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New Bounds for Some Spectrum–Based Topological Indices of Graphs

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Abstract

The spectrum-based graph invariant $\mathcal{E}(G)$, known as (ordinary) energy of a graph G, is defined by $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ are the eigenvalues of G. Recently introduced resolvent energy of a graph is a type of graph energy based on resolvent matrix and defined by $ER(G) = \sum_{i=1}^{n}(n-\lambda_i)^{-1}$. The resolvent Estrada index $EE_r(G)$ and resolvent signless Laplacian Estrada index $SLEE_r(G)$ are defined by $EE_r(G) = \sum\limits_{i=1}^{n} \left(1 - \frac{\lambda_i}{n-1}\right)^{-1}$ and $SLEE_r(G) = \sum\limits_{i=1}^{n} \left(1 - \frac{q_i}{2n-2}\right)^{-1}$, respectively, where $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$ are signless Laplacian eigenvalues of graph G. Using some classical and recently obtained analytic inequalities we obtain several new lower and upper bounds for these graph invariants and improve some of the existing ones. In addition, some relations between the ordinary graph energy $\mathcal{E}(G)$ and the resolvent energy $ER(G)$ are established.

1 Introduction

The topological index of a graph is a graph invariant that represents the number associated with the graph which correlates its structure. The interest in studying topological indices is mainly due to their use as one of the fundamental tools in QSPR/QSAR modeling employed in different fields of chemistry in order to describe and predict physical

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properties and biological activities of organic compounds from their molecular structures. In parallel, graph theory and complex network analysis tools are expanding to new potential fields of application from molecules to populations, social or technological networks such as genome, protein-protein networks, power electric power network or internet.

Let $G = (V(G), E(G))$, $V(G) = \{v_1, v_2, \ldots, v_n\}$, be a simple graph on n vertices and m edges.

Denote by $A(G)$ the adjacency matrix of G, and by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ its eigenvalues. The (ordinary) energy of graph G is defined as [14]

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

This graph invariant was introduced in the 1978, and since then hundreds of papers have been published concerning its chemical and mathematical properties. Due to the success of the concept of graph energy, a number of other "graph energies" have been introduced, based on different matrices associated with graphs. The most important properties of graph energy can be found in the monographs [22] and [19], and the references cited therein.

For a square $n \times n$ matrix M with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, its resolvent matrix, denoted by $\mathcal{R}_M(z)$, is defined as [24]

$$\mathcal{R}_M(z) = (zI_n - M)^{-1},$$

where I_n is the unit matrix of order n, and z is a complex variable which is different from eigenvalues of matrix M.

Recall that spectral norm of matix M is defined as $\|M\| = \max_i |\lambda_i|$. For any symmetric matrix M and $|z| > ||M||$, the resolvent matrix $\mathcal{R}_M(z)$ exists and $||\mathcal{R}_M(z)|| \leq \frac{1}{|z|-||M||}$.

Having in mind that all eigenvalues of n-vertex graph satisfy the condition $\lambda_i \leq n-1$, $i = 1, 2, \ldots, n$, [6], in paper [18] it was proposed to choose $z = n$. Thus, the numbers $\dfrac{1}{n-\lambda_i}$, $i = 1, 2, \ldots, n$, represent eigenvalues of matrix $\mathcal{R}_A(n) = (nI_n - A)^{-1}$ and $\det(\mathcal{R}_A(n)) = \prod_{i=1}^{n} \dfrac{1}{n-\lambda_i}$.

By analogy with ordinary graph energy, the resolvent energy of graph G is defined as [18]

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n-\lambda_i}.$$

Article [18] provides some interesting properties of $ER(G)$ related to the definition of $ER(G)$ via spectral moments and characteristic polynomial of a graph such as

$$ER(G) = \frac{1}{n}\sum_{k=0}^{\infty}\frac{M_k(G)}{n^k},$$

where $M_k(G) = \sum_{i=1}^{k}\lambda_i^k$, $k = 0, 1, 2, \ldots$ is the k-th spectral moment of G which is equal to the number of self-returning walks of length k, and

$$ER(G) = \frac{\phi'(G,n)}{\phi(G,n)},$$

where $\phi(G, x)$ is the characteristic polynomial of the graph G.

Notice that the resolvent energy belongs to a general class of cumulative vertex centrality measures based on closed walks [11]. The mention class of functions contains graph invariants of the form

$$\varphi(G) = \sum_{k=0}^{\infty} c_k M_k(G),$$

with the sequence of positive real numbers c_0, c_1, $\ldots$ chosen such that Maclaurin series $\sum_{k=0}^{\infty} c_k x^k$ converges to some function $f(x)$.

Some bounds for $ER(G)$ in terms of parameters n, m and n_0, where n_0 is the nullity of a graph, have also been obtained in [18]. Additional properties of $ER(G)$ can be found in the recent papers [1], [10], [13], [31]. Recently, in the paper [32] several new bounds for ER are obtained.

The resolvent Estrada index of a graph, put forward by Estrada and Higham in [11], is defined as

$$EE_r(G) = \sum_{i=1}^{n}\left(1 - \frac{\lambda_i}{n-1}\right)^{-1}.$$

The resolvent signless Laplacian Estrada index [16] is defined as

$$SLEE_r(G) = \sum_{i=1}^{n}\left(1 - \frac{q_i}{2n-2}\right)^{-1},$$

where $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$ are signless Laplacian eigenvalues of a graph. These graph invariants are defined for all graphs on n vertices except for complete graph K_n.

