Ordering connected graphs by their Kirchhoff indices [*]

Kexiang Xu[a], Kinkar Ch. Das[b], Xiao-Dong Zhang[c]

[a] College of Science, Nanjing University of Aeronautics & Astronautics,
Nanjing, Jiangsu 210016, P.R. China
[b] Department of Mathematics, Sungkyunkwan University,
Suwon 440-746, Republic of Korea
[c] Department of Mathematics, Shanghai Jiao Tong University,
800 Dongchuan road, Shanghai, 200240, P.R. China

Abstract

The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distances between all unordered pairs of vertices, which was introduced by Klein and Randić. In this paper we characterized all extremal graphs with Kirchhoff index among all graphs obtained by deleting p edges from a complete graph K_n with $p \leq \lfloor \frac{n}{2} \rfloor$ and obtained a sharp upper bound on the Kirchhoff index of these graphs. In addition, all the graphs with the first to ninth maximal Kirchhoff indices are completely determined among all connected graphs of order $n > 27$.

1 Introduction

Let G be a connected graph with vertices labeled as $v_1, v_2, \ldots, v_n$. The distance between vertices v_i and v_j, denoted by $d_G(v_i, v_j)$, is the length of a shortest path between

them. The famous Wiener index $W(G)$ [22] is the sum of distances between all unordered pairs of vertices, that is, $W(G) = \sum_{i<j} d_G(v_i, v_j)$.

In 1993, Klein and Randić [17] introduced a new distance function named resistance distance based on electrical network theory. They viewed G as an electrical network N by replacing each edge of G with a unit resistor, the resistance distance between v_i and v_j, denoted by $r_G(v_i, v_j)$, is defined to be the effective resistance between them 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 and physical interpretations [17, 18], but with a substantial potential for chemical applications.

In fact, the shortest-path might be imagined to be more relevant when there is corpuscular communication (along edges) between two vertices, whereas the resistance distance might be imagined to be more relevant when the communication is wave- or fluid-like. Then the chemical communication in molecules is rather wavelike suggests the utility of this concept in chemistry. So in recent years, the resistance distance was well studied in mathematical and chemical literatures [1, 2, 4, 8–12].

Analogue to Wiener index, the Kirchhoff index (or resistance index) [4] is defined as

$$Kf(G) = \sum_{i<j} r_G(v_i, v_j).$$

As a useful structure-descriptor, the computation of Kirchhoff index is a hard problem [1], but one may compute the specific classes of graphs. Since for trees, the Kirchhoff index and the Wiener index coincide. It is possible to study the Kirchhoff index of topological structures containing cycles. Throughout this paper we denote by P_n (resp. C_n, K_n) denote the path graph (resp. cycle graph, complete graph) on n vertices. Some nice mathematical results can be found in [20, 24].

All graphs considered in this paper are finite and simple. For two nonadjacent vertices v_i and v_j, we use $G + e$ to denote the graph obtained by inserting a new edge $e = v_i v_j$ in G. Similarly, for $e \in E(G)$ of graph G, let $G - e$ be the subgraph of G obtained by deleting the edge e from $E(G)$. The complement of graph G is always denoted by $\overline{G}$. For two vertex disjoint graphs G_1 and G_2, we denote by $G_1 \bigcup G_2$ the graph which consists of two connected components G_1 and G_2. The *join* of G_1 and G_2, denoted by $G_1 \bigvee G_2$,

2

is the graph with vertex set $V(G_1) \bigcup V(G_2)$ and edge set $E(G_1) \bigcup E(G_2) \bigcup \{u_i v_j : u_i \in V(G_1), v_j \in V(G_2)\}$. For other undefined notation and terminology from graph theory, the readers are referred to [5].

