper bounds on $E(G)$ are obtained.

Keywords: Energy of a graph, topological indices.

1 Introduction

Let $G = (V,E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple connected graph with $n = |V|$ vertices, $m = |E|$ edges, with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$, $d_i = d(v_i)$. Denote by $D = diag(d_1, d_2, \dots, d_n)$ the diagonal matrix of vertex degrees. The greatest, the second greatest, the smallest and second smallest vertex degrees with be, respectively, denoted by $\Delta = d_1$, $\Delta_2 = d_2$, $\delta = d_n$, and $\delta_2 = d_{n-1}$. If vertices v_i and v_j are adjacent in G, we will denote it as $i \sim j$.

The adjacency matrix $A = (a_{ij})$ of G is the $(0,1)$ of order $n \times n$ defined as

$$a_{ij} = \begin{cases} 1, & \text{if } i \sim j \\ 0, & \text{otherwise}. \end{cases}$$

The eigenvalues of matrix A, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, are the (ordinary) eigenvalues of G. The graph energy is spectrum–based graph invariant introduced in [7] as

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

More on this invariant one can find in monographs [11, 15] and papers [9, 10].

The sum of the α-th powers of the degrees of a graph G

$${}^{0}R_{\alpha}(G) = \sum_{i=1}^{n} d_i^{\alpha},$$

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is known as general zeroth–order Randić index [20]. It is also met under names general first Zagreb index [12] and variable first Zagreb index [16] (see also [18]). Here we are interested in the following special cases of ${}^0R_\alpha(G)$:

- Zeroth–order connectivity index or zeroth–order Randić index, ${}^0R(G) = {}^0R_{-1/2}(G)$ [13].
- Inverse degree or modified total adjacency index, $ID(G) = {}^0R_{-1}(G)$ [4,21].
- First Zagreb index, $M_1(G) = {}^0R_2(G)$, [5]. For more details on its properties see, for example, [2,6,8,21].

2 Preliminaries

In this section we recall some results from the literature that are of interest for the present paper.

Lemma 2.1. [3] *Let G be a graph with $n \geq 2$ vertices. Then*

$$E(G) \leq \sum_{i=1}^{n} \sqrt{d_i}\,. \tag{2.1}$$

Equality holds if and only if $G \cong \overline{K_n}$, or $G \cong t\,K_2 \cup (n-2t)K_1$, $1 \leq t \leq \frac{n}{2}$.

The following inequalities for the sequence of real number sequences will be used in the proofs of theorem in the present paper.

Lemma 2.2. [17] *Let $a = (a_i)$, $i = 1,2,\ldots,n$, $a_1 \geq a_2 \geq \cdots \geq a_n$, be a sequence of positive real numbers. Then*

$$\sum_{i=1}^{n} a_i \sum_{i=1}^{n} \frac{1}{a_i} \leq n^2 \left(1 + \alpha(n)\left(\sqrt{\frac{a_1}{a_n}} - \sqrt{\frac{a_n}{a_1}}\right)^2\right), \tag{2.2}$$

where

$$\alpha(n) = \frac{1}{4}\left(1 - \frac{(-1)^{n+1}+1}{2n^2}\right).$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_n$.

Lemma 2.3. [14] *Let $a = (a_i)$, $i = 1,2,\ldots,n$, be a sequence of positive real numbers. Then*

$$\left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \leq (n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{1/n}. \tag{2.3}$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_n$.

Lemma 2.4. [1] *Let $a=(a_i)$ and $b=(b_i)$, $i=1,2,\dots,n$, be two sequences of non–negative real numbers such that*

$$0 \le r_1 \le a_i \le R_1 \quad \textit{and} \quad 0 \le r_2 \le b_i \le R_2 \,.$$

Then

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le n^2 \alpha(n)(R_1-r_1)(R_2-r_2)\,. \tag{2.4}$$

Equality holds if and only if $r_1=a_1=\cdots=a_n=R_1$ or $r_2=b_1=\cdots=b_n=R_2$.

Lemma 2.5. [20] *Let $a=(a_i)$ and $b=(b_i)$, $i=1,2,\dots,n$, be two sequences of non–negative real numbers of similar monotonicity, and $p=(p_i)$, $i=1,2,\dots,n$, sequence of positive real numbers. Then*

$$\sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i \ge \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \tag{2.5}$$

When $a=(a_i)$ and $b=(b_i)$ are of opposite monotonicity, the reverse inequality is valid in (2.5). *Equality holds if and only if $a_1=\cdots=a_n$, or $b_1=\cdots=b_n$.*

3 Main results

In the next theorem we establish an upper bound for (G) in terms of n, Δ, δ and $\det D$.