Analytic inequalities plays an important role in obtaining and improving bounds for many spectrum-based graph invariants.

Using some classical and recently obtained analytic inequalities we estimate $ER(G)-1$ and $ER(G)-\det(\mathcal{R}_A(n))$. By using these results we obtained some new bounds for $ER(G)$ in terms of n, m, λ_1, λ_n and $\det(\mathcal{R}_A(n))$.

In the same manner we obtain new bounds for $ER(G)$, and upper bounds for $EE_r(G)$ and $SLEE_r(G)$, which are stronger than upper bounds previously reported in the literature.

In addition, we establish some relations between ordinary and resolvent graph energy which are of significant interest due to the paper [28].

2 Preliminaries

In this section we recall some analytic inequalities for real number sequences that are of interest for the subsequent considerations. In addition, we prove an equality that will be used in the rest of paper.

Lemma 2.1. [23] *Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, n$, be two sequences of non-negative real numbers of the same monotonicity and $p = (p_i)$, $i = 1, 2, \ldots, n$ sequence of positive real numbers. Then*

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

Equality in (1) *holds if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.*

Lemma 2.2. [23, 29] *Let $a = (a_i)$ and $p = (p_i)$, $i = 1, 2, \ldots, n$, be two sequences of positive real numbers such that $\sum\limits_{i=1}^{n} p_i = 1$ and $0 < r \leq a_i \leq R < +\infty$, $i = 1, \ldots, n$, $r, R \in \mathbb{R}$. Then*

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \leq r + R, \tag{2}$$

with equality if and only if $R = a_1 = a_2 = \cdots = a_n = r$ or $R = a_1 = a_2 = \cdots = a_k \geq a_{k+1} = \cdots = a_n = r$, for some k, $1 \leq k \leq n - 1$.

Lemma 2.3. [26] *Let $a = (a_i)$ and $p = (p_i)$, $i = 1, 2, \ldots, n$, be two sequences of positive real numbers such that $\sum\limits_{i=1}^{n} p_i = 1$ and $0 < r \leq a_i \leq R < +\infty$, $i = 1, \ldots, n$, $r, R \in \mathbb{R}$. Then*

$$\sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} \frac{p_i}{a_i} \leq \frac{1}{4} \left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}} \right)^2. \tag{3}$$

The equality holds if and only if $R = a_1 = a_2 = \cdots = a_n = r$.

Lemma 2.4. [21] *Let $a = (a_i)$ be a sequence of positive real numbers such that $0 < r \leq a_i \leq R < +\infty$, $i = 1, \ldots, n$, $r, R \in \mathbb{R}$. Then*

$$\sum_{i=1}^{n} a_i \sum_{i=1}^{n} \frac{1}{a_i} \leq \left(1 + \alpha(n) \left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}} \right)^2 \right) n^2, \tag{4}$$

where $\alpha(n) = \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right) = \frac{1}{4}\left(1 - \frac{(-1)^{n+1}+1}{2n^2}\right)$.
The equality holds if and only if $R = a_1 = a_2 = \cdots = a_n = r$ *or* $R = a_1 = a_2 = \cdots = a_k \geq a_{k+1} = \cdots = a_n = r$, *for* $k = \lfloor \frac{n}{2} \rfloor$.

Lemma 2.5. [3, 23] *Let* $a = (a_i)$ *and* $b = (b_i)$, $i = 1, 2, \ldots, n$, *be two sequences of real numbers such that* $a \leq a_i \leq A < +\infty$ *and* $b \leq b_i \leq B < +\infty$, $i = 1, \ldots, n$, $a, b, A, B \in \mathbb{R}$. *Then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq n^2 \alpha(n)(A-a)(B-b), \tag{5}$$

where $\alpha(n) = \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right) = \frac{1}{4}\left(1 - \frac{(-1)^{n+1}+1}{2n^2}\right)$.
The equality holds if and only if $a_1 = a_2 = \cdots = a_n$ *or* $b_1 = b_2 = \cdots = b_n$.

Lemma 2.6. [5] *Let* $a_1 \geq a_2 \geq \cdots \geq a_n > 0$ *be real numbers. Then*

$$\sum_{i=1}^{n} a_i - n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \geq (\sqrt{a_1} - \sqrt{a_n})^2, \tag{6}$$

with equality if $a_2 = a_3 = \cdots = a_{n-1} = \sqrt{a_1 a_n}$.

Lemma 2.7. [25, 30] *Let* $a_i \in \mathbb{R}^+, i = 1, \ldots, n$. *Then*

$$(n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \geq \left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \geq \sum_{i=1}^{n} a_i + n(n-1)\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}. \tag{7}$$

Equalities on both sides of inequalities (7) *hold if and only if* $a_1 = a_2 = \cdots = a_n$.

