On the Kirchhoff Index of Graphs

Kinkar C. Das

Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea

Reprint requests to K. C. D.; E-mail: kinkardas2003@googlemail.com

Z. Naturforsch. **68a,** 531 – 538 (2013) / DOI: 10.5560/ZNA.2013-0031
Received December 20, 2012 / revised March 15, 2013 / published online May 22, 2013

Let G be a connected graph of order n with Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n-1} > \mu_n = 0$. The Kirchhoff index of G is defined as $\mathrm{Kf} = \mathrm{Kf}(G) = n\sum_{k=1}^{n-1} 1/\mu_k$.

In this paper. we give lower and upper bounds on Kf of graphs in terms on n, number of edges, maximum degree, and number of spanning trees. Moreover, we present lower and upper bounds on the Nordhaus–Gaddum-type result for the Kirchhoff index.

Key words: Graph Spectrum; Laplacian Spectrum (of Graph); Kirchhoff Index; Nordhaus–Gaddum-Type.
Mathematics Subject Classification 2000: 05C50, 15A18

1. Introduction

It is well known that the resistance distance between two arbitrary vertices in an electrical network can be obtained in terms of the eigenvalues and eigenvectors of the combinatorial Laplacian matrix and normalized Laplacian matrix associated with the network. By studying the Laplacian matrix, people have proved many properties of resistance distances [1, 2]. The resistance distance is a novel distance function on a graph proposed by Klein and Randić [3]. The term 'resistance distance' was used because of the physical interpretation (see [4], for details).

Throughout this paper G will denote a simple, undirected, connected graph, and the vertices of it will be labelled by $v_1, v_2, \ldots, v_n$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The maximum vertex degree is denoted by Δ. In [5], it has been depicted that the standard distance between two vertices v_i and v_j of a connected graph G, denoted by d_{ij}, is defined as the length (= number of edges) of a shortest path that connects v_i and v_j. Moreover in order to examine other distances in graphs (or more formally, molecular graphs), Klein and Randić [3] considered the resistance distance between vertices of a graph G, denoted by r_{ij}, as defined in [1]. In fact, the resistance distance concept has been much studied in the chemical studies (see, for instance, [2, 3]). In [3, 6], it has been introduced the sum of resistance distances of all pairs of vertices of a molecular graph G,

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

that is named as the 'Kirchhoff index'.

Let J denote the square matrix of order n such that all of whose elements are unity. Then for all connected graphs (with two or more vertices) the matrix $L + \frac{1}{n}J$ is non-singular, its inverse

$$X = ||x_{ij}|| = \left(L + \frac{1}{n}J\right)^{-1}$$

exists and, as depicted in [1], $r_{ij} = x_{ii} + x_{jj} - 2x_{ij}$. The matrix whose (i, j)-entry is r_{ij}, is called the resistance distance matrix and will be denoted by $\mathrm{RD} = \mathrm{RD}(G)$. This matrix is symmetric and has a zero diagonal.

The Laplacian matrix of a graph G is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees, and $A(G)$ is the $(0, 1)$-adjacency matrix of graph G. Let $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$ denote the eigenvalues of $L(G)$. They are usually called the Laplacian eigenvalues of G.

As well known [7], a graph of order n has

$$t = t(G) = \frac{1}{n}\prod_{i=1}^{n-1} \mu_i \qquad (1)$$

spanning trees and

$$\sum_{i=1}^{n-1} \mu_i = 2m\,. \qquad (2)$$

The Kirchhoff index $\mathrm{Kf}(G)$ can also be written as

$$\mathrm{Kf}(G) = n \sum_{k=1}^{n-1} \frac{1}{\mu_k}, \tag{3}$$

where $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$ are the eigenvalues of the Laplacian matrix $L(G)$. The Kirchhoff index found noteworthy applications in chemistry, as a molecular structure descriptor [6, 8–10], and many of its mathematical properties have been established [1, 2, 11–18]. As usual, K_n, $K_{1,n-1}$, and $K_{p,q}$ $(n = p+q)$ denote respectively the complete graph, the star, and the complete bipartite graph.

Now we study the Kirchhoff index in more detail, especially its relationship with the number of vertices (atoms), the number of edges (bonds), maximum vertex degree (valency), the number of spanning trees, and the first Zagreb index. The paper is organized as follows. In Section 2, we present the lower and upper bounds on the Kirchhoff index of a graph. In Section 3, we obtain lower and upper bounds on the Nordhaus–Gaddum-type result for the Kirchhoff index.