For a graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, we denote by d_i the degree of the vertex v_i in G for $i = 1, 2, \ldots, n$. Assume that $A(G)$ is the $(0,1)$-adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. The Laplacian polynomial $Q(G, \lambda)$ of G is the characteristic polynomial of its Laplacian matrix, $Q(G, \lambda) = det(\lambda I_n - L(G)) = \sum_{k=0}^{n} (-1)^k c_k \lambda^{n-k}$. The Laplacian matrix $L(G)$ has nonnegative eigenvalues $n \geq \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ [6]. Denote by $S(G) = \{\mu_1, \mu_2, \ldots, \mu_n\}$ the spectrum of $L(G)$, i.e., the Laplacian spectrum of G. If the eigenvalue μ_i appears $l_i > 1$ times in $S(G)$, we write them as $\mu_i^{(l_i)}$ for the sake of convenience.

In 1996, Gutman and Mohar [14] obtained the following nice result, by which a relation is established between Kirchhoff index and Laplacian spectrum:

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

for any connected graphs of order $n \geq 2$.

Let $\mathcal{G}(n)$ be the set of connected graphs of order n. In this paper, we determined the first to ninth minimal Kirchhoff indices of graphs from $\mathcal{G}(n)$ with $n > 9$; also characterized all the graphs from $\mathcal{G}(n)$ with $n > 27$ with the first to ninth maximal Kirchhoff indices.

2　Preliminaries

In this section we will list some known lemmas as necessary preliminaries.

Lemma 2.1. ([15]) *Let G be a graph and $G' = G + e$ the graph obtained by inserting a new edge into G. Then we have*

$$\mu_1(G') \geq \mu_1(G) \geq \mu_2(G') \geq \mu_2(G) \geq \cdots \geq \mu_n(G') = \mu_n(G) = 0.$$

Combining Lemma 2.1 and the fact that $\sum_{i=1}^{n-1} \mu_i(G+e) - \sum_{i=1}^{n-1} \mu_i(G) = 2$, by the equation (1), the following lemma can be easily obtained.

3

Lemma 2.2. ([20]) Let G be a connected graph with $e \in E(G)$ and two nonadjacent vertices v_i and v_j in $V(G)$. Then we have

(1) $Kf(G - e) > Kf(G)$ where $G - e$ is connected;

(2) $Kf(G) > Kf(G + e')$ where $e' = v_i v_j$.

Based on Lemma 2.2 (1), the corollary below follows immediately.

Corollary 2.1. *Suppose that G is a connected graph of order n and with $m \geq n$ edges and with T as its spanning tree. Then we have $Kf(G) < Kf(T)$.*

Lemma 2.3. ([21]) *Let G be a graph of order n with $S(G) = \{\mu_1, \mu_2, \ldots, \mu_{n-1}, 0\}$. Then $S(\overline{G}) = \{n - \mu_1, n - \mu_2, \ldots, n - \mu_{n-1}, 0\}$.*

Lemma 2.4. ([17]) *Let G be a connected graph. Then we have $W(G) \geq Kf(G)$, with equality if and only if G is a tree.*

Before listing this problem, we first introduce some necessary notations and definitions. A vertex v of a tree T is called a *branching point* if $d(v) \geq 3$. A tree is said to be starlike if exactly one of its vertices has degree greater than two. Let P_n denote the path on n vertices. By $T_n(n_1, n_2, \ldots, n_k)$ we denote the starlike tree which has a vertex v of degree $k \geq 3$ and which has the property

$$T_n(n_1, n_2, \ldots, n_k) - v = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k}.$$

This tree has $n_1 + n_2 + \ldots + n_k + 1 = n$ vertices and assumed that $n_1 \geq n_2 \geq \ldots \geq n_k \geq 1$. We say that the starlike tree $T_n(n_1, n_2, \ldots, n_k)$ has k branches, the lengths of which are $n_1, n_2, \ldots, n_k$, respectively.