Lemma 2.8. [2, 27] *Let* $x = (x_i)$ *be a sequence of non-negative and* $a = (a_i)$, $i = 1, 2, \ldots, n$, *a sequence of positive real numbers. Then, for any* $r \geq 0$, *holds*

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum\limits_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum\limits_{i=1}^{n} a_i\right)^{r}}. \tag{8}$$

Equality is attained if and only if $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

Two sequences of real numbers $a = (a_i)$ and $b = (b_i), i = 1, 2, \ldots, n$, are said to be of similar monotonicity if and only if for each pair (i, j), $i, j = 1, 2, \ldots, n$, the pairs (a_i, a_j) and (b_i, b_j) are similarly ordered, i.e., it holds $(a_i - a_j)(b_i - b_j) \geq 0$.

Let $I = \{1, 2, \ldots, n\}, J_k = \{i_1, i_2, \ldots, i_k\}, J_k \subset I, 1 < i_1 < i_2 < \cdots < i_k < n$, $0 \leq k \leq n-2$, $J_0 = \emptyset$, be index sets and $I_{n-k} = I - J_k$, where $I_n = I, I_2 = \{1, n\}$ and $I_1 = \{1\}$.

Denote by $a = (a_i)$ and $p = (p_i)$ two sequences of non-negative real numbers. A weighted mean of order r of a sequence $a = (a_i)$ with respect to a sequence $p = (p_i)$ is defined as

$$M_r(a, p; I) = \left(\frac{\sum\limits_{i \in I} p_i a_i^r}{\sum\limits_{i \in I} p_i} \right)^{\frac{1}{r}}.$$

Lemma 2.9. [17] *Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, n$, be two sequences of non-negative real numbers of similar monotonicity, and $p = (p_i), i = 1, 2, \ldots, n$, a sequence of positive real numbers. If the pairs $(M_1(a, p; I - I_2), M_1(a, p; I_2))$ and $(M_1(b, p; I - I_2), M_1(b, p; I_2))$ are similarly ordered, then*

$$\sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i - \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \geq \frac{p_1 p_n (a_1 - a_n)(b_1 - b_n)}{p_1 + p_n} \sum_{i=1}^{n} p_i. \tag{9}$$

Equality holds if and only if $a_2 = a_3 = \cdots = a_{n-1} = \dfrac{a_1 + a_n}{2}$ or $b_2 = b_3 = \cdots = b_{n-1} = \dfrac{b_1 + b_n}{2}$.

Lemma 2.10. [6] *A graph has one eigenvalue if and only if it is totally disconnected. A graph has two distinct eigenvalues $\lambda_1 > \lambda_2$ with multiplicities m_1 and m_2 if and only if it consists of m_1 complete graphs of order $\lambda_1 + 1$. In that case, $\lambda_2 = -1$ and $m_2 = m_1 \lambda_1$.*

Remark 2.1. *In paper [7] it was proved that the same is true in the case of graphs with at most two different signless Laplacian eigenvalues.*

At the end of this section we prove one useful equality needed for further considerations.

Lemma 2.11. *Let G be an n-vertex graph with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then*

$$\sum_{i=1}^{n} \frac{\lambda_i^2}{n - \lambda_i} = n^2 (ER(G) - 1). \tag{10}$$

Proof. Using the fact that $\sum\limits_{i=1}^{n} \lambda_i = 0$, we obtain

$$\begin{aligned} n^2(ER(G) - 1) &= n^2 \left(\sum_{i=1}^{n} \frac{1}{n - \lambda_i} - \sum_{i=1}^{n} \frac{1}{n} \right) = n^2 \sum_{i=1}^{n} \left(\frac{1}{n - \lambda_i} - \frac{1}{n} \right) \\ &= n^2 \sum_{i=1}^{n} \frac{\lambda_i}{n^2 - n\lambda_i} = \sum_{i=1}^{n} \frac{\lambda_i (n^2 - n\lambda_i) + n\lambda_i^2}{n^2 - n\lambda_i} \\ &= \sum_{i=1}^{n} \lambda_i + \sum_{i=1}^{n} \frac{n\lambda_i^2}{n(n - \lambda_i)} = \sum_{i=1}^{n} \frac{\lambda_i^2}{n - \lambda_i}. \end{aligned}$$

∎

3 Some new bounds for the resolvent energy, resolvent Estrada and resolvent signless Laplacian Estrada indices

It was proved in [18] that $ER(G) \geq 1$, with equality if and only if $G \cong \overline{K}_n$. We now prove the following result.

Lemma 3.1. *For any real number k, such that $\frac{1}{n-\lambda_1} \geq k \geq (\det \mathcal{R}_A(n))^{\frac{1}{n}}$, the following inequality holds*

$$ER(G) \geq k + (n-1)\left(\frac{\det \mathcal{R}_A(n)}{k}\right)^{\frac{1}{n-1}}. \tag{11}$$

Proof. Consider the function (in variable x)

$$f(x) = x + (n-1)\left(\frac{\det \mathcal{R}_A(n)}{x}\right)^{\frac{1}{n-1}}, \; x > 0.$$

As

$$f'(x) = 1 - \left(\frac{\det \mathcal{R}_A(n)}{x^n}\right)^{\frac{1}{n-1}},$$

it follows that $f(x)$ is non-increasing function for $x \geq (\det \mathcal{R}_A(n))^{\frac{1}{n}}$.

