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REMARK ON ORDINARY AND RANDIĆ ENERGY OF GRAPHS

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Abstract. Let G be an undirected simple graph with n vertices and m edges. Denote with $|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_n|$ and $|\rho_1| \geqslant |\rho_2| \geqslant \cdots \geqslant |\rho_n|$ absolute eigenvalues and Randić eigenvalues of G arranged in non-increasing order, respectively. Upper bound of graph invariant $E(G) = \sum_{i=1}^n |\lambda_i|$, and lower and upper bounds of invariant $RE(G) = \sum_{i=1}^n |\rho_i|$ are obtained in this paper.

1. Introduction and preliminaries

Let G be an undirected simple graph with n vertices and m edges. If i-th and j-th vertices of graph G are adjacent, we denote it as $i \sim j$. Then the adjacency matrix $\mathbf{A} = (a_{ij})$ of G is defined as

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

Denote by $|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_n|$ absolute ordinary eigenvalues of G arranged in non-increasing order. Some well known results on graph eigenvalues are (see [6])

$$\sum_{i=1}^n \lambda_i = 0 \qquad \text{and} \qquad \sum_{i=1}^n \lambda_i^2 = 2m. \tag{1}$$

Energy of graph G is determined from [9]

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

The following inequality that establishes an upper bound for $E(G)$ in terms of parameters n and m was proved in [13]

$$E(G) \leqslant \sqrt{2mn}. \tag{2}$$

Energy-like spectral invariants have been introduced also for other graph matrices.

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Let $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ be a sequence of vertex degrees of G arranged in non-increasing order. Denote by $\mathbf{D}$ diagonal matrix of its vertex degrees. Then $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix of G. Let the eigenvalues of $\mathbf{L}$ be $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{n-1} \geqslant \mu_n = 0$ (see [2, 6, 8, 14]). If G is a simple graph with no isolated vertices, then matrix $\mathbf{D}^{-1/2}$ is well–defined. The normalized Laplacian matrix of the graph G is calculated as $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$. Its eigenvalues are $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_{n-1} \geqslant \gamma_n = 0$.

Some well known properties of the normalized Laplacian eigenvalues are (see [18]):

$$\sum_{i=1}^{n-1} \gamma_i = n \qquad \text{and} \qquad \sum_{i=1}^{n-1} \gamma_i^2 = n + 2R_{-1}, \tag{3}$$

where $R_{-1} = \sum_{i\sim j} \frac{1}{d_i d_j}$ is the general Randić index (see [3, 11, 17]).

The normalized Laplacian energy of G is defined as [4, 10]

$$NLE(G) = \sum_{i=1}^{n} |\gamma_i - 1|.$$

It is convenient to write the normalized Laplacian matrix as $\mathbf{L}^* = \mathbf{I} - \mathbf{R}$, where $\mathbf{R} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ is the so-called Randić matrix [3]. Denote with $|\rho_1| \geqslant |\rho_2| \geqslant \cdots \geqslant |\rho_n|$ absolute eigenvalues of $\mathbf{R}$ arranged in non-increasing order. Then, Randić energy of graph G is defined as

$$RE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Having in mind that $\gamma_i = 1 - \rho_{n-i+1}$, $i = 1, 2, \ldots, n$, Randić energy coincides with the normalized Laplacian energy (see [10]). The following inequality that determines an upper bound for $RE(G)$ in terms of n and R_{-1}, was proved in [3]

$$RE(G) \leqslant \sqrt{2nR_{-1}}. \tag{4}$$

In this paper we are going to prove inequalities that establish upper bounds for graph invariants $E(G)$ and lower and upper bounds for $RE(G)$.

2. Main results

The following theorem provides an upper bound for $E(G)$ in terms of n, m, $|\lambda_1|$ and $|\lambda_n|$.