2. Main Results

We now give some lower and upper bounds on $\mathrm{Kf}(G)$ in terms of n, m, Δ, t, and $M_1(G)$. First we give some well-known results:

Lemma 1. *[19] Let G be a graph on n vertices which has at least one edge. Then*

$$\mu_1 \geq \Delta + 1. \tag{4}$$

Moreover, if G is connected, then the equality holds in (4) if and only if $\Delta = n-1$.

Lemma 2. *[7] Let G be a connected graph of order n. Then $\mu_1 = \mu_2 = \ldots = \mu_{n-1}$ if and only if $G \cong K_n$.*

Lemma 3. *[7] Let G be a connected graph with $n \geq 3$ vertices. Then $\mu_2 = \mu_3 = \ldots = \mu_{n-1}$ if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ or $G \cong K_{\Delta,\Delta}$.*

Let $a_1, a_2, \ldots, a_r$ be positive real numbers. We define P_k to be the average of all products of k of the a_i's, that is

$$P_1 = \frac{a_1 + a_2 + \cdots + a_r}{r},$$
$$P_2 = \frac{a_1a_2 + a_1a_3 + \cdots + a_1a_r + a_2a_3 + \cdots + a_{r-1}a_r}{\frac{1}{2}r(r-1)},$$
$$\vdots$$
$$P_{r-1} = \frac{a_1a_2\cdots a_{r-1} + a_1a_2\cdots a_{r-2}a_r + \cdots + a_2a_3\cdots a_{r-1}a_r}{r},$$
$$P_r = a_1a_2\cdots a_r.$$

Hence the AM is simply P_1 and the GM is $P_r^{1/r}$. The following result generalize this:

Lemma 4 (Maclaurin's symmetric mean inequality)**.** *[20] For positive real numbers $a_1, a_2, \ldots, a_r$,*

$$P_1 \geq P_2^{1/2} \geq P_3^{1/3} \geq \cdots \geq P_r^{1/r}.$$

Equality holds if and only if $a_1 = a_2 = \ldots = a_r$.

Another structure descriptor introduced long time ago [9] is the so-called first Zagreb index (M_1) equal to the sum of the squares of the degrees of all vertices of G. Some basic properties of M_1 can be found in [21, 22]. Now we are ready to give lower and upper bounds on $\mathrm{Kf}(G)$ in terms of n, m, Δ, t, and $M_1(G)$.

Theorem 1. *Let G be a connected graph of order n with maximum degree Δ and the number of spanning trees t. Then*

$$\frac{n}{\Delta+1} + n(n-2)\left(\frac{\Delta+1}{nt}\right)^{1/(n-2)} \leq \mathrm{Kf}(G) \leq \frac{(n-1)}{t}\left[\frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)}\right]^{(n-2)/2}. \tag{5}$$

Moreover, the lower bound is attained if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$, and the upper bound is attained if and only if $G \cong K_n$.

Proof. By (1), we have

$$\frac{\mu_1^{n-1}}{nt} = \prod_{i=2}^{n-1} \frac{\mu_1}{\mu_i} \geq 1 \text{ as } \mu_1 \geq \mu_i, \; i = 2, 3, \ldots, n-1,$$

that is,

$$\mu_1^{n-1} \geq nt. \tag{6}$$

Lower Bound: Setting $r = n-2$ and $a_i = \mu_i$, $i = 2, 3, \ldots, n-1$, by Lemma 4, we get

$$P_{n-3}^{1/(n-3)} \geq P_{n-2}^{1/(n-2)},$$

where

$$P_{n-2} = \prod_{j=2}^{n-1} \mu_j$$

and

$$P_{n-3} = \frac{\sum_{i=2}^{n-1} \prod_{j=2,j\neq n-i+1}^{n-1} \mu_j}{n-2}.$$
$$= \frac{\prod_{j=2}^{n-1} \mu_j}{n-2} \cdot \sum_{i=2}^{n-1} \frac{1}{\mu_i}$$
$$= \frac{\prod_{j=2}^{n-1} \mu_j}{n(n-2)} \left(\mathrm{Kf}(G) - \frac{n}{\mu_1}\right) \text{ by (3)}.$$

From the above, we get

$$\frac{\prod_{j=2}^{n-1} \mu_j}{n(n-2)} \left(\mathrm{Kf}(G) - \frac{n}{\mu_1}\right) \geq \left(\prod_{j=2}^{n-1} \mu_j\right)^{(n-3)/(n-2)},$$

that is,

$$\mathrm{Kf}(G) \geq \frac{n}{\mu_1} + n(n-2) \left(\prod_{j=2}^{n-1} \mu_j\right)^{-1/(n-2)}.$$

Using (1) in the above, we get

$$\mathrm{Kf}(G) \geq \frac{n}{\mu_1} + n(n-2) \left(\frac{\mu_1}{nt}\right)^{1/(n-2)}. \qquad (7)$$

