Filomat 29:8 (2015), 1869–1877
DOI 10.2298/FIL1508869M

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

On Kirchhoff and Degree Kirchhoff Indices

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Abstract. Let G be an undirected connected graph with n vertices and m edges. If $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ and $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$ are the Laplacian and the normalized Laplacian eigenvalues of G, then the Kirchhoff and the degree Kirchhoff indices obey the relations $Kf(G) = n \sum_{i=1}^{n-1} 1/\mu_i$ and $DKf(G) = 2m \sum_{i=1}^{n-1} 1/\rho_i$, respectively. Upper bounds for $Kf(G)$ and $DKf(G)$ are obtained.

1. Introduction

In 1993 Klein and Randić [15] introduced a new distance function, named resistance distance, based on the theory of electrical networks. They viewed the graph G as an electrical network N by replacing each edge of G with a unit resistor. The resistance distance between the vertices u and v of the graph G, denoted by $R(u,v) = R(u,v|G)$, is then defined to be the effective resistance between the nodes u and v in N. Similar to the long recognized shortest–path distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical properties, but also with a substantial potential for chemical applications.

The Wiener index is the sum of ordinary distances between all pairs of vertices of a (connected) graph; for details and further references see [26]. The *Kirchhoff index* is defined in analogy to the Wiener index as [4, 15]:

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} R(u,v|G) \, .$$

In 2007 a closely related graph invariant, named *degree Kirchhoff index*, was put forward by Chen and Zhang [5], defined as

$$DKf(G) = \sum_{\{u,v\} \subseteq V(G)} d_u \, d_v \, R(u,v|G)$$

where d_v is the degree of the vertex v.

2010 *Mathematics Subject Classification*. Primary 05C12; Secondary 05C50
Keywords. Distance (in graph), Resistance distance (in graph), Kirchhoff index, Degree Kirchhoff index, Laplacian spectrum (of graph).
Received: 06 November 2013; Accepted: 12 April 2014
Communicated by Francesco Belardo
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The graph invariants Kf and DKf are currently much studied in the mathematical and mathematico–chemical literature; see the recent papers [2, 8, 11, 12, 17, 25] and [10, 14, 21], and the references cited therein.

Denote by $\mathbf{A}$ the adjacency matrix of the (connected) (n, m)-graph G, and by $\mathbf{D}$ the diagonal matrix of its vertex degrees. Then $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix of the G. Let the eigenvalues of $\mathbf{L}$ be $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$.

A long time known result for the Kirchhoff index is [13]:

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

The transition matrix $\mathbf{P}$ of connected graph G is defined as [3, 22, 23]

$$\mathbf{P} = \mathbf{D}^{-1}\mathbf{A} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{L}.$$

Its eigenvalues are $1 = \bar{\mu}_1(P) > \bar{\mu}_2(P) \geq \ldots \geq \bar{\mu}_n(P) \geq -1$.

Because the graph G is assumed to be connected, it has no isolated vertices and therefore the matrix $\mathbf{D}^{-1/2}$ is well–defined. Then $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$ is the normalized Laplacian matrix of the graph G. Its eigenvalues are $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$. For details on the spectral theory of the normalized Laplacian matrix see [6]. A remarkable analogy between the Kirchhoff and degree Kirchhoff indices is the formula [5]:

$$DKf(G) = 2m \sum_{i=1}^{n-1} \frac{1}{\rho_i} .$$

In earlier works [3, 8, 16, 20, 27, 29, 30], several bounds for the Kirchhoff index were reported. These depend on usual structural parameters (number of vertices, number of edges, vertex degrees, and similar). The bounds offered in the present work are of different nature: they reveal connections between the resistance-distance-based Kirchhoff index and the extremal (greatest, second-greatest, and smallest non-zero) Laplacian eigenvalues. For this reason, our bounds have not been designed to "compete with" or "outperform in accuracy" the previous ones. Neither is the purpose of our bounds to gain (approximate) numerical values of Kf of particular graphs, since their exact values are easily obtainable by direct calculation.

