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On Kirchhoff Index, Laplacian Energy and Their Relations

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Abstract

Let G be a simple connected graph with n vertices, m edges, a sequence of vertex degrees $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, and $\mathbf{D} = \operatorname{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. If $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ are the Laplacian eigenvalues of G, then the Kirchhoff index and Laplacian energy of G are defined as $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$ and $LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|$, respectively. In this paper we consider relation between Kf(G) and LE(G). Some new lower bounds for Kf(G) and LE(G) are also obtained.

1 Introduction

Let G = (V, E), $V = \{1, 2, ..., n\}$, be a simple connected graph with $n \ge 2$ vertices and m edges. If vertices i and j are adjacent, we write $i \sim j$. Denote by $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta > 0$, $d_i = d(i)$, a sequence of vertex degrees of G. Let \mathbf{A} be the adjacency matrix of G, and $\mathbf{D} = \text{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Eigenvalues of matrix \mathbf{L} , $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_{n-1} > \mu_n = 0$, form the so-called Laplacian spectrum of G.

In graph theory, an invariant is a property of graphs that depends only on the abstract structure, not on graph representations such as particular labellings or drawings of the graph. Such quantities are also called topological indices. Topological indices have gained

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considerable popularity in the mathematical chemistry literature in recent years. A large number of topological indices have been derived depending on vertex degrees. Among the oldest are the first and the second Zagreb index, M_1 and M_2 , defined as [15,16]

$$M_1 = M_1(G) = \sum_{i=1}^n d_i^2$$
 and $M_2 = M_2(G) = \sum_{i \sim j} d_i d_j$.

Details of the theory and applications of the two Zagreb indices can be found in surveys [4, 5, 18, 30] and in the references quoted therein.

Generalization of the second Zagreb index, reported in [2], known as general Randić index, R_{α} , is defined as

$$R_{\alpha} = R_{\alpha}(G) = \sum_{i \sim j} (d_i d_j)^{\alpha},$$

where α is an arbitrary real number. Here we are interested in two special cases, that is $\alpha = -1$ and $\alpha = 2$. The topological index R_{-1} is met in the literature under the names first-order overall index [3], modified second Zagreb index [30], and general Randić R_{-1} index [7]. The index R_2 is referred to as the second hyper Zagreb index [13].

A graph is said to be regular if all its vertices are of the same degree. Otherwise, it is an irregular. As the quantitative topological characterization of irregularity of graphs Albertson [1] proposed a measure defined as

$$Alb = Alb(G) = \sum_{i \sim j} |d_i - d_j|,$$

which is usually referred to as the Albertson index (see [20]) although the name "third Zagreb index" has also been proposed [14].

Here we are also interested in another irregularity measure which is defined as (see [38])

$$IRLF = IRLF(G) = \sum_{i \sim j} \frac{|d_i - d_j|}{\sqrt{d_i d_j}}.$$

In [22], Klein and Randić introduced the notion of resistance distance, r_{ij} . It 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 sum of resistance distances of all pairs of vertices of a graph *G* is named as the Kirchhoff index, i.e.

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

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As Gutman and Mohar [17] proved, the Kirchhoff index has the following connection with the Laplacian eigenvalues

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

For its basic mathematical properties, including various lower and upper bounds, see [9,24–27,31–33].

The Laplacian energy of a graph, LE, was defined in [19] as

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

In [23] Laplacian–energy–like invariant, LEL, was defined as

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

Since Kf(G), LE(G) and LEL(G) are all spectrum-based invariants of graph, it is interesting to find out their relationship. A number of relations between Kf(G) and LEL(G) as well as LEL(G) and LE(G) have been reported in the literature, see for example [11, 12, 21, 28, 34, 35]. However, to the best of our knowledge, relations between Kf(G) and LE(G) have not been studied so far.