From the geometric-arithmetic mean inequality it is easily obtained that $(\det \mathcal{R}_A(n))^{\frac{1}{n}} \leq \frac{1}{n-\lambda_1}$, implying $f\left(\det \mathcal{R}_A(n))^{\frac{1}{n}}\right) \leq f\left(\frac{1}{n-\lambda_1}\right)$.

Using the geometric-arithmetic mean inequality we obtain

$$f\left(\frac{1}{n-\lambda_1}\right) = \frac{1}{n-\lambda_1} + (n-1)\left(\frac{\det \mathcal{R}_A(n)}{\frac{1}{n-\lambda_1}}\right)^{\frac{1}{n-1}} = \frac{1}{n-\lambda_1} + (n-1)\left(\frac{\prod_{i=1}^{n} \frac{1}{n-\lambda_i}}{\frac{1}{n-\lambda_1}}\right)^{\frac{1}{n-1}} =$$

$$= \frac{1}{n-\lambda_1} + (n-1)\left(\prod_{i=2}^{n}\left(\frac{1}{n-\lambda_i}\right)\right)^{\frac{1}{n-1}} \leq \frac{1}{n-\lambda_1} + \sum_{i=2}^{n} \frac{1}{n-\lambda_i} = ER(G).$$

Thus, for any real number k, such that $\frac{1}{n-\lambda_1} \geq k \geq (\det \mathcal{R}_A(n))^{\frac{1}{n}}$, it holds

$$ER(G) \geq f\left(\frac{1}{n-\lambda_1}\right) \geq f(k) \geq f\left((\det \mathcal{R}_A(n))^{\frac{1}{n}}\right),$$

wherefrom we obtain the inequality (11). ∎

Remark 3.1. *Since $f\left(\det \mathcal{R}_A(n))^{\frac{1}{n}}\right) = n\,(\det \mathcal{R}_A(n))^{\frac{1}{n}}$, from (11) it can be concluded that*

$$ER(G) \geq n(\det \mathcal{R}_A(n))^{\frac{1}{n}}. \tag{12}$$

Equality holds if and only if $G \cong \overline{K}_n$. The inequality (12) can also be proved by using the geometric-arithmetic mean inequality.

As $\lambda_1 \geq \frac{2m}{n}$ [6], it holds that $\frac{1}{n-\lambda_1} \geq \frac{n}{n^2-2m}$. Besides, by using the inequality

$$ER(G) \leq 1 + \frac{2m(2n-1)}{n^2(n^2-2m)},$$

proved in [18], it can be concluded that

$$(\det \mathcal{R}_A(n))^{\frac{1}{n}} \leq \frac{1}{n} ER(G) \leq \frac{n^2(n^2-2m)+2m(2n-1)}{n^3(n^2-2m)}.$$

In addition, it is easy to verify that $\frac{n^2(n^2-2m)+2m(2n-1)}{n^3(n^2-2m)} \leq \frac{n}{n^2-2m}$, implying $\frac{1}{n-\lambda_1} \geq \frac{n}{n^2-2m} \geq (\det \mathcal{R}_A(n))^{\frac{1}{n}}$.

Remark 3.2. *Since* $\frac{1}{n-\lambda_1} \geq \frac{n}{n^2-2m} \geq (\det \mathcal{R}_A(n))^{\frac{1}{n}}$, *for* $k = \frac{1}{n-\lambda_1}$ *and* $k = \frac{n}{n^2-2m}$, *respectively, from (11), the following inequalities are obtained*

$$ER(G) \geq \frac{1}{n-\lambda_1} + (n-1)\cdot((n-\lambda_1)\det \mathcal{R}_A(n))^{\frac{1}{n-1}}, \tag{13}$$

$$ER(G) \geq \frac{n}{n^2-2m} + (n-1)\left(\frac{n^2-2m}{n}\det \mathcal{R}_A(n)\right)^{\frac{1}{n-1}}. \tag{14}$$

Theorem 3.1. *Let G be a simple graph on n vertices. Then*

$$ER(G) \geq 1 + \frac{1}{n}|\det A|^{\frac{2}{n}}(\det \mathcal{R}_A(n))^{\frac{1}{n}}. \tag{15}$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. Using the geometric-arithmetic mean inequality and relation (10), we obtain

$$n^2(ER(G)-1) = \sum_{i=1}^{n} \frac{\lambda_i^2}{n-\lambda_i} \geq n\left(\prod_{i=1}^{n}\frac{\lambda_i^2}{n-\lambda_i}\right)^{\frac{1}{n}} = n|\det A|^{\frac{2}{n}}(\det \mathcal{R}_A(n))^{\frac{1}{n}}.$$

Equality is attained if and only if $\frac{\lambda_1^2}{n-\lambda_1} = \frac{\lambda_2^2}{n-\lambda_2} = \cdots = \frac{\lambda_n^2}{n-\lambda_n}$, wherefrom it can be easily verified that $\lambda_1 = \lambda_2 = \cdots = \lambda_n$, and consequently, by Lemma 2.10, $G \cong \overline{K}_n$. ■

In the next theorems we establish some lower and upper bounds for $ER(G)-1$ and $ER(G) - n(\det \mathcal{R}_A(n))^{\frac{1}{n}}$ which depend on parameters n, λ_1, λ_n and $\det \mathcal{R}_A(n)$. These results lead straightforwardly to some new lower and upper bounds on resolvent energy of a graph.