Note that any tree with exactly one branching point is a starlike tree. Assume that T is a tree of order n with exactly two branching points v_1 and v_2 with $d(v_1) = r$ and $d(v_2) = t$. The orders of $r - 1$ components, which are paths, of $T - v_1$ are $p_1, \ldots, p_{r-1}$, the order of the component which is not a path of $T - v_1$ is $p_r = n - p_1 - \cdots - p_{r-1} - 1$. The orders of $t - 1$ components, which are paths, of $T - v_2$ are $q_1, \ldots, q_{t-1}$, the order of the
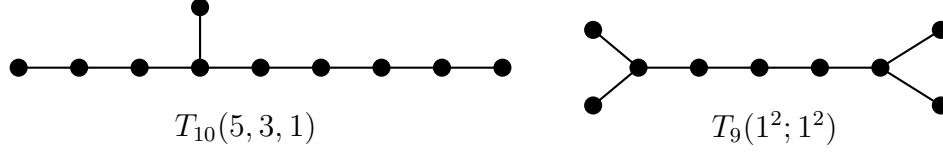
Figure 1: The trees $T_{10}(5, 3, 1)$ and $T_9(1^2; 1^2)$

component which is not a path of $T - v_2$ is $q_t = n - q_1 - \cdots - q_{t-1} - 1$. We denote this tree by $T = T_n(p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})$, where $r \leq t$, $p_1 \geq \cdots \geq p_{r-1}$ and $q_1 \geq \cdots \geq q_{t-1}$.

For convenience, when considering the trees $T_n(n_1, n_2, \ldots, n_k, \ldots, n_m)$ or $T_n(p_1, \ldots, p_k,$ $\ldots, p_{r-1}; q_1, \ldots, q_k, \ldots, q_{t-1})$, we use the symbols $n_k^{l_k}$ or $p_k^{l_k}$ (resp. $q_k^{l_k}$) to indicate that the number of n_k or p_k (resp. q_k) is $l_k > 1$ in the following. For example, $T_{15}(2, 2, 3, 3, 4)$ will be written as $T_{15}(2^2, 3^2, 4)$. As another two examples, the trees $T_{10}(5, 3, 1)$ and $T_9(1^2; 1^2)$ are shown in Figure 1.

In the following lemma the partial result in [19] are summarized.

Lemma 2.5. ([19]) *Suppose that T is a tree of order $n \geq 9$. Then we have*

$$
\begin{aligned}
W(P_n) \;>\;& W(T_n(n - 3, \, 1^2)) > W(T_n(n - 4, \, 2, \, 1)) > W(T_n(1^2; \, 1^2)) > W(T_n(n - 5, \, 3, \, 1)) \\
>\;& W(T_n(n - 4, \, 1^3)) = W(T_n(1^2; \, 2, \, 1)) > W(T_n(n - 6, \, 4, \, 1)) > W(T).
\end{aligned}
$$

Combining Lemmas 2.4 and 2.5, the following corollary can be easily obtained.

Corollary 2.2. *Suppose that T is a tree of order $n \geq 9$. Then we have*

$$
\begin{aligned}
Kf(P_n) \;>\;& Kf(T_n(n - 3, \, 1^2)) > Kf(T_n(n - 4, \, 2, \, 1)) > Kf(T_n(1^2; \, 1^2)) > Kf(T_n(n - 5, \, 3, \, 1)) \\
>\;& Kf(T_n(n - 4, \, 1^3)) = Kf(T_n(1^2; \, 2, \, 1)) > Kf(T_n(n - 6, \, 4, \, 1)) > Kf(T).
\end{aligned}
$$

Let P_n^k be the graph obtained by identifying a pendent vertex of a path of length $n - k + 1$ with one vertex of a cycle C_k.

Lemma 2.6. ([24]) *For any connected graph G of order $n > 3$ and with $n > 3$ edges, we have*

$$
Kf(G) \leq \frac{n^3 - 11n + 18}{6}
$$

with equality if and only if $G \cong P_n^3$.