2. Preliminaries

In this section we recall some results from spectral graph theory, and state a few analytical inequalities needed for our work.

Let G be undirected, connected graph with n vertices and m edges and let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n > 0$ be the sequence of vertex degrees of G.

Lemma 2.1. [18] *Let G be a graph of order n with at least one edge. Then* $\mu_1 \geq \Delta + 1$. *Moreover, if G is connected, then the equality* $\mu_1 = \Delta + 1$ *holds if and only if* $\Delta = n - 1$.

Lemma 2.2. [16] *Let G be a graph of order n. Then* $\mu_1 \leq n$, *with equality holding if and only if* $\bar{G}$ *is disconnected, where* $\bar{G}$ *stands for the complement of G.*

Lemma 2.3. [7, 18] *Let G be a simple graph of order n. Then* $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$ *holds if and only if* $G \cong K_n$ *or* $G \cong \bar{K}_n$.

Lemma 2.4. [7, 18, 28] *Let G be a connected graph on n vertices. Then* $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$ *if and only if* $G \cong K_{1,n-1}$ *or* $G \cong K_n$ *or* $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Lemma 2.5. [6] *Let G be a graph of order n. Then* $\rho_1 \geq n/(n-1)$.

Lemma 2.6. *Let*

$$\alpha(n-1) := \frac{1}{n-1}\left\lfloor \frac{n-1}{2} \right\rfloor\left(1-\frac{1}{n-1}\left\lfloor \frac{n-1}{2} \right\rfloor\right). \tag{1}$$

Then $\alpha(n-1) \le 1/4$ holds for each natural number n , $n \ge 3$. Equality holds if and only if n is odd.

Proof. Lemma 2.6 is obtained from the inequality between arithmetic and geometric means. ∎

Lemma 2.7. [1]. *Let $p_1, p_2, \dots, p_n$ and $a_1, a_2, \dots, a_n$ be non-negative real numbers for which there exist real constants r and R so that $0 < r \le a_i \le R < +\infty$, $i = 1, 2, \dots, n$. In addition, let S be a subset of $I = \{1, 2, \dots, n\}$ that minimizes the expression*

$$\left| \sum_{i\in S} p_i - \frac{1}{2}\sum_{i=1}^{n} p_i \right| . \tag{2}$$

Then

$$\left(\sum_{i=1}^{n} p_i\, a_i\right)\left(\sum_{i=1}^{n} \frac{p_i}{a_i}\right) - \left(\sum_{i=1}^{n} p_i\right)^2 \le \frac{(R-r)^2}{rR}\sum_{i\in S} p_i\left(\sum_{i=1}^{n} p_i - \sum_{i\in S} p_i\right). \tag{3}$$

Lemma 2.8. [19, 24] *Let $p_1, p_2, \dots, p_n$ be non-negative real numbers with the property $\sum\limits_{i=1}^{n} p_i = 1$. Further, let $a_1, a_2, \dots, a_n$ be real numbers for which there exist real constants r and R so that for each i , $i = 1, 2, \dots, n$, the inequalities $0 < r \le a_i \le R < +\infty$ hold. Then*

$$\sum_{i=1}^{n} p_i\, a_i + rM \sum_{i=1}^{n} \frac{p_i}{a_i} \le r + R\,. \tag{4}$$

Equality in (4) is attained if and only if $a_1 = a_2 = \dots = a_k = R$ and $a_{k+1} = a_{k+2} = \dots = a_n = r$ for some k , $1 \le k \le n$.

The complete split graph $CS(n, k)$, $1 \le k \le n-1$, is a graph on n vertices consisting of a clique on k vertices and a stable set on the remaining $n-k$ vertices, in which each vertex of the clique is adjacent to each vertex of the stable set. Thus, $CS(n, k)$ has $\frac{1}{2}\,k(k-1) + (n-k)k = nk - \frac{1}{2}\,k(k+1)$ edges.

Note that the complete graph K_n and the star $K_{1,n-1}$ are complete split graphs for $k = n-1$, and $k = 1$, respectively.

