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A note on the Laplacian resolvent energy, Kirchhoff index and their relations

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Abstract

Let G be a simple graph of order n and let L be its Laplacian matrix. Eigenvalues of the matrix L are denoted by $\mu_1, \mu_2, \cdots, \mu_n$ and it is assumed that $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$. The Laplacian resolvent energy and Kirchhoff index of the graph G are defined as $RL(G) = \sum_{i=1}^{n} \frac{1}{n+1-\mu_i}$ and $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$, respectively. In this paper, we derive some bounds on the invariant $RL(G)$ and establish a relation between $RL(G)$ and $Kf(G)$.

Keywords: Graph energy; Laplacian resolvent energy; Kirchhoff index.

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1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $|E(G)| = m$. Denote by $A(G)$ the adjacency matrix of G, and by $\lambda_1, \lambda_2, \cdots, \lambda_n$ its eigenvalues satisfying $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. The (ordinary) energy of the graph G is defined [7] as

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

Concept of graph energy has many applications, especially in chemistry. The most important properties of graph energy can be found in the monographs [11, 13] and in the references cited therein.

There are graph energies which are based on different matrices associated with graphs. One of them is the Laplacian resolvent energy. Before defining this energy, we need some basic definitions.

Let L be the Laplacian matrix of the graph G and $\mu_1, \mu_2, \cdots, \mu_n$ be its Laplacian eigenvalues satisfying $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$. The Laplacian resolvent matrix $\mathcal{R}_L(z)$ of the matrix L is defined as

$$\mathcal{R}_L(z) = (zI_n - L)^{-1}.$$

Since all the Laplacain eigenvalues satisfy the condition $\mu_i \le n$, $i = 1, 2, ..., n$, in the paper [3] it was proposed to choose $z = n + 1$. The Laplacian resolvent energy is defined [3] as

$$RL(G) = \sum_{i=1}^{n} \frac{1}{n+1-\mu_i}.$$

Some of the basic properties and various bounds of the Laplacian resolvent energy can be found in the papers [3, 14, 20, 21].

In the paper [17], Klein and Randić introduced the notion of resistance distance r_{ij} which is defined as the resistance between the nodes i and j in an electrical network corresponding to the graph G in which all edges are replaced by unit resistors. The Kirchhoff index is defined as

$$Kf(G) = \sum_{i<j} r_{ij}.$$

Gutman and Mohar in the paper [8] and Zhy *et al.* in the paper [25] independently proved that Kirchhoff index can be represented as

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

For some basic properties and various bounds of $Kf(G)$, see the monograph [9].

Now, we recall some analytic inequalities for real number sequences that are of interest for the subsequent considerations.

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Lemma 1.1. [15] *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 $p = (p_i)$, $i = 1, 2, \ldots, n$, be a sequence of positive real numbers. Then*

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

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

Lemma 1.2. [4] *Let $a_1 \geqslant a_2 \geqslant \cdots \geqslant a_n > 0$. Then*

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

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

Lemma 1.3. [4] *Let $0 < a_1 \leq \cdots \leq a_i \leq \cdots \leq a_k \leq \cdots \leq a_n$ and $p_1, p_2, ..., p_n$ be positive real numbers such that $p_1 + p_2 + \cdots + p_n = 1$ and $Q_i = p_1 + p_2 + \cdots + p_i, R_k = p_k + p_{k+1} + \cdots p_n$. Then*

$$\frac{p_1}{a_1} + \frac{p_2}{a_2} + \cdots + \frac{p_n}{a_n} - \frac{1}{p_1 a_1 + p_2 a_2 + \cdots + p_n a_n} \geqslant \frac{Q_i R_k (a_k - a_i)^2}{a_i a_k (Q_i a_i + R_k a_k)}, \tag{3}$$

with equality for

$$a_1 = a_2 = \cdots = a_i, a_k = a_{k+1} = \cdots = a_n, a_{i+1} = a_{i+2} = \cdots = a_{k-1} = \frac{Q_i a_i + R_k a_k}{Q_i + R_k}.$$

Lemma 1.4. [2, 15] *Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, n$, be two sequences of real numbers such that $a \leqslant a_i \leqslant A < +\infty$ and $b \leqslant b_i \leqslant B < +\infty$ for $i = 1, \ldots, n$ where $a, b, A, B \in \mathbb{R}$. Then*

$$n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \leqslant n^2 \alpha(n)(A - a)(B - b), \tag{4}$$

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 sign in (4) holds if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