Theorem 3.2. *Let G be a graph on n vertices, $n > 1$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then*

$$ER(G) - n(\det \mathcal{R}_A(n))^{\frac{1}{n}} \geq \frac{\left(\sqrt{n-\lambda_n} - \sqrt{n-\lambda_1}\right)^2}{(n-\lambda_1)(n-\lambda_n)} \tag{16}$$

$$ER(G) - n(\det \mathcal{R}_A(n))^{\frac{1}{n}} \leq n^2\alpha(n) \cdot \frac{\left(\sqrt{n-\lambda_n} - \sqrt{n-\lambda_1}\right)^2}{(n-\lambda_1)(n-\lambda_n)}, \tag{17}$$

where $\alpha(n) = \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right) = \frac{1}{4}\left(1 - \frac{(-1)^{n+1}+1}{2n^2}\right)$.
Equalities in both (16) *and* (17) *are attained if and only if G is an empty graph.*

Proof. Lower bound (16). The proof follows from inequality (6) for $a_i = \frac{1}{n-\lambda_i}$, $i = 1, \ldots, n$.
Upper bound (17). For $a_i = b_i = \frac{1}{\sqrt{n-\lambda_i}}$, $i = 1, \ldots, n$, $A = B = \frac{1}{\sqrt{n-\lambda_1}}$, $a = b = \frac{1}{\sqrt{n-\lambda_n}}$, by inequality (5) we obtain

$$ER(G) - \frac{1}{n}\left(\sum_{i=1}^{n} \frac{1}{\sqrt{n-\lambda_i}}\right)^2 \leq n^2\alpha(n) \frac{\left(\sqrt{n-\lambda_n} - \sqrt{n-\lambda_1}\right)^2}{(n-\lambda_1)(n-\lambda_n)}.$$

Using the left-hand side of the inequality (7) we get

$$ER(G) \leq \frac{1}{n}\left((n-1)ER(G) + n(\det \mathcal{R}_A(n))^{\frac{1}{n}}\right) + n\alpha(n)\frac{(\sqrt{n-\lambda_n} - \sqrt{n-\lambda_1})^2}{(n-\lambda_1)(n-\lambda_n)},$$

and the proof follows.

By Lemma 2.6, the equality in (16) is attained if and only if $\frac{1}{n-\lambda_2} = \frac{1}{n-\lambda_3} = \cdots = \frac{1}{n-\lambda_{n-1}} = \sqrt{\frac{1}{(n-\lambda_1)(n-\lambda_n)}}$, that is if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = n - \sqrt{(n-\lambda_1)(n-\lambda_n)}$.

If $\lambda_n = \lambda_1$, then $n - \sqrt{(n-\lambda_1)(n-\lambda_n)} = \lambda_1$, implying $\lambda_1 = \lambda_2 = \cdots = \lambda_n$. Consequently, by Lemma 2.10, G is an empty graph.

If $\lambda_n < \lambda_1$ then G has three distinct eigenvalues

$$\left\{\lambda_1, \left[n - \sqrt{(n-\lambda_1)(n-\lambda_n)}\right]^{n-2}, \lambda_n\right\}.$$

As $n - \sqrt{(n-\lambda_1)(n-\lambda_n)} > 0$, the latter case is impossible, since then $|\lambda_n| > \lambda_1$.

Equality in (17) is attained if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_n$ and consequently, G is an empty graph. ∎

Remark 3.3. *The lower bound* (16) *is better than the lower bound* (8) *from [32].*

Theorem 3.3. *Let G be a graph on n vertices, $n > 1$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then*

$$\frac{(\lambda_1-\lambda_n)^2}{(n-\lambda_1)(n-\lambda_n)(2n-\lambda_1-\lambda_n)} \leq ER(G)-1 \leq \alpha(n)\frac{(\lambda_1-\lambda_n)^2}{(n-\lambda_1)(n-\lambda_n)}, \qquad (18)$$

where $\alpha(n) = \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor \left(1-\frac{1}{n}\left\lfloor \frac{n}{2}\right\rfloor\right) = \frac{1}{4}\left(1-\frac{(-1)^{n+1}+1}{2n^2}\right)$.
Equality at the left-hand side of (18) *holds if only if and only if $G \cong \overline{K}_n$, and equality at the right-hand side of* (18) *is attained if and only if $G \cong \overline{K}_n$ or (provided n is even) $G \cong \frac{n}{2}K_2$.*

Proof. Lower bound in (18). Left hand-side of (18) is obtained from (9) for $p_i = n-\lambda_i, a_i = b_i = \dfrac{1}{n-\lambda_i}, i = 1,2,\ldots,n$.
Upper bound in (18). For $a_i = \dfrac{1}{n-\lambda_i}, i = 1,2,\ldots,n, r = \dfrac{1}{n-\lambda_n}, R = \dfrac{1}{n-\lambda_1}$, the inequality (4) transforms into

$$n^2 ER(G) \leq \left(1+\alpha(n)\cdot\frac{(\lambda_1-\lambda_n)^2}{(n-\lambda_1)(n-\lambda_n)}\right)\cdot n^2,$$

and the proof follows.