Theorem 3.1. *Let G be a graph of order $n \ge 3$ without isolated vertices. Then*

$$E(G) \le \sqrt{\Delta} + \sqrt{\delta} + (n-2)\left(\frac{\det D}{\Delta\delta}\right)^{\frac{1}{2(n-2)}} \left(1+\alpha(n-2)\left(\sqrt[4]{\frac{\Delta}{\delta}} - \sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right)\,. \tag{3.1}$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Proof. The inequality (2.2) can be considered in the following form

$$\sum_{i=2}^{n-1} a_i \sum_{i=2}^{n-1} \frac{1}{a_i} \le \left(1+\alpha(n-2)\left(\sqrt{\frac{a_2}{a_{n-1}}} - \sqrt{\frac{a_{n-1}}{a_2}}\right)^2\right)(n-2)^2\,,$$

For $a_i=\sqrt{d_i}$, $a_2=\sqrt{\Delta_2}$, $a_{n-1}=\sqrt{\delta_2}$, $i=2,\dots,n-1$, the above inequality becomes

$$\sum_{i=2}^{n-1} \sqrt{d_i} \sum_{i=2}^{n-1} \frac{1}{\sqrt{d_i}} \le \left(1+\alpha(n-2)\left(\sqrt[4]{\frac{\Delta_2}{\delta_2}} - \sqrt[4]{\frac{\delta_2}{\Delta_2}}\right)^2\right)(n-2)^2\,, \tag{3.2}$$

On the other hand, based on the arithmetic–geometric mean inequality (AM–GM) [20], we have that

$$\sum_{i=2}^{n-1} \frac{1}{\sqrt{d_i}} \geq (n-2)\left(\prod_{i=2}^{n-1} \frac{1}{\sqrt{d_i}}\right)^{\frac{1}{n-2}} = (n-2)\left(\prod_{i=2}^{n-1} \frac{1}{d_i}\right)^{\frac{1}{2(n-2)}} = (n-2)\left(\frac{\det D}{\Delta\delta}\right)^{-\frac{1}{2(n-2)}}. \tag{3.3}$$

From the above and inequality (3.2) we obtain

$$(n-2)\left(\frac{\det D}{\Delta\delta}\right)^{-\frac{1}{2(n-2)}} \sum_{i=2}^{n-1} \sqrt{d_i} \leq (n-2)^2 \left(1+\alpha(n-2)\left(\sqrt[4]{\frac{\Delta_2}{\delta_2}} - \sqrt[4]{\frac{\delta_2}{\Delta_2}}\right)^2\right),$$

that is

$$\sum_{i=2}^{n-1} \sqrt{d_i} \leq (n-2)\left(\frac{\det D}{\Delta\delta}\right)^{\frac{1}{2(n-2)}} \left(1+\alpha(n-2)\left(\sqrt{\frac{\Delta_2}{\delta_2}} + \sqrt{\frac{\delta_2}{\Delta_2}} - 2\right)\right). \tag{3.4}$$

The function $f(x) = \sqrt{x} + \frac{1}{\sqrt{x}}$ is monotone increasing for every real $x \geq 1$. Since $1 \leq \frac{\Delta_2}{\delta_2} \leq \frac{\Delta}{\delta}$, from (3.4) we have that

$$\sum_{i=2}^{n-1} \sqrt{d_i} \leq (n-2)\left(\frac{\det D}{\Delta\delta}\right)^{\frac{1}{2(n-2)}} \left(1+\alpha(n-2)\left(\sqrt[4]{\frac{\Delta}{\delta}} - \sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right).$$

that is

$$\sum_{i=1}^{n} \sqrt{d_i} \leq \sqrt{\Delta} + \sqrt{\delta} + (n-2)\left(\frac{\det D}{\Delta\delta}\right)^{\frac{1}{2(n-2)}} \left(1+\alpha(n-2)\left(\sqrt[4]{\frac{\Delta}{\delta}} - \sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right).$$

Now, from the above and (2.1) we arrive at (3.1).