Lemma 1.5. [12] *Let $a = (a_i)$, $i = 1, \ldots, n$, be a sequence of positive real numbers such that $0 < r \leq a_i \leq R < +\infty$ for $i = 1, \ldots, n$ where $r, R \in \mathbb{R}$. Then*

$$\sum_{i=1}^{n} a_i \sum_{i=1}^{n} \frac{1}{a_i} \leqslant \left(1 + \alpha(n) \left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}} \right)^2 \right) n^2, \tag{5}$$

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 sign in (5) holds if and only if $R = a_1 = a_2 = \cdots = a_n = r$ or $R = a_1 = a_2 = \cdots = a_k \geqslant a_{k+1} = \cdots = a_n = r$, for $k = \lfloor \frac{n}{2} \rfloor$.

Lemma 1.6. [15, 23] *Let $a = (a_i)$ and $p = (p_i)$, $i = 1, 2, \ldots, n$, be two sequences of positive real numbers such that $\sum_{i=1}^{n} p_i = 1$ and $0 < r \leq a_i \leq R < +\infty$ for $i = 1, \ldots, n$ where $r, R \in \mathbb{R}$. Then*

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \leqslant r + R, \tag{6}$$

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

Lemma 1.7. [18, 24] *Let $a_i \in \mathbb{R}^+, i = 1, \ldots, n$. Then*

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

Both Equality signs in (7) hold if and only if $a_1 = a_2 = \cdots = a_n$.

Lemma 1.8. [1, 22] *Let $x = (x_i)$ be a sequence of non-negative and $a = (a_i)$, $i = 1, 2, \ldots, n$, be a sequence of positive real numbers. Then, for any $r \geqslant 0$, it holds that*

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

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

Lemma 1.9. [5] *A graph has one eigenvalue if and only if its size is zero. A graph has two distinct eigenvalues λ_1 and λ_2, $\lambda_1 > \lambda_2$, with multiplicities m_1 and m_2, respectively, 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 1.1. [6] *A result similar to Lemma 1.9 holds for the graphs with at most two different Laplacian eigenvalues.*

2. Main results

In this section, we are present some new lower and upper bounds for $RL(G)$ in the terms of number of vertices n, number of edges m, $\det \mathcal{R}_L(n+1)$, the greatest and the second-smallest Laplacian eigenvalues μ_1 and μ_{n-1}, respectively.

2.1 Lower bounds

Theorem 2.1. *For $n \geq 3$, let G be a graph with n vertices. Then*

$$RL(G) \geqslant \frac{1}{n+1} + (n-1)\left((n+1)\det \mathcal{R}_L(n+1)\right)^{\frac{1}{n-1}}. \tag{9}$$

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

Proof. Taking $n := n-1$, $p_i = 1, a_i = b_i = \frac{1}{\sqrt{n+1-\mu_i}}, i = 1, 2, \ldots, n-1$ in (1) and using the right-hand side of (7), we get

$$\begin{aligned}
(n-1)\sum_{i=1}^{n-1}\frac{1}{n+1-\mu_i} &\geqslant \left(\sum_{i=1}^{n-1}\frac{1}{\sqrt{n+1-\mu_i}}\right)^2 \\
&\geqslant \sum_{i=1}^{n-1}\frac{1}{n+1-\mu_i} + (n-1)(n-2)\left(\prod_{i=1}^{n-1}\frac{1}{n+1-\mu_i}\right)^{\frac{1}{n-1}} \\
&= \sum_{i=1}^{n-1}\frac{1}{n+1-\mu_i} + (n-1)(n-2)((n+1)\det \mathcal{R}_L(n+1))^{\frac{1}{n-1}}
\end{aligned}$$

which is equivalent to

$$(n-2)\sum_{i=1}^{n-1}\frac{1}{n+1-\mu_i} \geqslant (n-1)(n-2)((n+1)\det \mathcal{R}_L(n+1))^{\frac{1}{n-1}},$$

and the proof follows for $n \geq 3$.
Equality holds if and only if

$$\frac{1}{\sqrt{n+1-\mu_1}} = \frac{1}{\sqrt{n+1-\mu_2}} = \cdots = \frac{1}{\sqrt{n+1-\mu_{n-1}}}$$

i.e., if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1} \geqslant \mu_n = 0$ and by Remark 1.1 this is equivalent to $G \cong \overline{K_n}$ or $G \cong K_n$. □