Let us consider a function

$$g(x) = \frac{n}{x} + n(n-2) \left(\frac{x}{nt}\right)^{1/(n-2)},$$
$$x \geq \Delta + 1 \text{ and } x^{n-1} \geq nt.$$

Then we have

$$g'(x) = -\frac{n}{x^2} + \frac{n}{(nt)^{1/(n-2)} x^{(n-3)/(n-2)}}$$
$$\geq -\frac{n}{x^2} + \frac{n}{x^{(n-1)/(n-2)} x^{(n-3)/(n-2)}}$$
$$= 0 \text{ as } x^{n-1} \geq nt.$$

Thus $g(x)$ is an increasing function on $x \geq \Delta + 1$ and $x^{n-1} \geq nt$. Hence we have

$$g(x) \geq \frac{n}{\Delta+1} + n(n-2) \left(\frac{\Delta+1}{nt}\right)^{1/(n-2)}.$$

Using the above result in (7), we get the lower bound in (5) by (4) and (6).

Upper Bound: Setting $r = n-1$ and $a_i = \mu_i$, $i = 1, 2, \ldots, n-1$, by Lemma 4, we get

$$P_2^{1/2} \geq P_{n-2}^{1/(n-2)},$$

where

$$P_2 = \frac{1}{(n-1)(n-2)} \sum_{i=1}^{n-1} \sum_{j=1, j\neq i}^{n-1} \mu_i \mu_j$$
$$= \frac{1}{(n-1)(n-2)} \left[\left(\sum_{i=1}^{n-1} \mu_i\right)^2 - \sum_{i=1}^{n-1} \mu_i^2\right]$$
$$= \frac{1}{(n-1)(n-2)} \left[4m^2 - M_1(G) - 2m\right]$$

as $\sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n} d_i(d_i+1)$,

$M_1(G) = \sum_{i=1}^{n} d_i^2$, and $2m = \sum_{i=1}^{n} d_i$

and

$$P_{n-2} = \frac{\sum_{i=1}^{n-1} \prod_{j=1,j\neq n-i+1}^{n-1} \mu_j}{n-1}$$
$$= \frac{\prod_{j=1}^{n-1} \mu_j}{n-1} \cdot \sum_{i=1}^{n-1} \frac{1}{\mu_i} = \frac{t}{(n-1)} \mathrm{Kf}(G) \text{ by (3)}.$$

From the above, we get

$$\frac{t}{(n-1)} \mathrm{Kf}(G) \leq \left[\frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)}\right]^{(n-2)/2},$$

that is,

$$\mathrm{Kf}(G) \leq \frac{(n-1)}{t} \left[\frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)}\right]^{(n-2)/2},$$

which gives the upper bound in (5). First part of the proof is over.

Now suppose that the equality (left and right) hold in (5). Then all the inequalities in above must be equalities. The equality for lower bound, we have $\mu_1 = \Delta + 1$ and $\mu_2 = \mu_3 = \ldots = \mu_{n-1}$, by Lemma 4. By Lemmas 1 and 3, we have $G \cong K_n$ or $G \cong K_{1,n-1}$. The equality for upper bound, we have $\mu_1 = \mu_2 = \ldots = \mu_{n-1}$ by Lemma 4. By Lemma 2, we have $G \cong K_n$.

Conversely, one can see easily that the left equality holds in (5) for complete graph K_n or star $K_{1,n-1}$ and the right equality holds in (5) for complete graph K_n. □

Corollary 1. *Let T be a tree of order n with maximum degree Δ. Then*

$$\frac{n}{\Delta+1} + n(n-2) \left(\frac{\Delta+1}{n}\right)^{1/(n-2)} \leq \mathrm{Kf}(G)$$

$$< (n-1)\left[\frac{2(n-1)(2n-3)-M_1(T)}{(n-1)(n-2)}\right]^{(n-2)/2}.$$

The lower bound is attained if and only if $G \cong K_{1,n-1}$.

Proof. Since T is a tree, $t = 1$. From Theorem 1, we get the required result. □

Corollary 2. *Let U be a connected unicyclic graph of order n with maximum degree Δ. Then*

$$\frac{n}{\Delta+1}+n(n-2)\left(\frac{\Delta+1}{n^2}\right)^{1/(n-2)} \le \mathrm{Kf}(U) \le \frac{(n-1)}{3}\left[\frac{2n(2n-1)-M_1(U)}{(n-1)(n-2)}\right]^{(n-2)/2} \tag{8}$$

with equality (left and right) holding if and only if $U \cong K_3$.