THEOREM 1. *Let G be an undirected simple graph with n vertices and m edges. Then*

$$E(G) \leqslant \sqrt{2mn - \frac{n}{2}(|\lambda_1| - |\lambda_n|)^2}. \tag{5}$$

Equality holds if and only if $G \cong \bar{K}_n$ or if n is even and G is disjoint union of $\frac{n}{2}$ paths K_2.

Proof. According to

$$n\sum_{i=1}^{n}|\lambda_i|^2-\left(\sum_{i=1}^{n}|\lambda_i|\right)^2=\sum_{1\leqslant i\leqslant j\leqslant n}(|\lambda_i|-|\lambda_j|)^2,$$

we have that

$$n\sum_{i=1}^{n}|\lambda_i|^2-\left(\sum_{i=1}^{n}|\lambda_i|\right)^2\geqslant\sum_{i=2}^{n-1}\left((|\lambda_1|-|\lambda_i|)^2+(|\lambda_i|-|\lambda_n|)^2\right)+(|\lambda_1|-|\lambda_n|)^2. \quad (6)$$

Based on Jensen's inequality (see [16]) we have that

$$\sum_{i=2}^{n-1}((|\lambda_1|-|\lambda_i|)^2+(|\lambda_i|-|\lambda_n|)2)\geqslant\frac{n-2}{2}(|\lambda_1|-|\lambda_n|)^2. \quad (7)$$

According to equality (1) and inequalities (6) and (7) we obtain the inequality (5).

Equality in (6) holds if and only if $|\lambda_2|=|\lambda_3|=\cdots=|\lambda_n|$, whereas in (7) if and only if $|\lambda_1|-|\lambda_i|=|\lambda_i|-|\lambda_n|$, for each $i=2,\ldots,n-1$. This means that equality in (5) holds if and only if $|\lambda_1|=|\lambda_2|=\cdots=|\lambda_n|$. Consequently, the equality in (5) holds if and only if $G\cong\overline{K}_n$, or if n is even and G is disjoint union of $\frac{n}{2}$ paths K_2. □

REMARK 1. Since for every undirected simple graph with n vertices and m edges, with the property $|\lambda_1|\neq|\lambda_n|$ holds

$$\sqrt{2mn-\frac{n}{2}(|\lambda_1|-|\lambda_n|)^2}\leqslant\sqrt{2mn},$$

it follows that inequality (5) is stronger than (2).

COROLLARY 1. *Let G be an undirected simple graph with n vertices and m edges, with the property $|\lambda_1|\neq|\lambda_n|$. Then*

$$E(G)\leqslant\frac{\sqrt{2}nm}{|\lambda_1|-|\lambda_n|}. \quad (8)$$

Proof. Inequality (5) can be rewritten as

$$E(G)^2+\frac{n}{2}(|\lambda_1|-|\lambda_n|)^2\leqslant 2mn.$$

Having in mind inequality between arithmetic and geometric means, A-G inequality, (see [16]), we have that

$$2\sqrt{\frac{n}{2}E(G)^2(|\lambda_1|-|\lambda_n|)^2}\leqslant 2mn$$

wherefrom the inequality (8) follows. □

REMARK 2. Inequalities (8) and (2) are not comparable. For the graphs with the property $|\lambda_1|-|\lambda_n|>\sqrt{m}$, inequality (8) is stronger than inequality (2). When $G\cong K_n$, the inequality (8) is stronger than (2) if $n\geqslant 6$. When $2\leqslant n\leqslant 5$, the opposite is valid. In the case of complete bipartite graph, bounds (8) and (2) are identical.

REMARK 3. Let us note that inequality (5) is opposite to the inequalities

$$E(G)\geqslant\sqrt{2mn-n^2(|\lambda_1|-|\lambda_n|)^2\alpha(n)}\geqslant\sqrt{2mn-\frac{n^2}{4}(|\lambda_1|-|\lambda_n|)^2}, \tag{9}$$

where

$$\alpha(n)=\frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\left(1-\frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\right)=\frac{1}{4}\left(1-\frac{1+(-1)^{n+1}}{2n^2}\right)=\begin{cases}\frac{1}{4}, & \text{if } n \text{ is even}\\ \frac{(n-1)(n+1)}{4n^2}, & \text{if } n \text{ is odd}\end{cases}. \tag{10}$$

The first inequality in (9) was proved in [15] and the second one in [7].