Lemma 2.9. [9] *The Laplacian spectrum of $CS(n, k)$, $1 \le k \le n-1$, satisfies the conditions: $\mu_1 = \dots = \mu_k = n$ and $\mu_{k+1} = \dots = \mu_{n-1} = k$, i.e.,*

$$\mathrm{Spec}(CS(n, k)) = \{\underbrace{n, n, \dots, n}_{k-\text{times}}\,,\ \underbrace{k, k, \dots, k}_{(n-k-1)-\text{times}}\,,\ 0\}\,.$$

This spectrum is unique to $CS(n, k)$.

Lemma 2.10. [18, 28] *The Laplacian spectrum of the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ is*

$$\mathrm{Spec}(K_{\frac{n}{2},\frac{n}{2}}) = \{n\ ,\ \underbrace{n/2, n/2, \dots, n/2}_{(n-2)-\text{times}}\ , 0\}\,.$$

This spectrum is unique to $K_{\frac{n}{2},\frac{n}{2}}$.

Proposition 2.11. [23] *Let G be a connected d-regular graph with n vertices and m edges, then*

$$Kf(G) \leq \frac{n(n-1)}{d(1-\mu_2(P))} \tag{5}$$

Proposition 2.12. [3] *For any simple connected graph G*

$$KF(G) \leq \frac{n}{d_n}\left(\frac{n-k-2}{1-\mu_2(P)} + \frac{k}{2} + \frac{1}{\theta}\right), \tag{6}$$

where $k = \left\lfloor \frac{\mu_2(P)(n-1)+1}{\mu_2(P)+1} \right\rfloor$ *and* $\theta = \mu_2(P)(n-k-2) - k + 2$.

3. Main Results

3.1. On Kirchhoff index

We now obtain an upper bound for $Kf(G)$ in terms of the parameters n, m, μ_1, and μ_{n-1}.

Theorem 3.1. *Let G be an undirected connected graph with* n, $n \geq 3$, *vertices and m edges. Then*

$$Kf(G) \leq \frac{n(n-1)^2}{2m}\left(1 + \frac{(\mu_1 - \mu_{n-1})^2}{\mu_1\,\mu_{n-1}}\,\alpha(n-1)\right) \tag{7}$$

where $\alpha(n-1)$ *is given by Eq. (1). Equality in (7) holds if and only if* $G \cong K_n$.

Proof. Let $n := n-1$, $p_i := 1$, $i = 1, 2, \ldots, n-1$, and $S = \{1, 2, \ldots, k\}$, $1 \leq k \leq n-1$. Then the minimum in (2) is reached for $k = \left\lfloor \frac{n-1}{2} \right\rfloor$. Therefore $S = \{1, 2, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor\}$. Now for $n := n-1$, $p_i := 1$, $a_i := \mu_i$, $i = 1, 2, \ldots, n-1$, $R := \mu_1$, $r := \mu_{n-1}$ and $S = \{1, 2, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor\}$, inequality (3) becomes

$$\left(\sum_{i=1}^{n-1} \mu_i\right)\left(\sum_{i=1}^{n-1} \frac{1}{\mu_i}\right) - (n-1)^2 \leq \frac{(\mu_1 - \mu_{n-1})^2}{\mu_1\,\mu_{n-1}} \left\lfloor \frac{n-1}{2} \right\rfloor \left((n-1) - \left\lfloor \frac{n-1}{2} \right\rfloor\right). \tag{8}$$

Since $\sum_{i=1}^{n-1} \mu_i = 2m$ and $\left\lfloor \frac{n-1}{2} \right\rfloor \left(n - 1 - \left\lfloor \frac{n-1}{2} \right\rfloor\right) = (n-1)^2\,\alpha(n-1)$, inequality (8) becomes

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i} \leq \frac{(n-1)^2}{2m} + \frac{(n-1)^2}{2m}\frac{(\mu_1 - \mu_{n-1})^2}{\mu_1\,\mu_{n-1}}\,\alpha(n-1)\,.$$