Equality at the left-hand side of (18) is attained if and only if $\frac{1}{n-\lambda_2} = \frac{1}{n-\lambda_3} = \cdots = \frac{1}{n-\lambda_{n-1}} = \frac{\frac{1}{n-\lambda_1}+\frac{1}{n-\lambda_n}}{2}$. Using the similar arguments as in the proof of Theorem 3.2, it is concluded that $G \cong \overline{K}_n$ or G has three distinct eigenvalues

$$\left\{\lambda_1, \left[\frac{\lambda_1+\lambda_n}{2}+\frac{(\lambda_1-\lambda_n)^2}{4(n-\frac{\lambda_1+\lambda_n}{2})}\right]^{n-2}, \lambda_n\right\}.$$

The latter case is impossible since $\frac{\lambda_1+\lambda_n}{2}+\frac{(\lambda_1-\lambda_n)^2}{4(n-\frac{\lambda_1+\lambda_n}{2})} > 0$, implying $|\lambda_n| > \lambda_1$.

Equality at the right-hand side of (18) is attained if and only if $\frac{1}{n-\lambda_1} = \frac{1}{n-\lambda_2} = \cdots = \frac{1}{n-\lambda_n}$ or $\frac{1}{n-\lambda_1} = \frac{1}{n-\lambda_2} = \cdots = \frac{1}{n-\lambda_k} \geq \frac{1}{n-\lambda_{k+1}} = \cdots = \frac{1}{n-\lambda_n}$ for $k = \lfloor \frac{n}{2} \rfloor$. By Lemma 2.10, in the first case $G \cong \overline{K}_n$, and in in the second case (provided n is even) $G \cong \frac{n}{2}K_2$. ■

Theorem 3.4. *Let G be an n-vertex graph with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then*

$$ER(G)-1 \leq -\frac{\lambda_1\lambda_n}{(n-\lambda_n)(n-\lambda_1)}. \qquad (19)$$

Equality is attained if and only if $G \cong \overline{K}_n$ or $G \cong kK_s$ for some k and s, $1 \leq k \leq n-1$, such that $n = ks$.

Proof. In Rennie's inequality (2) we choose $a_i = \dfrac{1}{n-\lambda_i}, i = 1, \ldots, n,\ r = \dfrac{1}{n-\lambda_n}, R = \dfrac{1}{n-\lambda_1}, p_i = \dfrac{1}{n}$. Then

$$\sum_{i=1}^{n} \frac{1}{n} \cdot \frac{1}{n-\lambda_i} + rR \sum_{i=1}^{n} \frac{\frac{1}{n}}{\frac{1}{n-\lambda_i}} \leq \frac{1}{n-\lambda_n} + \frac{1}{n-\lambda_1},$$

i.e.,

$$\frac{1}{n} ER(G) + \frac{1}{(n-\lambda_n)(n-\lambda_1)} \cdot \frac{1}{n} \sum_{i=1}^{n} (n-\lambda_i) \leq \frac{2n-\lambda_1-\lambda_n}{(n-\lambda_n)(n-\lambda_1)}.$$

As $\sum_{i=1}^{n}(n-\lambda_i) = n^2$, the last inequality can be transformed into

$$\frac{1}{n} ER(G) + \frac{n}{(n-\lambda_n)(n-\lambda_1)} \leq \frac{2n-\lambda_1-\lambda_n}{(n-\lambda_n)(n-\lambda_1)},$$

which straightforwardly leads to the upper bound in (19).

Equality in (19) is attained if and only if $\frac{1}{n-\lambda_1} = \frac{1}{n-\lambda_2} = \cdots = \frac{1}{n-\lambda_n}$ or $\frac{1}{n-\lambda_1} = \frac{1}{n-\lambda_2} = \cdots = \frac{1}{n-\lambda_k} \geq \frac{1}{n-\lambda_{k+1}} = \cdots = \frac{1}{n-\lambda_n}$ for some k, $1 \leq k \leq n-1$. In the first case $G \cong \overline{K}_n$, while in the second case $G \cong kK_s$, for some k and s, $1 \leq k \leq n-1$, such that $n = ks$. ■

Theorem 3.5. *Let G be a graph on n vertices, $G \neq K_n$, with eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ and signless Laplacian eigenvalues $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$. Then*

(a)

$$EE_r(G) \leqslant n + \alpha(n) \cdot \frac{n(\lambda_1-\lambda_n)^2}{(n-1-\lambda_1)(n-1-\lambda_n)}, \tag{20}$$

and

(b)

$$SLEE_r(G) \leqslant \frac{n^2(n-1)}{n(n-1)-m} \left(1 + \alpha(n) \frac{(q_1-q_n)^2}{(2n-2-q_1)(2n-2-q_n)}\right), \tag{21}$$

where $\alpha(n) = \dfrac{1}{n}\left\lfloor \dfrac{n}{2} \right\rfloor \left(1 - \dfrac{1}{n}\left\lfloor \dfrac{n}{2} \right\rfloor\right) = \dfrac{1}{4}\left(1 - \dfrac{(-1)^{n+1}+1}{2n^2}\right)$.
Both equalities are attained if and only if $G \cong \overline{K}_n$ or (provided n is even, $n > 2$) $G \cong \frac{n}{2}K_2$.