In the following theorem we establish lower and upper bounds for $RE(G)$ in terms of parameters n, R_{-1}, $|\rho_1|$ and $|\rho_n|$.

THEOREM 2. *Let G be an undirected simple graph of order n with no isolated vertices. Then*

$$2nR_{-1}-n^2(|\rho_1|-|\rho_n|)^2\alpha(n)\leqslant RE^2(G)\leqslant 2nR_{-1}-\frac{n}{2}(|\rho_1|-|\rho_n|)^2. \tag{11}$$

Equality holds if and only if n is even and G is disjoint union of $\frac{n}{2}$ paths K_2.

Proof. If in inequality (see [1])

$$\left|n\sum_{i=1}^{n}a_ib_i-\sum_{i=1}^{n}a_i\sum_{i=1}^{n}b_i\right|\leqslant(A-a)(B-b)n\left\lfloor\frac{n}{2}\right\rfloor\left(1-\frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\right) \tag{12}$$

we substitute a_i and b_i with $|\rho_i|$, $i=1,2,\dots n$, a and b with $|\rho_n|$, and A and B with $|\rho_1|$, we obtain

$$\left|n\sum_{i=1}^{n}|\rho_i|^2-\left(\sum_{i=1}^{n}|\rho_i|\right)^2\right|\leqslant n^2\alpha(n)(|\rho_1|-|\rho_n|)^2. \tag{13}$$

Since

$$\sum_{i=1}^{n}|\rho_i|^2=\sum_{i=1}^{n}|\gamma_{n-i+1}-1|^2=2R_{-1}\qquad\text{and}\qquad 2nR_{-1}-RE(G)^2\geqslant 0,$$

inequality (13) becomes

$$2nR_{-1}-RE(G)^2\leqslant n^2\alpha(n)(|\rho_1|-|\rho_n|)^2.$$

By rearranging the above inequality, left part of inequality (11) is obtained.

Equality in (13) holds if and only if $|\rho_1| = |\rho_2| = \cdots = |\rho_n|$. This means that equality in the left part of (11) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_2$. Since G has no isolated vertices, it must be $G \ncong \overline{K}_n$, thus equality in the left part of (11) holds if and only if G is isomorphic to disjoint union of $\frac{n}{2}$ paths K_2, where n is even.

By the similar procedure used in proof of Theorem 1, the right side of inequality (11) is proved. □

REMARK 4. Since $(|\rho_1| - |\rho_n|)^2 \geqslant 0$, right side of inequality (11) is stronger than (4).

COROLLARY 2. *Let G be an undirected simple graph of order n with no isolated vertices. If n is even then*

$$\frac{n^2}{n-1} - \frac{n^2}{4}(|\rho_1| - |\rho_n|)^2 \leqslant RE^2(G) \leqslant n^2 - \frac{n}{2}(|\rho_1| - |\rho_n|)^2.$$

If n is odd then

$$\frac{n^2}{n-1} - \frac{(n-1)(n+1)}{4}(|\rho_1| - |\rho_n|)^2 \leqslant RE^2(G) \leqslant n(n-1) - \frac{n}{2}(|\rho_1| - |\rho_n|)^2.$$

Proof. Inequalities are obtained from Theorem 2 and inequality

$$\frac{n}{2(n-1)} \leqslant R_{-1} \leqslant \left\lfloor \frac{n}{2} \right\rfloor$$

proved in [12]. □

COROLLARY 3. *Let G be an undirected simple graph of order n with no isolated vertices. If $|\rho_1| \neq |\rho_n|$, then*

$$RE(G) \leqslant \frac{\sqrt{2n}R_{-1}}{|\rho_1| - |\rho_n|}.$$

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