By multiplying the above inequality with n, we obtain (7). Equality in (7) holds if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$. Since G is connected, according to Lemma 2.3, equality in (7) holds if and only if $G \cong K_n$. ■

Corollary 3.2. *Let G be an undirected connected graph with* n, $n \geq 3$, *vertices and m edges. Then*

$$Kf(G) \leq \frac{n(n-1)^2}{8m}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2. \tag{9}$$

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

Proof. Inequality (9) is obtained from inequality (7) and Lemma 2.6. ■

Our next result is an upper bound for $Kf(G)$ in terms of n, m, Δ, μ_2, and μ_{n-1}.

Theorem 3.3. *Let G be undirected connected graph with n , n ≥ 4, vertices and m edges. Then*

$$Kf(G) \leq \frac{n}{1+\Delta} + \frac{n(n-2)^2}{2m-n}\left(1 + \frac{(\mu_2-\mu_{n-1})^2}{\mu_2\,\mu_{n-1}}\,\alpha(n-2)\right). \tag{10}$$

Equality holds if and only if $G \cong K_n$ *or* $G \cong K_{1,n-1}$.

Proof. For $n := n-1$ and $p_i := 1$, $i = 2,3,\dots,n-1$, according to Lemma 2.7,

$$\left(\sum_{i=2}^{n-1} a_i\right)\left(\sum_{i=2}^{n-1}\frac{1}{a_i}\right) - (n-2)^2 \leq \frac{(R-r)^2}{mM}\left\lfloor\frac{n-2}{2}\right\rfloor\left((n-2) - \left\lfloor\frac{n-2}{2}\right\rfloor\right).$$

For $a_i := \mu_i$, $i = 2,3,\dots,n-1$, $R = \mu_2$, and $r = \mu_{n-1}$, the above inequality becomes

$$\sum_{i=2}^{n-1}\frac{1}{\mu_i} \leq \frac{(n-2)^2}{2m-\mu_1} + \frac{(n-2)^2}{2m-\mu_1}\frac{(\mu_2-\mu_{n-1})^2}{\mu_2\,\mu_{n-1}}\,\alpha(n-2)\,.$$

Accordingly, we have that

$$\begin{aligned} Kf(G) &= \sum_{i=1}^{n-1}\frac{n}{\mu_i} = \frac{n}{\mu_1} + \sum_{i=2}^{n-1}\frac{n}{\mu_i} \\ &\leq \frac{n}{\mu_1} + \frac{(n-2)^2}{2m-\mu_1}\left(1 + \frac{(\mu_2-\mu_{n-1})^2}{\mu_2\,\mu_{n-1}}\,\alpha(n-2)\right). \end{aligned}$$

Since by Lemma 2.1, $\mu_1 \geq \Delta + 1$, i.e., $\frac{1}{\mu_1} \leq \frac{1}{\Delta+1}$, whereas by Lemma 2.2, $\mu_1 \leq n$, i.e., $\frac{1}{2m-\mu_1} \leq \frac{1}{2m-n}$, from the above inequality, (10) follows.

Since the graph G is connected, by Lemma 2.1, if $\mu_1 = 1 + \Delta$, then $\Delta = n-1$, i.e., $\mu_1 = n$. Equality in (10) holds if and only if $\mu_1 = n$ and $\mu_2 = \mu_3 \cdots = \mu_{n-1}$. Then by Lemmas 2.4, 2.9, and 2.10, equality in (10) holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$. ∎

Bearing in mind Lemma 2.4 and inequality (10), the following result can be derived.

Corollary 3.4. *Let G be an undirected connected graph with n , n ≥ 4, vertices and m edges. Then*

$$Kf(G) \leq \frac{n}{1+\Delta} + \frac{n(n-2)^2}{4(2m-n)}\left(\sqrt{\frac{\mu_2}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_2}}\right)^2\,. \tag{11}$$

Equality holds if and only if $G \cong K_n$ *or* $G \cong K_{1,n-1}$.