Proof. For unicyclic graph U, $3 \le t \le n$. From Theorem 1, we get the required result (8). Using the above result in Theorem 1, we conclude that the equality (left and right) hold in (8) if and only if $U \cong K_3$. □

Example 1. Consider a graph $G = K_{1,n-1} + \{e\}$, where e is an edge. For G, the Laplacian spectrum is

$$S(G) = \{n, 3, \underbrace{1, 1, \ldots, 1}_{n-3}, 0\}.$$

One can see easily that the lower and upper bounds of the Kirchhoff index in (5) are

$$1+n(n-2)\left(\frac{1}{3}\right)^{1/(n-2)}$$

$$\text{and}\quad \frac{(n-1)}{3}\left[\frac{3n^2-n-6}{(n-1)(n-2)}\right]^{(n-2)/2},$$

respectively, while the exact value of the Kirchhoff index is

$$n^2-\frac{8n}{3}+1.$$

Lemma 5. *[23] Let $a_1, a_2, \ldots, a_n \ge 0$ and $p_1, p_2, \ldots, p_n \ge 0$ with $\sum_{i=1}^{n} p_i = 1$. Then*

$$\sum_{i=1}^{n} p_i a_i - \prod_{i=1}^{n} a_i^{p_i} \ge n\lambda\left(\frac{1}{n}\sum_{i=1}^{n} a_i - \prod_{i=1}^{n} a_i^{1/n}\right), \tag{9}$$

where $\lambda = \min\{p_1, p_2, \ldots, p_n\}$. Moreover, the equality holds in (9) if and only if $a_1 = a_2 = \ldots = a_n$.

We now give a lower bound on Kf in terms of n, t, and Δ.

Theorem 2. *Let G be a connected graph of order n with maximum degree Δ and the number of spanning trees t. Then*

$$\mathrm{Kf}(G) \ge 2n(n-2)\left[\left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)} \cdot (\Delta+1)^{1/2(n-2)} - \frac{1}{2}\left(\frac{1}{nt}\right)^{1/(n-1)}\right] + \frac{n}{\Delta+1} \tag{10}$$

with equality holding if and only if $G \cong K_n$.

Proof. Setting $a_i = \frac{1}{\mu_i}$, $i = 1, 2, \ldots, n-1$, and $p_1 = \frac{1}{2(n-1)}$, $p_i = \frac{2n-3}{2(n-1)(n-2)}$, $i = 2, 3, \ldots, n-1$, in (9), we get

$$\frac{1}{2(n-1)}\cdot\frac{1}{\mu_1}+\frac{2n-3}{2(n-1)(n-2)}\sum_{i=2}^{n-1}\frac{1}{\mu_i} - \left(\frac{1}{\mu_1}\right)^{1/2(n-1)} \cdot \prod_{i=2}^{n-1}\left(\frac{1}{\mu_i}\right)^{(2n-3)/2(n-1)(n-2)} \ge \frac{1}{2(n-1)}\sum_{i=1}^{n-1}\frac{1}{\mu_i} - \frac{1}{2}\prod_{i=1}^{n-1}\left(\frac{1}{\mu_i}\right)^{1/(n-1)},$$

that is,

$$\frac{1}{2(n-1)}\cdot\frac{1}{\mu_1}+\frac{2n-3}{2(n-1)(n-2)}\left(\frac{1}{n}\mathrm{Kf}(G)-\frac{1}{\mu_1}\right) - \mu_1^{1/2(n-2)}\cdot\left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)} \ge \frac{1}{2n(n-1)}\mathrm{Kf}(G) - \frac{1}{2}\left(\frac{1}{nt}\right)^{1/(n-1)},$$

that is,

$$\mathrm{Kf}(G) \ge 2n(n-2)\left[\left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)}\mu_1^{1/2(n-2)} - \frac{1}{2}\left(\frac{1}{nt}\right)^{1/(n-1)} + \frac{1}{2(n-2)\mu_1}\right]. \tag{11}$$

By Lemma 1 and from (6), we have

$$\mu_1 \ge \Delta+1 \quad\text{and}\quad \mu_1^{n-1} \ge nt.$$

Let us consider a function

$$f(x) = \left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)} x^{1/2(n-2)} + \frac{1}{2(n-2)x},$$
$$x \geq \Delta + 1 \text{ and } x^{n-1} \geq nt.$$

Then we have

$$f'(x) = \left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)} \cdot \frac{1}{2(n-2)} \frac{1}{x^{1-1/2(n-2)}} - \frac{1}{2(n-2)x^2}$$
$$= \frac{1}{2(n-2)x^2}\left[\left(\frac{x^{n-1}}{nt}\right)^{\frac{2n-3}{2(n-1)(n-2)}} - 1\right] \geq 0$$
$$\text{as } x^{n-1} \geq nt.$$

Thus $f(x)$ is an increasing function on $x \geq \Delta + 1$ and $x^{n-1} \geq nt$. Hence we have

$$f(x) \geq \left(\frac{1}{nt}\right)^{(2n-3)/2(n-1)(n-2)} (\Delta+1)^{1/2(n-2)} + \frac{1}{2(n-2)(\Delta+1)}.$$

Using the above result in (11), we get the required result (10). First part of the proof is over.