Proof. (a) Setting $a_i = \dfrac{n-1}{n-1-\lambda_i}$, $i = 1, 2, \ldots, n$, $R = \dfrac{n-1}{n-1-\lambda_1}$, $r = \dfrac{n-1}{n-1-\lambda_n}$, the inequality (4) transforms into

$$EE_r(G) \leqslant n + \alpha(n) \cdot \frac{n(\lambda_1-\lambda_n)^2}{(n-1-\lambda_1)(n-1-\lambda_n)},$$

where we used that $\sum_{i=1}^{n} \dfrac{1}{a_i} = \sum_{i=1}^{n}\left(1 - \dfrac{1}{n-1}\lambda_i\right) = n$.

(b) Letting $a_i = \dfrac{2n-2}{2n-2-q_i}$, $i=1,2,\dots,n$, $R = \dfrac{2n-2}{2n-2-q_1}$, $r = \dfrac{2n-2}{2n-2-q_n}$, the inequality (4) transforms into

$$SLEE_r(G) \leqslant \frac{n^2(n-1)}{n(n-1)-m}\left(1+\alpha(n)\frac{(q_1-q_n)^2}{(2n-2-q_1)(2n-2-q_n)}\right),$$

where we used that $\sum\limits_{i=1}^{n}\dfrac{1}{a_i} = \sum\limits_{i=1}^{n}\left(1-\dfrac{1}{2n-2}q_i\right) = n - \dfrac{2m}{2n-2} = n - \dfrac{m}{n-1}$.

According to Lemmas 2.4 and 2.10 and Remark 2.1, in both relations (20) and (21), equalities are attained if and only if $G \cong \overline{K}_n$ or (provided n is even, $n>2$) $G \cong \frac{n}{2}K_2$. ■

Remark 3.4. *The upper bound (20) is stronger than previously reported upper bound from [16, Lemma 3.6, (5)] and the upper bound (21) strengthens the upper bound from [16, Lemma 4.10 (5)], since* $\alpha(n) < \frac{1}{3}$.

4 Relations between ordinary and resolvent graph energy

Determining the connection between different types of graph energies is a very interesting and important problem in chemical graph theory. In recent papers [8], [4] and [9] some relations between ordinary, Randić and Laplacian graph energy were established.

In the paper [28] the authors provide some experimentally obtained relations between ordinary and resolvent graph energy of trees.

In the sequel we obtain some relations between ordinary and resolvent graph energy of general graphs.

Theorem 4.1. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}^2(G)\left(\frac{1}{ER(G)} + \frac{(n-\lambda_1)(n-\lambda_n)}{n^2}\right) \le 2m(2n-\lambda_1-\lambda_n). \tag{22}$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. For $p_i = \dfrac{\lambda_i^2}{2m}$, $a_i = n-\lambda_i$, $i=1,2,\dots,n$, $r = n-\lambda_1$ and $R = n-\lambda_n$, the inequality (2) transforms into

$$\sum_{i=1}^{n}\lambda_i^2(n-\lambda_i) + (n-\lambda_1)(n-\lambda_n)\sum_{i=1}^{n}\frac{\lambda_i^2}{n-\lambda_i} \le 2m(2n-\lambda_1-\lambda_n). \tag{23}$$

From inequality (8), letting $r = 1$, $x_i = |\lambda_i|$, $a_i = \dfrac{1}{n-\lambda_i}$, $i = 1, 2, \dots, n$, we obtain the inequality

$$\sum_{i=1}^{n} \lambda_i^2 (n-\lambda_i) \geq \frac{\left(\sum\limits_{i=1}^{n} |\lambda_i|\right)^2}{\sum\limits_{i=1}^{n} \dfrac{1}{n-\lambda_i}},$$

that is

$$\sum_{i=1}^{n} \lambda_i^2 (n-\lambda_i) \geq \frac{\mathcal{E}^2(G)}{ER(G)}. \tag{24}$$

For $r = 1$, $x_i = |\lambda_i|$, $a_i = n - \lambda_i$, $i = 1, 2, \dots, n$, the inequality (8) transforms into

$$\sum_{i=1}^{n} \frac{\lambda_i^2}{n-\lambda_i} \geq \frac{\left(\sum\limits_{i=1}^{n} |\lambda_i|\right)^2}{\sum\limits_{i=1}^{n} (n-\lambda_i)},$$

i.e.,

$$\sum_{i=1}^{n} \frac{\lambda_i^2}{n-\lambda_i} \geq \frac{\mathcal{E}^2(G)}{n^2}. \tag{25}$$

Now, the inequality (22) follows from inequalities (23), (24) and (25).