Theorem 3.5. *Let G be an undirected connected graph with n , n ≥ 3, vertices and m edges. Then*

$$Kf(G) \leq n\,\frac{(\mu_1+\mu_{n-1})(n-1) - 2m}{\mu_1\,\mu_{n-1}} \tag{12}$$

Equality holds if and only if G is a complete split graph or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. For $n := n-1$, $p_i := \frac{1}{n-1}$, $a_i := \mu_i$, $i = 1,2,\dots,n-1$, $R := \mu_1$, and $r := \mu_{n-1}$, from inequality (4) it follows that

$$\frac{1}{n-1}\sum_{i=1}^{n-1}\mu_i + \frac{\mu_1\,\mu_{n-1}}{n-1}\sum_{i=1}^{n-1}\frac{1}{\mu_i} \leq \mu_1 + \mu_{n-1}$$

i.e.,

$$2mn + \mu_1 \, \mu_{n-1} \, Kf(G) \le n(n-1)(\mu_1 + \mu_{n-1}) \, . \tag{13}$$

Inequality (12) follows directly from (13).

Since the equality in (4) holds if and only if $a_1 = \cdots = a_k = R$ and $a_{k+1} = \cdots = a_n = r$ for some k , $1 \le k \le n-1$, it means that equality in (12) holds if and only if $\mu_1 = \cdots = \mu_k$ and $\mu_{k+1} = \cdots = \mu_{n-1}$ for some k , $1 \le k \le n-1$. Bt Lemmas 2.9 and 2.10, equality in (12) holds if and only if $G \cong CS(n,k)$ for $1 \le k \le n-1$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$. ∎

Corollary 3.6. *Inequality (12) includes the inequality (9), i.e., it is stronger than (9).*

Proof. If on the left side of (13), the inequality between arithmetic and geometric means of two positive real numbers is applied, then

$$2\sqrt{2mn \, \mu_1 \, \mu_{n-1} \, Kf(G)} \le 2mn + \mu_1 \, \mu_{n-1} \, Kf(G) \le n(n-1)(\mu_1 + \mu_{n-1})$$

is obtained. From the left and the right terms of the above inequality, we arrive at (9). ∎

Theorem 3.7. *Let G be an undirected connected graph with n , $n \ge 4$, vertices and m edges. Then*

$$Kf(G) \le \frac{n}{1+\Delta} + n \, \frac{(\mu_2 + \mu_{n-1})(n-2) - (2m-n)}{\mu_2 \, \mu_{n-1}} \, . \tag{14}$$

Equality holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Proof. Rewriting the inequality (4) as

$$\sum_{i=2}^{n-1} p_i \, a_i + rR \sum_{i=2}^{n-1} \frac{p_i}{a_i} \le r + R \tag{15}$$

for $p_i := \frac{1}{n-2}$, $a_i := \mu_i$, $i = 2, \ldots, n-1$, $R := \mu_2$, and $r := \mu_{n-1}$, we obtain

$$\sum_{i=2}^{n-1} \frac{n}{\mu_i} \le \frac{n((\mu_2 + \mu_{n-1})(n-2) - (2m - \mu_1))}{\mu_2 \, \mu_{n-1}} \, .$$

This implies

$$Kf(G) = \frac{n}{\mu_1} + \sum_{i=2}^{n-1} \frac{n}{\mu_i} \le \frac{n}{\mu_1} + \frac{n((\mu_1 + \mu_{n-1})(n-2) - (2m - \mu_1))}{\mu_2 \, \mu_{n-1}} \, .$$

Since $1 + \Delta \le \mu_1 \le n$, we arrive at (14).