The rest of the paper is organized as follows. In Section 2 we give some results reported in the literature that will be used throughout the paper. In Section 3.1 we prove some inequalities that establish relations between Kirchhoff index and Laplacian energy of a graph. The new lower bounds for Kf(G) depending on the structural graph parameters and some of the above mentioned vertex-degree-based indices are presented in Section 3.2. At the end of the section we give a conjecture with the upper bound for R_{-1} that depends solely on n and m. We believe that it is the best possible in its class. We perform a number of testing to find counterexample(s), but we couldn't. However, we were not able to prove it explicitly. Under this assumption, the lower bound for Kf(G) obtained in this paper that depends on n, m and R_{-1} is the best possible in its class. Finally, in Section 3.3 we give some new lower bounds for the LE(G).

2 Preliminaries

In this section we recall some results for lower bounds of Kf(G) and LE(G) reported in the literature and some analytic inequalities for real number sequences that will be used subsequently. Before we proceed, let us define one special class of *d*-regular graphs Γ_d [33].

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Let N(i) be the set of all neighborhoods of the vertex i, i.e. $N(i) = \{k \mid k \in V, k \sim i\}$, and d(i, j) the distance between vertices i and j. Denote by Γ_d a set of all d-regular graphs, $1 \leq d \leq n-1$, with the properties that diameter is D = 2 and $|N(i) \cap N(j)| = d$ for $i \nsim j$.

In [40] the following lower bound for Kf(G) was established

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

Equality holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

In [25] (see also [26]) it was proven that

$$Kf(G) \ge \frac{n^2(n-1) - 2m}{2m},$$
 (2)

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

In [26] (see also [27]) the following bound was reported

$$Kf(G) \ge -1 + 2(n-1)R_{-1},$$
(3)

with equality holding if and only if $G \cong K_n$, or $G \in \Gamma_d$.

The following lower bound for the Laplacian energy of simple connected graphs was proven in [10]

$$LE(G) \ge 2 + \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right|.$$
 (4)

For the bipartite graphs in [39] it was shown that

$$LE(G) \ge \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right| \,. \tag{5}$$

Let $x = (x_i)$ and $a = (a_i)$, i = 1, 2, ..., n, be two positive real number sequences. In [36] it was proven that for any $r \ge 0$,

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^r}.$$
(6)

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

Let $a = (a_i), i = 1, 2, ..., n$, be a positive real number sequence. Then, for any real r, $r \leq 0$ or $r \geq 1$, holds (see e.g. [29])

$$\sum_{i=1}^{n} a_i^r \ge n^{1-r} \left(\sum_{i=1}^{n} a_i\right)^r.$$
(7)

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Equality holds if and only if $a_1 = a_2 = \cdots = a_n$. If $0 \le r \le 1$, then the sense of (7) reverses.

Let $p = (p_i)$ and $a = (a_i)$, i = 1, 2, ..., n, be two positive real number sequences with the properties $p_1 + p_2 + \cdots + p_n = 1$ and $0 < r \le a_i \le R < +\infty$. In [37] the following inequality was proven

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \le r + R.$$
(8)

Denote by $p = (p_i)$ and $a = (a_i)$, i = 1, 2, ..., n, real number sequences with the properties $p_i \ge 0$, $p_1 + p_2 + \cdots + p_n = 1$ and $r \le a_i \le R$. For such sequences the following inequalities are valid [8]:

$$0 \le \sum_{i=1}^{n} p_i a_i^2 - \left(\sum_{i=1}^{n} p_i a_i\right)^2 \le \frac{1}{2} (R-r) \sum_{i=1}^{n} p_i \left| a_i - \sum_{j=1}^{n} p_j a_j \right|.$$
(9)

3 Main results

3.1 Relation between Kirchhoff index and Laplacian energy

In the following theorem we determine relation between Kirchhoff index and Laplacian energy of a graph.

Theorem 1. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then for any real k such that $\mu_{n-1} \ge k > 0$, holds

$$\left(\left(n+k-\frac{4m}{n}\right)(M_1+2m)-2nkm+\frac{8m^3}{n^2}\right)Kf(G) \ge n\left(LE(G)-\frac{2m}{n}\right)^2.$$
 (10)

Equality holds if k = n and $G \cong K_n$.