Now suppose that the equality holds in (10). Then all the inequalities in the above must be equalities. Thus we must have $\mu_1 = \Delta + 1$ and $\mu_1 = \mu_2 = \ldots = \mu_{n-1}$ by Lemma 5. By Lemmas 1 and 2, we have $G \cong K_n$.

Conversely, one can see easily that the equality holds in (10) for complete graph K_n. □

Corollary 3. *Let T be a tree of order n with maximum degree Δ. Then*

$$\mathrm{Kf}(T) > 2n(n-2)\left[\left(\frac{1}{n}\right)^{(2n-3)/2(n-1)(n-2)} \cdot (\Delta+1)^{1/2(n-2)} - \frac{1}{2}\left(\frac{1}{n}\right)^{1/(n-1)}\right] + \frac{n}{\Delta+1}.$$

Corollary 4. *Let U be a connected unicyclic graph of order n with maximum degree Δ. Then*

$$\mathrm{Kf}(U) \geq 2n(n-2)\left[\left(\frac{1}{n^2}\right)^{(2n-3)/2(n-1)(n-2)} \cdot (\Delta+1)^{1/2(n-2)} - \frac{1}{2}\left(\frac{1}{3n}\right)^{1/(n-1)}\right] + \frac{n}{\Delta+1} \tag{12}$$

with equality holding in (12) if and only if $U \cong K_3$.

Example 2. Consider a graph $G = K_n$. For G, the Laplacian spectrum is

$$S(G) = \{\underbrace{n, n, \ldots, n}_{n-1}, 0\}.$$

One can see easily that both the lower bound in (10) and the exact value of the Kirchhoff index are $n-1$.

Lemma 6 (Newton's inequality)**.** *[24] Let a_1, $a_2, \ldots, a_r$ be the positive real numbers. Also let P_k, $k = 1, 2, \ldots, r$ be defined before Lemma 4. Then*

$$P_{k-1}P_{k+1} \leq P_k^2 \quad (k = 1, 2, \ldots, r-1;\ P_0 = 1)$$

with equality holding if and only $a_1 = a_2 = \ldots = a_r$.

Now we give another lower bound on $\mathrm{Kf}(G)$ in terms of n, m, and $M_1(G)$.

Theorem 3. *Let G be a connected graph of order n with m edges and the first Zagreb index $M_1(G)$. Then*

$$\mathrm{Kf}(G) \geq \frac{2mn(n-1)(n-2)}{4m^2 - M_1(G) - 2m} \tag{13}$$

with equality holding in (13) if and only if $G \cong K_n$.

Proof. From Lemma 6, we get

$$\frac{P_1}{P_2} \leq \frac{P_2}{P_3} \leq \frac{P_3}{P_4} \leq \cdots \leq \frac{P_{r-1}}{P_r}.$$

From the above, we get

$$P_1 P_r \leq P_{r-1} P_2, \quad r \geq 3. \tag{14}$$

Setting $r = n-1$ and $a_i = \mu_i$, $i = 1, 2, \ldots, n-1$, in (14), we get

$$P_1 = \frac{\sum_{i=1}^{n-1} \mu_i}{n-1} = \frac{2m}{n-1},$$
$$P_2 = \frac{2\sum_{i<j} \mu_i \mu_j}{(n-1)(n-2)} = \frac{\left(\sum_{i=1}^{n-1} \mu_i\right)^2 - \sum_{i=1}^{n-1} \mu_i^2}{(n-1)(n-2)}$$
$$= \frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)},$$
$$\text{as } \sum_{i=1}^{n-1} \mu_i^2 = M_1(G) + 2m,$$
$$P_{n-2} = \frac{\prod_{i=1}^{n-1} \mu_i \sum_{i=1}^{n-1} \frac{1}{\mu_i}}{n-1} = \frac{tn}{n-1} \sum_{i=1}^{n-1} \frac{1}{\mu_i},$$
$$\text{and } P_{n-1} = \prod_{i=1}^{n-1} \mu_i = nt.$$

From (14), we get

$$\frac{2mnt}{n-1} \le \frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)} \cdot \frac{tn}{n-1} \sum_{i=1}^{n-1} \frac{1}{\mu_i},$$

that is,

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i} \ge \frac{2m(n-1)(n-2)}{4m^2 - M_1(G) - 2m}.$$

Using the above result in (3), we get the lower bound in (13). First part of the proof is over.