Equality in (14) holds if and only if $\mu_1 = n$ and $\mu_2 = \cdots = \mu_{n-1}$. By Lemmas 2.4, 2.9, and 2.10, this happens if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$. ∎

Corollary 3.8. *The upper bound (14) includes inequality (11), i.e., it is stronger than (11).*

Proof. Inequality (14) can be rewritten in the form

$$\mu_2 \, \mu_{n-1} \left(Kf(G) - \frac{n}{1+\Delta} \right) + n(2m-n) \le n(n-2)(\mu_2 + \mu_{n-1}) \, .$$

By applying the inequality between arithmetic and geometric means for two positive real numbers, on the left side of the above inequality, we obtain

$$2\sqrt{\mu_2 \, \mu_{n-2} \left(Kf(G) - \frac{1}{1+\Delta} \right) n(2m-n)} \le n(n-2)(\mu_1 + \mu_{n-1})$$

which is equivalent with (11). ∎

3.2. On degree Kirchhoff index

In the following theorem we establish an uper bound for $DKf(G)$ depending on the parameters n, m, ρ_1, ρ_{n-1}, and $\alpha(n-1)$.

Theorem 3.9. *Let G be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$DKf(G) \leq \frac{2m(n-1)^2}{n} \left(1 + \frac{(\rho_1 - \rho_{n-1})^2}{\rho_1 \, \rho_{n-1}} \, \alpha(n-1)\right). \tag{16}$$

Equality in (16) holds if and only if $G \cong K_n$.

Proof. Similarly as in the proof of Theorem 3.1, for $n := 1$, $p_i := 1$, $a_i := \mu_i$, $i = 1, 2, \dots, n-1$, $R := \rho_1$, $r := \rho_{n-1}$, and $S = \{1, 2, \dots, \left\lfloor \frac{n-1}{2} \right\rfloor\}$, the inequality (3) yields

$$\left(\sum_{i=1}^{n-1} \rho_i\right)\left(\sum_{i=1}^{n-1} \frac{1}{\rho_i}\right) - (n-1)^2 \leq \frac{(\rho_1 - \rho_{n-1})^2}{\rho_1 \, \rho_{n-1}} \left\lfloor \frac{n-1}{2} \right\rfloor \left(n - 1 - \left\lfloor \frac{n-1}{2} \right\rfloor\right).$$

Since $\sum\limits_{i=1}^{n-1} \rho_i = n$ and $\left\lfloor \frac{n-1}{2} \right\rfloor \left(n - 1 - \left\lfloor \frac{n-1}{2} \right\rfloor\right) = (n-1)^2 \, \alpha(n-1)$, the above inequality becomes

$$\sum_{i=1}^{n-1} \frac{1}{\rho_i} \leq \frac{(n-1)^2}{n} \left(1 + \frac{(\rho_1 - \rho_{n-1})^2}{\rho_1 \, \rho_{n-1}} \, \alpha(n-1)\right).$$

By multiplying the above inequality with $2m$, inequality (16) is obtained. Equality in (16) holds if and only if $\rho_1 = \rho_2 = \cdots = \rho_{n-1} = \frac{n}{n-1}$, i.e., if and only if $G \cong K_n$. ∎

Since $\alpha(n-1) \leq \frac{1}{4}$, we obtain:

Corollary 3.10. *Let G be undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$DKf(G) \leq \frac{m(n-1)^2}{2n} \left(\sqrt{\frac{\rho_1}{\rho_{n-1}}} + \sqrt{\frac{\rho_{n-1}}{\rho_1}}\right)^2 . \tag{17}$$

Equality in (17) holds if and only if $G \cong K_n$.

Theorem 3.11. *Let G be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$DKf(G) \leq 2m \, \frac{(n-1)(\rho_1 + \rho_{n-1}) - n}{\rho_1 \, \rho_{n-1}} . \tag{18}$$

Equality in (18) holds if and only if G is a (connected) graph with normalized Laplacian spectrum $\{\underbrace{\rho_1, \dots, \rho_1}_{k\text{-times}}, \underbrace{\rho_{n-1}, \dots, \rho_{n-1}}_{(n-k-1)\text{-times}}, 0\}$, for some k, $1 \leq k \leq n-1$.