Proof. For r = 1, n := n - 1, $x_i := \left| \mu_i - \frac{2m}{n} \right|$, $a_i := \frac{1}{\mu_i}$, $i = 1, 2, \dots, n - 1$, the inequality (6) becomes

$$\sum_{i=1}^{n-1} \mu_i \left| \mu_i - \frac{2m}{n} \right|^2 \ge \frac{\left(\sum_{i=1}^{n-1} \left| \mu_i - \frac{2m}{n} \right| \right)^2}{\sum_{i=1}^{n-1} \frac{1}{\mu_i}},$$

that is

$$\sum_{i=1}^{n-1} \mu_i \left| \mu_i - \frac{2m}{n} \right|^2 \ge \frac{n \left(LE(G) - \frac{2m}{n} \right)^2}{Kf(G)}.$$
(11)

For n := n - 1, $p_i := \frac{\mu_i^2}{M_1 + 2m}$, $a_i := \mu_i$, $r = \mu_{n-1}$, $R = \mu_1$, i = 1, 2, ..., n - 1, the inequality (8) transforms into

$$\sum_{i=1}^{n-1} \mu_i^3 + \mu_1 \mu_{n-1} \sum_{i=1}^{n-1} \mu_i \le (\mu_1 + \mu_{n-1})(M_1 + 2m),$$

i.e.

$$\sum_{i=1}^{n-1} \mu_i^3 \le (\mu_1 + \mu_{n-1})(M_1 + 2m) - 2m\mu_1\mu_{n-1}.$$
(12)

Consider the function

$$f(x) = (x + \mu_{n-1})(M_1 + 2m) - 2xm\mu_{n-1}.$$

This is an increasing function. Hence, for $x = \mu_1 \leq n$ holds $f(x) = f(\mu_1) \leq f(n)$. From (12) we get

$$\sum_{i=1}^{n-1} \mu_i^3 \le (n+\mu_{n-1})(M_1+2m) - 2nm\mu_{n-1}.$$
(13)

Since the function

$$g(x) = (n+x)(M_1 + 2m) - 2nmx$$

is decreasing, for $x = \mu_{n-1} \ge k > 0$ holds $g(x) = g(\mu_{n-1}) \le g(k)$. Therefore from (13) follows

$$\sum_{i=1}^{n-1} \mu_i^3 \le (n+k)(M_1+2m) - 2nmk.$$
(14)

On the other hand, the following identity is valid

$$\sum_{i=1}^{n-1} \mu_i \left| \mu_i - \frac{2m}{n} \right|^2 = \sum_{i=1}^{n-1} \mu_i^3 - \frac{4m}{n} \sum_{i=1}^{n-1} \mu_i^2 + \frac{4m^2}{n^2} \sum_{i=1}^{n-1} \mu_i$$

$$= \sum_{i=1}^{n-1} \mu_i^3 - \frac{4m}{n} (M_1 + 2m) + \frac{8m^3}{n^2}.$$
(15)

The inequality (10) is obtained according to inequalities (14) and (11) and equality (15).

Corollary 1. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then

$$\left(M_1 + 2m - \frac{4m^2(n+1)}{n^2}\right) Kf(G) \ge \left(LE(G) - \frac{2m}{n}\right)^2.$$
 (16)

Equality holds if $G \cong K_n$.

Proof. Since $\mu_1 \leq n$, it follows

$$\sum_{i=1}^{n-1} \mu_i \left| \mu_i - \frac{2m}{n} \right|^2 \le n \sum_{i=1}^{n-1} \left| \mu_i - \frac{2m}{n} \right|^2 = n \left(M_1 + 2m - \frac{4m^2(n+1)}{n^2} \right).$$

From the above and (11) we arrive at (16).

Corollary 2. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then

$$\left(\frac{2m^2}{n-1} + mn - \frac{4m^2(n+1)}{n^2}\right) Kf(G) \ge \left(LE(G) - \frac{2m}{n}\right)^2.$$
 (17)

Equality holds if $G \cong K_n$.