5

Denote by $C_{p,q}^l$ the graph which is formed by two disjoint cycles C_p and C_q linked by a path of length l (see Figure 2). In [25], the authors determined the graph which maximizes the Kirchhoff index among all connected graphs of order n with n edges and exactly two cycles. Recently, Feng, Yu et al. and one of the present authors [13] completely characterized the extremal graph with maximal Kirchhoff index among all connected graphs of order n and with $n + 1$ edges.
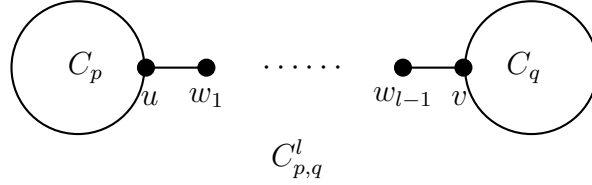

$$C_{p,q}^l$$

Figure 2: The graph $C_{p,q}^l$

Lemma 2.7. ([13]) *Let G be a connected graph of order n and with $n + 1$ edges $(n \geq 8)$. Then we have*

$$Kf(G) \leq \frac{n^3 - 21n + 36}{6}$$

with equality if and only if $G \cong C_{3,3}^{n-5}$.

An invariant related to Kirchhoff index is defined [24] as follows: $Kf_{v_i}(G) = \sum_{j \neq i} r_G(v_i, v_j)$. In the following lemma a nice formula is presented on Kirchhoff index of a graph with cut vertices.

Lemma 2.8. ([25]) *Let x be a cut vertex of connected graph G such that $G = G_1 \bigcup G_2$, $V(G_1) \bigcap V(G_2) = \{x\}$ and $|V(G_i)| = n_i$ for $i = 1, 2$. Then we have*

$$Kf(G) = Kf(G_1) + Kf(G_2) + (n_1 - 1)Kf_x(G_2) + (n_2 - 1)Kf_x(G_1).$$

Note that ([23]) P_n has uniquely the largest Wiener index among all trees of order n. From Lemma 2.8, the corollary below follows immediatey.

Corollary 2.3. *Let G_0 be a connected graph with $v_0 \in V(G_0)$ and T_t a tree of order $t \geq 2$ with $x \in V(T_t)$. Assume that G is a graph obtained by identifying the vertex v_0 in G_0 with*

6

$x \in T$ and G' is obtained by identifying $v_0 \in G_0$ with a pendent vertex of path P_t. Then

$$Kf(G) \leq Kf(G')$$

with equality holding if and only if $G \cong G'$, i.e., $T_t \cong P_t$ with x being a pendent in T_t.

Lemma 2.9. ([24]) *Among all connected graph of order n with n edges and cycle length k, the graph P_n^k has uniquely the maximal Kirchhoff index.*

3 Main results

In this section, we will order all the graphs from $\mathcal{G}(n)$ with n being not very small by their Kirchhoff indices. In what follows, we will deal with the two cases, respectively, for graphs from $\mathcal{G}(n)$ with smaller Kirchhoff indices and with larger Kirchhoff indices.

3.1 The ordering of connected graphs with smaller Kirchhoff indices

Lukovits et al. [20] showed that, among all connected graphs of order n, $Kf(G) \geq n-1$ with equality if and only if G is complete graph K_n. In the following it suffices to order the graphs from $\mathcal{G}(n) \setminus \{K_n\}$ by their Kirchhoff indices.

For convenience, for a subgraph G_0 of K_n, we denote by $K_n - G_0$ the graph obtained by deleting all edges of G_0 from K_n. From the structure of $K_n - G_0$, we claim that $\overline{K_n - G_0} \cong \overline{K_{n-|V(G_0)|}} \bigcup G_0$. For the consistency of sign, we write $G_1(n) = K_n$ and $G_2(n) = K_n - K_2$. Moreover, let $G_3(n) = K_n - 2K_2$ and $G_4(n) = K_n - K_{1,2}$. Next we consider the graphs obtained by deleting three edges from K_n. Assume that

$$G_5(n) = K_n - 3K_2; \quad G_6(n) = K_n - (K_{1,2} \cup K_2); \quad G_7(n) = K_n - P_4;$$

$$G_8(n) = K_n - C_3; \quad G_9(n) = K_n - K_{1,3}.$$

In the following theorem the graphs from $\mathcal{G}(n)$ with $n \geq 11$ and with first to ninth minimal Kirchhoff indices are completely determined.