Corollary 3.12. *The upper bound (18) includes inequality (17), i.e., it is stronger than (17).*

Proof is analogous to the proof of Corollary 3.6. ∎

Theorem 3.13. *Let G be an undirected connected graph with n, $n \geq 4$, vertices and m edges. Then*

$$DKf(G) \leq m + \frac{2m(n-2)(\rho_2 + \rho_{n-1} - 1)}{\rho_2 \, \rho_{n-1}} . \tag{19}$$

Equality in (19) holds if and only if $G \cong K_{1,n}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Using the inequality (15), for $p_i := \frac{1}{n-2}$, $a_i := \rho_i$, $i = 1, 2, \ldots, n-1$, $R := \rho_2$, and $r := \rho_{n-1}$, we arrive at

$$\sum_{i=2}^{n-1} \frac{2m}{\rho_i} \leq 2m \frac{(\rho_2 + \rho_{n-1})(n-2) - (n-\rho_1)}{\rho_2\, \rho_{n-1}}$$

resulting in

$$DKf(G) = \frac{2m}{\rho_1} + \sum_{i=2}^{n-1} \frac{2m}{\rho_i} \leq \frac{2m}{\rho_1} + 2m \frac{(\rho_2 + \rho_{n-2})(n-2) - (n-\rho_1)}{\rho_2\, \rho_{n-1}} .$$

Since $\rho_1 \leq 2$ and $2\rho_1 \geq \rho_2\, \rho_{n-2}$, from the above inequality it follows that

$$\frac{2m}{\rho_1} + \frac{2m((\rho_2 + \rho_{n-1})(n-2) - (n-\rho_1))}{\rho_2\, \rho_{n-1}} \leq \frac{2m}{2} + 2m \frac{(\rho_2 + \rho_{n-1})(n-2) - (n-2)}{\rho_2\, \rho_{n-1}}$$

which is the desired result. Equality in (19) holds if and only if $\rho_1 = 2$ and $\rho_2 = \cdots = \rho_{n-1}$. Since $\sum_{i=1}^{n-1} \rho_i = n$, equality in (19) holds if and only if $\rho_1 = 2$ and $\rho_2 = \cdots = \rho_{n-1} = 1$, i.e., if and only if $G \cong K_{1,n-1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$. ■

By a similar argument as in the case of Corollary 3.8, the following result can be proved:

Corollary 3.14. *Let G be an undirected connected graph with n , $n \geq 4$, vertices and m edges. Then*

$$DKf(G) \leq m\left(1 + \frac{n-2}{2}\left(\sqrt{\frac{\rho_2}{\rho_{n-1}}} + \sqrt{\frac{\rho_{n-1}}{\rho_2}}\right)^2\right). \tag{20}$$

Equality holds if and only if $G \cong K_{1,n-1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Corollary 3.15. *The inequality (19) includes the inequality (20), i.e. it is stronger than (20).*

Proof. The proof is similar to the proof of Corollary 3.6. ■

Note that the bounds obtained in (7), (10), (12) and (14), are, generally, incomparable. According to the numerical results,which are omitted for brevity, the following can be concluded:

- If $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even, bound in (12) is exact, while bounds (7), (10) and (14) are not. Consequently, bound (12) is better than the others. Bounds obtained by (10) and (14) are equal, and for $n \geq 8$ are stronger than the one obtained by (7).
- If $G \cong K_n - e$, bounds (12) and (14) are exact, but bounds (7) and (10) are not. On the other hand, bound (10) is stronger than (7) for each $n \geq 4$.
- If $G \cong P_n$, for $n \geq 4$, bound (7) is stronger than bounds obtained by (10), (12) and (14). Bound (12) is stronger than bounds (10) and (14), while (14) is stronger than (10).

Similarly, in general, bounds (7), (10), (12) and (14) are incomparable with (5) and (6). Thus, for example

- If $G \cong K_{1,n-1}$, bounds (10), (12) and (14) are exact, while (5), (6) and (7) are not. Bound (6) is stronger than (7).
- If $G \cong C_n$, bound (6) is stronger than bound (7) when $n \geq 6$, stronger than (10) and (14) when $n \geq 4$, and stronger than (12) when $n \geq 8$.

Acknowledgement. This work was supported by the Serbian Ministry of Education and Science, Project No. TR32012 and TR32009 .

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