Proof. The inequality (17) is obtained according to (16) and inequality

$$M_1 \le m\left(\frac{2m}{n-1} + n - 2\right),$$

which was proven in [6].

3.2 Some new lower bounds for Kf(G)

In the following theorem we establish lower bound for Kf(G) in terms of structural graph parameters n, m, and topological index R_{-1} .

Theorem 2. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{n^2(n-1)-m}{m} - 2(n-1)R_{-1}.$$
 (18)

Equality holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

Proof. The following equalities hold

$$\sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) = \sum_{i \sim j} \left(\frac{d_i + d_j}{d_i d_j} \right)^2 - \sum_{i \sim j} \frac{2}{d_i d_j} = \sum_{i \sim j} \left(\frac{d_i + d_j}{d_i d_j} \right)^2 - 2R_{-1}.$$
 (19)

For r = 2, $a_i := \frac{d_i + d_j}{d_i d_j}$, where the summation is performed over all edges of graph G, the inequality (7) becomes

$$\sum_{i \sim j} \left(\frac{d_i + d_j}{d_i d_j}\right)^2 \ge m^{-1} \left(\sum_{i \sim j} \frac{d_i + d_j}{d_i d_j}\right)^2 = \frac{n^2}{m}.$$
(20)

According to (19) and (20) follows

$$\sum_{i=1}^{n} \frac{1}{d_i} \ge \frac{n^2}{m} - 2R_{-1}.$$
(21)

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From the inequalities (1) and (21) we get

$$Kf(G) \ge -1 + (n-1)\left(\frac{n^2}{m} - 2R_{-1}\right),$$

wherefrom (18) is obtained.

Equality in (20) holds if and only if for any two pairs of adjacent vertices $i \sim j$ and $u \sim v$, i.e. for any two edges of graph G holds

$$\frac{1}{d_i} + \frac{1}{d_j} = \frac{1}{d_u} + \frac{1}{d_v}.$$

Let j and u be two vertices that are adjacent to vertex i. From the last equality we have that $d_j = d_u$. Since G is connected, equality in (20) holds if and only if G is regular or semiregular bipartite graph. Equality in (1) is attained if and only if $G \cong K_n$, or $G \cong K_{r,n-r}, 1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$. This means that equality in (18) holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}, 1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

Remark 1. According to (3) and (18) follows

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

where from we obtain (2).

Remark 2. The inequality (18) is stronger than the inequality (3), for example, when $G \cong P_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$. We could not find any connected graph for which the inequality (3) is stronger than the inequality (18). However, it is an open question whether the inequality (18) is always stronger than the inequality (3).

Remark 3. Let G be a connected d-regular graph, $1 \le d \le n-1$. According to (18) follows

$$Kf(G) \ge \frac{n(n-1)-d}{d},$$

with equality holding if and only if $G \in \Gamma_d$. This inequality was proven in [31].

In the following theorem we determine lower bound for Kf(G) in terms of parameters n, m, and topological indices M_2 and IRLF.

Theorem 3. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{n^2(n-1)-2m}{2m} + \frac{(n-1)(IRLF)^2}{2M_2}.$$
 (22)

Equality holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

Proof. The following identity holds

$$\sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i \sim j} \left(\frac{d_i - d_j}{d_i d_j}\right)^2 + \sum_{i \sim j} \frac{2}{d_i d_j} = \sum_{i \sim j} \left(\frac{d_i - d_j}{d_i d_j}\right)^2 + 2R_{-1}.$$
 (23)

For r = 1, $x_i := \frac{|d_i - d_j|}{\sqrt{d_i d_j}}$, $a_i := d_i d_j$, where the summation is performed over all edges of graph G, the inequality (6) transforms into

$$\sum_{i \sim j} \frac{\left(\frac{|d_i - d_j|}{\sqrt{d_i d_j}}\right)^2}{d_i d_j} \ge \frac{\left(\sum_{i \sim j} \frac{|d_i - d_j|}{\sqrt{d_i d_j}}\right)^2}{\sum_{i \sim j} d_i d_j} = \frac{(IRLF)^2}{M_2}.$$
(24)

From (23) and (24) follows

$$\sum_{i=1}^n \frac{1}{d_i} \geq \frac{(IRLF)^2}{M_2} + 2R_{-1}.$$

From the above and (21) we get

$$\sum_{i=1}^{n} \frac{1}{d_i} \ge \frac{n^2}{2m} + \frac{(IRLF)^2}{2M_2}.$$

The inequality (22) is obtained from the above and inequality (1).