Equality in (3.3) holds if and only if $d_2 = \cdots = d_{n-1}$. Equality in (2.1) holds if and only if $G \cong \overline{K_n}$, or $G \cong tK_2 \cup (n-2t)K_1$. Since G has no isolated vertices, equality in (3.1) holds if and only if $G \cong \frac{n}{2}K_2$, for even n. □

Corollary 3.1. *Let G be a graph of order $n \geq 3$ without isolated vertices. Then*

$$E(G) \leq \sqrt{\Delta} + \sqrt{\delta} + \frac{n-2}{4}\left(\frac{\det D}{\Delta\delta}\right)^{\frac{1}{2(n-2)}} \left(\sqrt[4]{\frac{\Delta}{\delta}} + \sqrt[4]{\frac{\delta}{\Delta}}\right)^2. \tag{3.5}$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Proof. For every $n \geq 3$ holds

$$\alpha(n-2) \leq \frac{1}{4}.$$

From the above and (3.1) the inequality (3.5) immediately follows. □

The proof of the next two theorems is analogous to that of Theorem 3.1, hence omitted.

Theorem 3.2. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq \sqrt{\Delta} + (n-1)\left(\frac{\det D}{\Delta}\right)^{\frac{1}{2(n-1)}}\left(1+\alpha(n-1)\left(\sqrt[4]{\frac{\Delta}{\delta}}-\sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right).$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Corollary 3.2. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq \sqrt{\Delta} + \frac{n-1}{4}\left(\frac{\det D}{\Delta}\right)^{\frac{1}{2(n-1)}}\left(\sqrt[4]{\frac{\Delta}{\delta}}+\sqrt[4]{\frac{\delta}{\Delta}}\right)^2.$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Theorem 3.3. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq n\left(\det D\right)^{\frac{1}{2n}}\left(1+\alpha(n)\left(\sqrt[4]{\frac{\Delta}{\delta}}-\sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right).$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Corollary 3.3. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq \frac{n}{4}\left(\det D\right)^{\frac{1}{2n}}\left(\sqrt[4]{\frac{\Delta}{\delta}}+\sqrt[4]{\frac{\delta}{\Delta}}\right)^2.$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Theorem 3.4. *Let G be a graph of order $n \geq 2$ and size m, without isolated vertices. Then*

$$E(G) \leq \min\left\{\sqrt{(2m-n)(n-ID(G))} + {}^0R(G),\ \sqrt{(2m+n)(n+ID(G))} - {}^0R(G)\right\}. \quad (3.6)$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Proof. In [19] it was proven that for any real α, $0 \leq \alpha \leq 1$ holds

$$^0R_\alpha(G) \leq \min\left\{\frac{(2m-n)^\alpha}{(n-ID(G))^{\alpha-1}} + {}^0R_{\alpha-1}(G),\ \frac{(2m+n)^\alpha}{(n+ID(G))^{\alpha-1}} - {}^0R_{\alpha-1}(G)\right).$$

For $\alpha = \frac{1}{2}$, the above inequality becomes

$$^0R_{\frac{1}{2}}(G) \leq \min\left\{(2m-n)^{\frac{1}{2}}(n-ID(G))^{\frac{1}{2}} + {}^0R_{-\frac{1}{2}}(G),\ (2m+n)^{\frac{1}{2}}(n+ID(G))^{\frac{1}{2}} - {}^0R_{-\frac{1}{2}}(G)\right\},$$

that is

$$\sum_{i=1}^{n} \sqrt{d_i} \le \min\left\{ \sqrt{(2m-n)(n-ID(G))} + {}^0R(G) \,,\, \sqrt{(2m+n)(n+ID(G))} - {}^0R(G) \right\} . \tag{3.7}$$

Now, from the above and inequality (2.1) we obtain (3.6).

Equality in (3.7) holds if and only if $d_1 = \cdots = d_n$. Equality in (2.1) holds if and only if $G \cong \overline{K_n}$, or $G \cong t\,K_2 + (n-2t)K_1$. Since G has no isolated vertices, equality in (3.6) holds if and only if $G \cong \frac{n}{2}K_2$, for even n. □

Theorem 3.5. *Let G be a graph with $n \ge 2$ vertices. Then*

$$E(G) \le n\,(\det D)^{\frac{1}{2n}} + n^2\alpha(n)\left(\Delta^{\frac{1}{4}} - \delta^{\frac{1}{4}}\right)^2 . \tag{3.8}$$

Equality holds if and only if $G \cong \overline{K_n}$, or $G \cong \frac{n}{2}K_2$, for even n.