Theorem 2.2. *Let G be a graph with n vertices. Then*

$$RL(G) \geqslant \frac{1}{n+1} + (n-1)\left((n+1)\det \mathcal{R}_L(n+1)\right)^{\frac{1}{n-1}} + \frac{(\sqrt{n+1-\mu_1} - \sqrt{n+1-\mu_{n-1}})^2}{(n+1-\mu_1)(n+1-\mu_{n-1})}. \tag{10}$$

Equality holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$ or G has four distinct Laplacian eigenvalues, namely

$$\mu_1, \left(n+1-\sqrt{(n+1-\mu_1)(n+1-\mu_{n-1})}\right)^{n-3}, \mu_{n-1}, \mu_n,$$

where $n+1-\sqrt{(n+1-\mu_1)(n+1-\mu_{n-1})}$ has multiplicity $n-3$.

Proof. Using Inequality (2) for $n := n-1$, $a_i = \dfrac{1}{n+1-\mu_i}$, $i = 1, \ldots, n-1$, we get (10).

By Lemma 1.2 equality sign in (10) holds if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-2} = n+1-\sqrt{(n+1-\mu_1)(n+1-\mu_{n-1})}$. If $\mu_1 = \mu_{n-1}$, then we have $\mu_1 = \mu_2 = \cdots = \mu_{n-1} \geqslant \mu_n = 0$, and equality sign in (10) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$. If $\mu_1 \neq \mu_{n-1}$, then equality sign in (10) holds if and only if G has four distinct Laplacian eigenvalues, namely

$$\mu_1, \left(n+1-\sqrt{(n+1-\mu_1)(n+1-\mu_{n-1})}\right)^{n-3}, \mu_{n-1}, \mu_n,$$

where $n+1-\sqrt{(n+1-\mu_1)(n+1-\mu_{n-1})}$ has multiplicity $n-3$. □

Theorem 2.3. *Let G be a graph with n vertices and m edges. Then*

$$RL(G) \geqslant \frac{1}{n+1} + \frac{(n-1)^2}{n^2-1-2m} + \frac{(\mu_1-\mu_{n-1})^2}{(n+1-\mu_1)(n+1-\mu_{n-1})(2n+2-\mu_1-\mu_{n-1})}, \tag{11}$$

Equality holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$ or G has four distinct Laplacian eigenvalues, namely

$$\mu_1, \left(\frac{\mu_1+\mu_{n-1}}{2}\right)^{n-3}, \mu_{n-1}, \mu_n,$$

where $\dfrac{\mu_1+\mu_{n-1}}{2}$ has multiplicity $n-3$.

Proof. By Inequality (3) for $n := n-1$, $a_i = n+1-\mu_i, p_i = \dfrac{1}{n-1}, i = 1, \ldots, n-1, Q_1 = R_n = \dfrac{1}{n-1}$, we get (11).

From Lemma 1.3 we have that equality sign in (11) holds if and only if

$$\mu_2 = \mu_3 = \cdots = \mu_{n-2} = \frac{\mu_1+\mu_{n-1}}{2}.$$

If $\mu_1 = \mu_{n-1}$ then $\mu_1 = \mu_2 = \cdots \mu_{n-1} \geqslant \mu_n = 0$ and equality sign in (11) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$. If $\mu_1 \neq \mu_{n-1}$ then equality sign in (11) holds if and only G has four distinct Laplacian eigenvalues, namely

$$\mu_1, \left(\frac{\mu_1+\mu_{n-1}}{2}\right)^{n-3}, \mu_{n-1}, \mu_n,$$

where $\dfrac{\mu_1+\mu_{n-1}}{2}$ has multiplicity $n-3$. □

Theorem 2.4. [14] *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$RL(G) \geqslant \frac{1}{n+1} + \frac{(n-1)^2}{n^2-1-2m}. \tag{12}$$

Equality holds if and only if $G \cong K_n$.

Remark 2.1. *Inequality (11) is better than (12).*

2.2 Upper bounds

Theorem 2.5. *Let G be a graph with n vertices. Then*

$$RL(G) \leqslant \frac{1}{n+1} + (n-1)((n+1)\det \mathcal{R}_L(n+1))^{\frac{1}{n-1}} + (n-1)^2\alpha(n-1)\frac{(\sqrt{n+1-\mu_1}-\sqrt{n+1-\mu_{n-1}})^2}{(n+1-\mu_1)(n+1-\mu_{n-1})}, \tag{13}$$

where

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

Equality sign in (13) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$.