Now suppose that the equality holds in (13). Then all the inequalities in the above must be equalities. Thus we have $\mu_1 = \mu_2 = \mu_3 = \ldots = \mu_{n-1}$ by Lemma 6. By Lemma 2, we have $G \cong K_n$.

Conversely, one can see easily that the equality holds in (13) for complete graph K_n. □

Example 3. Consider a graph $G = K_n \backslash \{e\}$, where e is any edge in K_n. For G, the Laplacian spectrum is

$$S(G) = \{\underbrace{n, n, \ldots, n}_{n-2}, n-2, 0\}.$$

One can see easily that the lower bound of the Kirchhoff index in (13) is

$$n - 1 + \frac{2(n-1)}{n^2 - n - 4},$$

while the exact value of the Kirchhoff index is

$$n - 1 + \frac{2}{n-2}.$$

3. Nordhaus–Gaddum-Type Results for the Kirchhoff Index

Zhou and Trinajstić [10] obtained the following Nordhaus–Gaddum-type result for the Kirchhoff index:

Lemma 7. *Let G be a connected (molecular) graph on $n \ge 5$ vertices with a connected $\overline{G}$. Then*

$$\mathrm{Kf}(G) + \mathrm{Kf}(\overline{G}) \ge 4n - 2.$$

We now give lower and upper bounds for $\mathrm{Kf}(G) + \mathrm{Kf}(\overline{G})$ in terms on n, $M_1(G)$, and number of spanning trees:

Theorem 4. *Let G be a connected graph of order n with m edges. Then*

$$\begin{aligned}(n-1)\left(\frac{n^{2(n-2)}}{t\bar{t}}\right)^{1/(n-1)} &\le \mathrm{Kf}(G) + \mathrm{Kf}(\overline{G}) \\ &\le \frac{(n-1)}{t\bar{t}}\left[\frac{2m(n-1) - M_1(G)}{n-1}\right]^{n-2},\end{aligned} \tag{15}$$

where t and $\bar{t}$ are the number of spanning trees of G and $\overline{G}$, respectively. Moreover, the equality (left and right) hold in (15) if and only if G is isomorphic to a graph H such that there exists a positive integer k $(1 \le k \le n-1)$ with

$$\mu_1(H) = \mu_2(H) = \ldots = \mu_k(H),$$
$$\mu_{k+1}(H) = \mu_{k+2}(H) = \ldots = \mu_{n-1}(H),$$

and $\mu_i(H) + \mu_j(H) = n$, $1 \le i \le k$, $k+1 \le j \le n-1$.

Proof. From (3), we have

$$\begin{aligned}\mathrm{Kf}(G) + \mathrm{Kf}(\overline{G}) &= n \sum_{i=1}^{n-1}\left(\frac{1}{\mu_i} + \frac{1}{n-\mu_i}\right) \\ &= n^2 \sum_{i=1}^{n-1} \frac{1}{\mu_i(n-\mu_i)}.\end{aligned} \tag{16}$$

Lower Bound: Setting $r = n-1$ and $a_i = \mu_i(n-\mu_i)$, $i = 1, 2, \ldots, n-1$, by Lemma 4, we get

$$P_{n-2}^{1/(n-2)} \ge P_{n-1}^{1/(n-1)},$$

that is,

$$P_{n-2} \ge P_{n-1}^{(n-2)/(n-1)},$$

that is,

$$\frac{1}{n-1} \prod_{i=1}^{n-1} \mu_i(n-\mu_i) \cdot \sum_{i=1}^{n-1} \frac{1}{\mu_i(n-\mu_i)} \ge \left[\prod_{i=1}^{n-1} \mu_i(n-\mu_i)\right]^{(n-2)/(n-1)},$$

that is,

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i(n-\mu_i)} \ge \frac{(n-1)}{\left[\prod_{i=1}^{n-1} \mu_i(n-\mu_i)\right]^{1/(n-1)}},$$

that is,

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i(n-\mu_i)} \geq \frac{(n-1)}{[n^2 t\bar{t}]^{1/(n-1)}} \quad \text{as } n\bar{t} = \prod_{i=1}^{n-1}(n-\mu_i) \text{ and by (1)}. \tag{17}$$

Using (17) in (16), we get the lower bound in (15).