Equality is attained if and only if equalities hold in (23), (24) and (25). Having in mind Lemmas 2.2 and 2.8, it is easy to conclude that these conditions are satisfied if and only if graph G has exactly one eigenvalue, that is when $G \cong \overline{K}_n$. ■

Corollary 4.1. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}^2(G) \leq \left(2m(2n-\lambda_1-\lambda_n) - n(n-\lambda_1)(n-\lambda_n)|\det A|^{\frac{2}{n}} (\det \mathcal{R}_A(n))^{\frac{1}{n}}\right) ER(G).$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. Using the geometric-arithmetic mean inequality we obtain

$$\sum_{i=1}^{n} \frac{\lambda_i^2}{n-\lambda_i} \geq n \left(\prod_{i=1}^{n} \frac{\lambda_i^2}{n-\lambda_i}\right)^{\frac{1}{n}} = n|\det A|^{\frac{2}{n}} (\det \mathcal{R}_A(n))^{\frac{1}{n}}.$$

By the last inequality and inequalities (23) and (24), we obtain the required result. ■

Corollary 4.2. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}^2(G) \leq \frac{n^2\left(2m(2n-\lambda_1-\lambda_n)\det \mathcal{R}_A(n)^{\frac{1}{n}} - n|\det A|^{\frac{2}{n}}\right)}{(n-\lambda_1)(n-\lambda_n)(\det \mathcal{R}_A(n))^{\frac{1}{n}}}.$$

Equality holds if and if $G \cong \overline{K}_n$.

Proof. As it holds

$$\sum_{i=1}^{n} \lambda_i^2(n-\lambda_i) \geq n\left(\prod_{i=1}^{n} \lambda_i^2(n-\lambda_i)\right)^{\frac{1}{n}} = \frac{n|\det A|^{\frac{2}{n}}}{(\det \mathcal{R}_A(n))^{\frac{1}{n}}},$$

having in mind the inequalities (23) and (25), the required inequality is obtained. ■

Corollary 4.3. *Let G be a simple graph of order n with m edges. Then*

$$\frac{\mathcal{E}^2(G)}{ER(G)} + n^2(n-\lambda_1)(n-\lambda_n)(ER(G)-1) \leq 2m(2n-\lambda_1-\lambda_n), \tag{26}$$

with equality if and only if $G \cong \overline{K}_n$.

Proof. Relation (10) and inequalities (23) and (24) imply the required inequality.

Equality is attained if and only if equalities hold in both (23) and (24). By Lemma 2.2, equality in (23) holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_n$ or $\lambda_1 = \lambda_2 = \cdots = \lambda_k \geq \lambda_{k+1} = \cdots = \lambda_n$, for some k, $1 \leq k \leq n-1$, implying that $G \cong \overline{K}_n$ or $G \cong kK_s$ for some k and s, $1 \leq k \leq n-1$, such that $n = ks$. Since equality in (24) is attained if and only if $|\lambda_1|(n-\lambda_1) = |\lambda_2|(n-\lambda_2) = \cdots = |\lambda_n|(n-\lambda_n)$, it is easily concluded that equality holds in (26) if and only if G is an empty graph. ■

Corollary 4.4. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}(G) \leq n^2\sqrt{ER(G)-1}, \tag{27}$$

with equality if and only if $G \cong \overline{K}_n$.

Proof. The inequality (27) follows directly from (10) and (25). Equality in (27) holds if and only if $\frac{|\lambda_1|}{n-\lambda_1} = \frac{|\lambda_2|}{n-\lambda_2} = \cdots = \frac{|\lambda_n|}{n-\lambda_n}$, wherefrom it is easily concluded that $\lambda_1 = \lambda_2 = \cdots = \lambda_n$, i.e., G is an empty graph. ■

Remark 4.1. *Let G be unicyclic and bipartite graph of order n. Bearing in mind that for unicyclic graph holds $m = n$, using the inequality (27) and*

$$ER(G) \leq 1 + \frac{2m}{n(n^2-m)}, \tag{28}$$

from [18] we get the upper bound

$$\mathcal{E}(G) \leq \sqrt{\frac{2n^3}{n-1}}, \tag{29}$$

which is stronger than the upper bound (3) from [20] in the case of unicylic graphs.

Theorem 4.2. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}^4(G) \leq \frac{n^2 m^2 (2n - \lambda_1 - \lambda_n)^2 ER(G)}{(n - \lambda_1)(n - \lambda_n)}. \tag{30}$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. For $p_i = \dfrac{\lambda_i^2}{2m}$, $a_i = n - \lambda_i$, $R = n - \lambda_n$, $r = n - \lambda_1$, $i = 1, 2, \ldots, n$, the inequality (3) transforms into

$$\sum_{i=1}^{n} \lambda_i^2 (n - \lambda_i) \sum_{i=1}^{n} \frac{\lambda_i^2}{n - \lambda_i} \leq \frac{m^2 (2n - \lambda_1 - \lambda_n)^2}{(n - \lambda_1)(n - \lambda_n)}. \tag{31}$$

Now, the inequalities (24),(25) and (31) imply the inequality (30).

Having in mind the cases of equality in relations (3),(24) and (25), it is easily obtained that equality in (30) is valid if and only if G is an empty graph. ■

Corollary 4.5. *Let G be a simple graph of order n with m edges. Then*

$$\mathcal{E}(G) \leq \frac{m(2n - \lambda_1 - \lambda_n)}{n} \sqrt{\frac{ER(G)}{(ER(G) - 1)(n - \lambda_1)(n - \lambda_n)}}, \tag{32}$$

with equality if and only if $G \cong \overline{K}_n$.

Proof. The proof follows from (10), (24) and (31). ■

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