Proof. Using Inequality (4) and right-hand side of (7) for

$$n := n-1, a_i = b_i = \frac{1}{\sqrt{n+1-\mu_i}}, i = 1, \ldots, n-1, A = B = \frac{1}{\sqrt{n+1-\mu_1}}, a = b = \frac{1}{\sqrt{n+1-\mu_{n-1}}},$$

we get (13). Similarly as in the proof of Theorem 2.1, equality sign in (13) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$. □

Theorem 2.6. *Let G be a graph with n vertices. Then*

$$RL(G) \leqslant \frac{1}{n+1} + \frac{(n-1)^2}{n^2-1-2m}\left(1+\alpha(n-1)\frac{(\mu_1-\mu_{n-1})^2}{(n+1-\mu_1)(n+1-\mu_{n-1})}\right), \tag{14}$$

where

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

Equality sign in (14) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_n$.

Proof. In (5) letting

$$n := n-1, a_i = \frac{1}{n+1-\mu_i}, i = 1, \ldots, n-1, r = \frac{1}{n+1-\mu_{n-1}}, R = \frac{1}{n+1-\mu_1}$$

we get (14).
By Lemma 1.5, equality sign in (14) holds if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1} \geqslant \mu_n = 0$ i.e., if and only if $G \cong \overline{K}_n$ or $G \cong K_n$. $\square$

Theorem 2.7. *Let G be a graph with n vertices and m edges. Then*

$$RL(G) \leqslant \frac{1}{n+1} + \frac{2m+(n-1)(n+1-\mu_1-\mu_{n-1})}{(n+1-\mu_1)(n+1-\mu_{n-1})}, \tag{15}$$

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

Proof. Inequality (15) follows from (6) when

$$n := n-1, a_i = \frac{1}{n+1-\mu_i}, r = \frac{1}{n+1-\mu_{n-1}}, R = \frac{1}{n+1-\mu_1}, p_i = \frac{1}{n-1}, i = 1, 2, \ldots, n-1.$$

By Lemma 1.6, equality sign in (15) holds if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1} > \mu_n = 0$ i.e., if and only if $G \cong \overline{K}_n$ or $G \cong K_n$. $\square$

2.3 Relations between $RL(G)$ and $Kf(G)$

In the next theorem we establish a relationship between Laplacian resolvent energy and Kirchhoff index of a graph.

Theorem 2.8. *Let G be connected graph with n vertices. Then*

$$Kf(G) \geqslant \frac{n}{n+1} \cdot \frac{((n+1)RL(G)-1)^2(n+1-\mu_1)^2}{(n+1-\mu_1)^2(1-(n+1)RL(G))+(n+1)(n^2-1)}. \tag{16}$$

Equality holds if and only if $G \cong K_n$.

Proof. In Radon's inequality (8) for $r = 1$, $n := n-1$, $a_i = \dfrac{1}{\mu_i}$, $x_i = \dfrac{1}{n+1-\mu_i}$, $i = 1, 2, ..., n-1$, we get

$$\sum_{i=1}^{n-1} \frac{\mu_i}{(n+1-\mu_i)^2} \geqslant \frac{\left(RL(G)-\dfrac{1}{n+1}\right)^2}{\dfrac{1}{n} \cdot Kf(G)}.$$

Since

$$\begin{aligned}
\sum_{i=1}^{n-1} \frac{\mu_i}{(n+1-\mu_i)^2} &= \sum_{i=1}^{n-1} \frac{\mu_i}{(\mu_i-n-1)^2} \\
&= \sum_{i=1}^{n-1} \frac{1}{\mu_i-n-1} + \sum_{i=1}^{n-1} \frac{n+1}{(\mu_i-n-1)^2} \\
&= -RL(G) + \frac{1}{n+1} + (n+1)\sum_{i=1}^{n-1} \frac{1}{(\mu_i-n-1)^2},
\end{aligned}$$

and

$$\frac{1}{(n+1-\mu_i)^2} \leq \frac{1}{(n+1-\mu_1)^2}$$

for all $i = 1, 2, ..., n-1$, and hence we have that

$$\sum_{i=1}^{n-1} \frac{\mu_i}{(n+1-\mu_i)^2} \leq -RL(G) + \frac{1}{n+1} + (n+1) \cdot \frac{n-1}{(n+1-\mu_1)^2},$$

and the proof follows. Equality in (16) holds if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1} \geqslant \mu_n = 0$ i.e. if and only if $G \cong K_n$, since G is connected graph. □

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