Upper Bound: Setting $r = n-1$ and $a_i = \mu_i(n-\mu_i)$, $i = 1, 2, \ldots, n-1$, by Lemma 4, we have

$$P_1 \geq P_{n-2}^{1/(n-2)},$$

that is,

$$\frac{\sum_{i=1}^{n-1} \mu_i(n-\mu_i)}{n-1} \geq \left[\frac{1}{n-1}\prod_{i=1}^{n-1}\mu_i(n-\mu_i) \cdot \sum_{i=1}^{n-1}\frac{1}{\mu_i(n-\mu_i)}\right]^{1/(n-2)},$$

that is,

$$\frac{2m(n-1)-M_1(G)}{n-1} \geq \left[\frac{n^2 t\bar{t}}{n-1}\sum_{i=1}^{n-1}\frac{1}{\mu_i(n-\mu_i)}\right]^{1/(n-2)}$$

as $\sum_{i=1}^{n-1}\mu_i^2 = M_1(G) + 2m$,

that is,

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i(n-\mu_i)} \leq \frac{(n-1)}{n^2 t\bar{t}} \cdot \left[\frac{2m(n-1)-M_1(G)}{n-1}\right]^{n-2}. \tag{18}$$

Using (18) in (16), we get the upper bound in (15). First part of the proof is over.

Now suppose that the equality (left and right) hold in (15). Then all the inequalities in above must be equalities. Thus we must have $\mu_1(n-\mu_1) = \mu_2(n-\mu_2) = \ldots = \mu_{n-1}(n-\mu_{n-1})$ by Lemma 4. For

$$\mu_i(n-\mu_i) = \mu_j(n-\mu_j),$$

we have

$$(\mu_i-\mu_j)(\mu_i+\mu_j-n) = 0, \quad \text{that is, } \mu_i = \mu_j \text{ or } \mu_i+\mu_j = n.$$

From the above we conclude that G is isomorphic to a graph H such that there exists a positive integer k $(1 \leq k \leq n-1)$ with

$$\mu_1(H) = \mu_2(H) = \ldots = \mu_k(H),$$
$$\mu_{k+1}(H) = \mu_{k+2}(H) = \ldots = \mu_{n-1}(H),$$

and $\mu_i(H)+\mu_j(H) = n$, $1 \leq i \leq k$, $k+1 \leq j \leq n-1$.

Conversely, let H be a graph such that there exists a positive integer k $(1 \leq k \leq n-1)$ with

$$\mu_1(H) = \mu_2(H) = \ldots = \mu_k(H),$$
$$\mu_{k+1}(H) = \mu_{k+2}(H) = \ldots = \mu_{n-1}(H),$$

and

$$\mu_i(H)+\mu_j(H) = n, \quad 1 \leq i \leq k, \quad k+1 \leq j \leq n-1.$$

Then

$$\begin{aligned} t\bar{t} &= \frac{1}{n}\mu_1^k(H)\mu_{n-1}^{n-k-1}(H)\frac{1}{n}(n-\mu_1(H))^k \cdot (n-\mu_{n-1}(H))^{n-k-1} \\ &= \frac{1}{n^2}\mu_1^{n-1}(H)\mu_{n-1}^{n-1}(H) \quad \text{as } \mu_1(H) = n-\mu_{n-1}(H) \end{aligned} \tag{19}$$

and

$$\begin{aligned} 2m(n-1)-M_1(H) &= n\sum_{i=1}^{n-1}\mu_i(H) - \sum_{i=1}^{n-1}\mu_i^2(H) \\ &= nk\mu_1(H) + n(n-k-1)\mu_{n-1}(H) - k\mu_1^2(H) - (n-k-1)\mu_{n-1}^2(H) \\ &= k\mu_1(H)\mu_{n-1}(H) + (n-k-1)\mu_1(H)\mu_{n-1}(H) \quad \text{as } \mu_1(H) = n-\mu_{n-1}(H) \\ &= (n-1)\mu_1(H)\mu_{n-1}(H). \end{aligned} \tag{20}$$

Hence

$$\begin{aligned} \mathrm{Kf}(H)+\mathrm{Kf}(\overline{H}) &= n^2\sum_{i=1}^{n-1}\frac{1}{\mu_i(H)(n-\mu_i(H))} \\ &= n^2\left[\frac{k}{\mu_1(H)(n-\mu_1(H))} + \frac{n-k-1}{\mu_{n-1}(H)(n-\mu_{n-1}(H))}\right] \\ &= \frac{n^2(n-1)}{\mu_1(H)\mu_{n-1}(H)} \quad \text{as } \mu_1(H) = n-\mu_{n-1}(H) \\ &= (n-1)\left(\frac{n^{2(n-2)}}{t\bar{t}}\right)^{1/(n-1)} \quad \text{by (19)} \end{aligned}$$

and

$$\begin{aligned}\mathrm{Kf}(H)+\mathrm{Kf}(\overline{H}) &= \frac{n^2(n-1)}{\mu_1(H)\mu_{n-1}(H)}\\ &= \frac{(n-1)n^2}{\mu_1^{n-1}(H)\mu_{n-1}^{n-1}(H)}\mu_1^{n-2}(H)\mu_{n-1}^{n-2}(H)\\ &= \frac{(n-1)}{t\bar{t}}\left[\frac{2m(n-1)-M_1(H)}{n-1}\right]^{n-2} \text{ by (19) and (20).}\end{aligned}$$