Proof. For $a_i = b_i = \sqrt[4]{d_i}$, $a_1 = b_1 = \sqrt[4]{\Delta}$, $a_n = b_n = \sqrt[4]{\delta}$, $i = 1,2,\ldots,n$, the inequality (2.4) becomes

$$\left| n\sum_{i=1}^{n} \sqrt{d_i} - \left(\sum_{i=1}^{n} \sqrt[4]{d_i} \right) \right|^2 \le n^2\alpha(n)\left(\Delta^{\frac{1}{4}} - \delta^{\frac{1}{4}}\right)^2 .$$

Since

$$n\sum_{i=1}^{n} \sqrt{d_i} - \left(\sum_{i=1}^{n} \sqrt[4]{d_i} \right)^2 \ge 0 ,$$

the above inequality becomes

$$n\sum_{i=1}^{n} \sqrt{d_i} - \left(\sum_{i=1}^{n} \sqrt[4]{d_i} \right)^2 \le n^2\alpha(n)\left(\Delta^{\frac{1}{4}} - \delta^{\frac{1}{4}}\right)^2 . \tag{3.9}$$

On the other hand, for $a_i = \sqrt{d_i}$, $i = 1,2,\ldots,n$, the inequality (2.3) becomes

$$\left(\sum_{i=1}^{n} \sqrt[4]{d_i} \right)^2 \le (n-1)\sum_{i=1}^{n} \sqrt{d_i} + n\left(\prod_{i=1}^{n} \sqrt{d_i} \right)^{\frac{1}{n}} ,$$

that is

$$\left(\sum_{i=1}^{n} \sqrt[4]{d_i} \right)^2 \le (n-1)\sum_{i=1}^{n} \sqrt{d_i} + n\,(\det D)^{\frac{1}{2n}} , \tag{3.10}$$

From the above and inequality (3.9) we obtain

$$\sum_{i=1}^{n} \sqrt{d_i} \le n\,(\det D)^{\frac{1}{2n}} + n^2\alpha(n)\left(\Delta^{\frac{1}{4}} - \delta^{\frac{1}{4}}\right)^2 .$$

Now, from the above and (2.1) we obtain (3.8).

Equality in (3.9) holds if and only if $d_1 = \cdots = d_n$. Equality in (2.1) holds if and only if $G \cong \overline{K_n}$, or $G \cong t\,K_2 \cup (n-2t)K_1$, $1 \le t \le \frac{n}{2}$. This implies that equality in (3.8) holds if and only if $G \cong \overline{K_n}$, or $G \cong \frac{n}{2}K_2$, for even n. □

In the next theorem we determine an upper bound for $E(G)$ in terms of $ID(G)$, $M_1(G)$ and parameters Δ and δ.

Theorem 3.6. *Let G be a graph of order $n \geq 3$ without isolated vertices. Then*

$$E(G) \leq \sqrt{\Delta} + \sqrt{\delta} + \sqrt{\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)\left(M_1(G) - \Delta^2 - \delta^2\right)}. \tag{3.11}$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Proof. The inequality (2.5) can be considered in a form

$$\sum_{i=2}^{n-1} p_i \sum_{i=2}^{n-1} p_i a_i b_i \geq \sum_{i=2}^{n-1} p_i a_i \sum_{i=2}^{n-1} p_i b_i .$$

For $p_i = \frac{1}{d_i}$, $a_i = b_i = d_i^{\frac{3}{2}}$, $i = 2, \ldots, n-1$, the above inequality becomes

$$\sum_{i=2}^{n-1} \frac{1}{d_i} \sum_{i=2}^{n-1} d_i^2 \geq \left(\sum_{i=2}^{n-1} \sqrt{d_i}\right)^2 , \tag{3.12}$$

that is

$$\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)\left(M_1(G) - \Delta^2 - \delta^2\right) \geq \left(\sum_{i=1}^{n} \sqrt{d_i} - \sqrt{\Delta} - \sqrt{\delta}\right)^2$$

From the above inequality we obtain

$$\sum_{i=1}^{n} \sqrt{d_i} \leq \sqrt{\Delta} + \sqrt{\delta} + \sqrt{\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)\left(M_1(G) - \Delta^2 - \delta^2\right)}.$$

Now, from the above inequality and (2.1) we obtain (3.11).

Equality in (3.12) holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$. Equality in (2.1) holds if and only if $G \cong \overline{K_n}$, or $G \cong t\,K_2 \cup (n-2t)K_1$, $1 \leq t \leq \frac{n}{2}$. Since G has no isolated vertices, the inequality (3.11) holds if and only if $G \cong \frac{n}{2}K_2$, for even n. □

By a similar procedure the following results are proved.

Theorem 3.7. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq \sqrt{\Delta} + \sqrt{\left(ID(G) - \frac{1}{\Delta}\right)\left(M_1(G) - \Delta^2\right)}.$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

Theorem 3.8. *Let G be a graph of order $n \geq 2$ without isolated vertices. Then*

$$E(G) \leq \sqrt{ID(G) M_1(G)}.$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$, for even n.

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