Equality in (24) holds if and only if for any two pairs of adjacent vertices $i \sim j$ and $u \sim v$ holds

$$\frac{|d_i - d_j|}{(d_i d_j)^{3/2}} = \frac{|d_u - d_v|}{(d_u d_v)^{3/2}}.$$

Let j and u be two vertices that are adjacent to vertex i. Then

$$\frac{d_i - d_j|}{d_i^{3/2}} = \frac{|d_i - d_u|}{d_u^{3/2}}.$$
(25)

Equality in (21) holds if and only if $d_j = d_u$. In that case in (25) equality is attained, also. Together, the equalities in (24) and (21) hold if and only if G is regular or semiregular bipartite graph. Equality in (1) is attained if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$, therefore equality in (22) holds under the same conditions.

Remark 4. Since

$$\frac{(n-1)(IRLF)^2}{2M_2}\geq 0,$$

the inequality (22) is stronger than (2).

By the similar arguments as in case of Theorem 3, the following result can be proved.

Theorem 4. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{n^2(n-1) - 2m}{2m} + \frac{(n-1)(Alb)^2}{2R_2}.$$
 (26)

Equality holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

Remark 5. Since

$$\frac{(n-1)(Alb)^2}{2R_2} \ge 0.$$

the inequality (26) is stronger than (2).

Since $2R_2 \leq n(n-1)^5$ (see [16]), we have the following corollary of Theorem 4.

Corollary 3. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{n^2(n-1) - 2m}{2m} + \frac{(Alb)^2}{n(n-1)^4}.$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

As we have adduced in Remark 2, even by exhaustive testing we couldn't find a graph for which the inequality (3) is stronger than (18), however we could not explicitly prove that. Having this in mind, we give the following conjecture for the equivalent problem.

Conjecture 1. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$R_{-1} \le \frac{n^2}{4m} \le \frac{n^2}{4(n-1)}.$$

3.3 Some new lower bounds for the Laplacian energy of a graph

In the next theorem we establish lower bound for LE(G) in terms of parameters n, m, Δ, δ and the first Zagreb index.

Theorem 5. Let G be a simple connected graph with $n \ge 2$ vertices and m edges, with the property $\Delta \neq \delta$. Then

$$LE(G) \ge 2 + \frac{2(nM_1 - 4m^2)}{n(\Delta - \delta)}$$

Proof. For $p_i = \frac{1}{n}$, $a_i = d_i$, $r = \delta$, $R = \Delta$, i = 1, 2, ..., n, the inequality (9) becomes

$$\frac{1}{n}\sum_{i=1}^{n}d_{i}^{2} - \left(\frac{1}{n}\sum_{i=1}^{n}d_{i}\right)^{2} \leq \frac{1}{2n}(\Delta-\delta)\sum_{i=1}^{n}\left|d_{i} - \frac{1}{n}\sum_{j+1}^{n}d_{j}\right|,$$

that is

$$nM_1 - 4m^2 \le \frac{n}{2}(\Delta - \delta) \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right|.$$
 (27)

Bearing in mind (4) and (27) we have that

$$nM_1 - 4m^2 \le \frac{n}{2}(\Delta - \delta)(LE(G) - 2).$$

Since $\Delta \neq \delta$, from the above follows the required result.

In the case of bipartite graphs, by a similar procedure, according to (5) and (27), the following result can be proved.

Theorem 6. Let G be a simple bipartite graph with $n \ge 2$ vertices and m edges, with $\Delta \neq \delta$. Then

$$LE(G) \ge \frac{2(nM_1 - 4m^2)}{n(\Delta - \delta)}.$$

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