This completes the proof. □

Corollary 5. *Let G be a self-complimentary graph of order n with m edges. Then*

$$\frac{(n-1)}{2}\left(\frac{n^{2(n-2)}}{t^2}\right)^{1/(n-1)} \leq \mathrm{Kf}(G) \leq \frac{(n-1)}{2t^2}\left[\frac{2m(n-1)-M_1(G)}{n-1}\right]^{n-2}, \tag{21}$$

where t is the number of spanning tree of G. Moreover, the equality (left and right) hold in (21) if and only if G is isomorphic to a graph H such that there exists a positive integer k $(1 \leq k \leq n-1)$ *with*

$$\mu_1(H)=\mu_2(H)=\ldots=\mu_k(H),$$
$$\mu_{k+1}(H)=\mu_{k+2}(H)=\ldots=\mu_{n-1}(H),$$

and $\mu_i(H)+\mu_j(H)=n,\ 1\leq i\leq k,\ k+1\leq j\leq n-1$.

Proof. Since G is self-complimentary graph, therefore G is connected and $G \cong \overline{G}$. Thus we have $t=\bar{t}$. From Theorem 4, we get the required result in (21). Moreover, the equality (left and right) hold in (21) if and only if G is isomorphic to a graph H (H is defined in the statement). □

Acknowledgement

The author is grateful to the four anonymous referees for their careful reading and valuable comments on this paper, which have considerably improved the presentation of this paper. This work is supported by the Faculty Research Fund, Sungkyunkwan University, 2012 and Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea.

[1] W. Xiao and I. Gutman, Theor. Chem. Acc. **110**, 284 (2003).
[2] W. Xiao and I. Gutman, Commun. Math. Comput. Chem. **49**, 67 (2003).
[3] D. J. Klein and M. Randić, J. Math. Chem. **12**, 81 (1993).
[4] H. Chen and F. Zhang, Discrete Appl. Math. **155**, 654 (2007).
[5] F. Buckley and F. Harray, Distance in Graphs, Addison–Wesley, Redwood 1990.
[6] D. Bonchev, A. T. Balaban, X. Liu, and D. J. Klein, Int. J. Quantum Chem. **50**, 1 (1994).
[7] K. C. Das, Graphs Combin. **23**, 625 (2007).
[8] K. C. Das, A. D. Güngör, and A. S. Çevik, Commun. Math. Comput. Chem. **67**, 541 (2012).
[9] E. Estrada and N. Hatano, Chem. Phys. Lett. **486**, 166 (2010).
[10] B. Zhou and N. Trinajstić, Chem. Phys. Lett. **455**, 120 (2008).
[11] K. C. Das, K. Xu, and I. Gutman, Lin. Alg. Appl. **436**, 3661 (2012).
[12] X. Gao, Y. Luo, and W. Liu, Discr. Appl. Math. **159**, 2050 (2011).
[13] J. L. Palacios, Int. J. Quantum Chem. **81**, 135 (2001).
[14] J. L. Palacios, Method. Comput. Appl. Prob. **6**, 381 (2004).
[15] Y. J. Yang and X. Y. Jiang, Commun. Math. Comput. Chem. **60**, 107 (2008).
[16] H. Wang, H. Hua, and D. Wang, Math. Commun. **15**, 347 (2010).
[17] H. P. Zhang, X. Y. Jiang, and Y. J. Yang, Commun. Math. Comput. Chem. **61**, 697 (2009).
[18] H. P. Zhang, Y. J. Yang, and C. W. Li, Discr. Appl. Math. **107**, 2918 (2009).
[19] R. Merris, Lin. Alg. Appl. **197 – 198**, 143 (1994).
[20] P. Biler and A. Witkowski, Problems in Mathematical Analysis, M. Dekker, New York 1990.
[21] K. C. Das, Discr. Math. **285**, 57 (2004).
[22] I. Gutman and K. C. Das, Commun. Math. Comput. Chem. **50**, 83 (2004).
[23] S. Furuichi, J. Math. Inequal. **5**, 21 (2011).
[24] S. Rosset, J. Am. Math. **96**, 815 (1989).