Theorem 3.1. ([10]) *Let* $n \geq 11$ *and* $G \in \mathcal{G}(n)$ *but other than any graph from the set* $\{G_i(n)|i \in \{1, 2, \ldots, 9\}\}$. *Then we have*

$$Kf(G) > Kf(G_9(n)) > Kf(G_8(n)) > Kf(G_7(n)) > Kf(G_6(n)) > Kf(G_5(n))$$
$$> Kf(G_4(n)) > Kf(G_3(n)) > Kf(G_2(n)) > Kf(G_1(n)).$$

In view of Theorem 3.1, naturally we will ask a related problem as follows:

For an integer $4 \leq p \leq \left\lfloor \dfrac{n}{2} \right\rfloor$, which graph has the extremal Kirchhoff index among all connected graphs obtained by deleting p edges from K_n?

Before solving the above problem, we need a related lemma as follows:

Lemma 3.1. ([7]) *Let* G *be a connected graph with at least one edge. Then*

$$\mu_1(G) \leq \max_{v_i v_j \in E(G)} |N_i \cup N_j| \tag{2}$$

where N_i *is the neighbor set of vertex* $v_i \in V(G)$. *This upper bound for* $\mu_1(G)$ *does not exceed* n.

In the following theorem we will give a complete solution of this problem for the minimal case.

Theorem 3.2. *For any integer* $2 \leq p \leq \left\lfloor \dfrac{n}{2} \right\rfloor$ *and any graph* G *obtained by deleting* p *edges from* K_n, *we have*

$$Kf(G) \geq n - 1 + \frac{2p}{n-2} \tag{3}$$

with equality holding in (3) *if and only if* $G \cong K_n - p\,K_2$.

Proof. Denote by $\overline{\mu}_i$ with $i = 1, 2, \ldots, n$ the non-increasing Laplacian eigenvalues of $\overline{G}$. By Lemma 2.3, we have $\overline{\mu}_i = n - \mu_{n-i}$ for $i = 1, 2, \ldots, n - 1$. Since $\overline{G}$ is the complement graph of G, we have $\overline{m} = p$ with $2 \leq p \leq \lfloor \frac{n}{2} \rfloor$, where $\overline{m}$ is the number of edges in $\overline{G}$. Since

$$\overline{m} = p \leq \left\lfloor \frac{n}{2} \right\rfloor,$$

$\overline{G}$ must be a disconnected graph. Let k be the number of connected components in $\overline{G}$. Also let $\overline{n}_i$ and $\overline{m}_i$ be the number of vertices and number of edges in the i-th component

of $\overline{G}$ such that $\overline{n}_1 \geq \overline{n}_2 \geq \cdots \geq \overline{n}_{k-1} \geq \overline{n}_k$. Thus we have

$$\sum_{i=1}^{k} \overline{n}_i = n \quad \text{and} \quad \sum_{i=1}^{k} \overline{m}_i = \overline{m} = p.$$

From the above, it follows that

$$p = \sum_{i=1}^{k} \overline{m}_i \geq \sum_{i=1}^{k} (\overline{n}_i - 1) = n - k, \quad \text{that is,} \quad k \geq n - p.$$

Therefore there are at least $n - p$ Laplacian eigenvalues which are zero in $\overline{G}$, that is,

$$\overline{\mu}_i = 0, \ i = p + 1, \ p + 2, \ldots, \ n. \tag{4}$$

Using the above, we get

$$\sum_{i=1}^{n-1} \overline{\mu}_i = \sum_{i=1}^{p} \overline{\mu}_i = 2p. \tag{5}$$

Since $\overline{G}$ is disconnected, by Lemma 3.1, we have

$$\overline{\mu}_i \leq n - 1, \ i = 1, 2, \ldots, n - 1.$$

Now we have

$$\begin{aligned}
Kf(G) &= \sum_{i=1}^{n-1} \frac{n}{\mu_i} \\
&= \sum_{i=1}^{n-1} \frac{n}{n - \overline{\mu}_{n-i}} \quad \text{as } \mu_i = n - \overline{\mu}_{n-i} \\
&= n - 1 - p + \sum_{i=1}^{p} \frac{n}{n - \overline{\mu}_i} \quad \text{by (4)} \\
&\geq n - 1 - p + \frac{p^2}{\displaystyle\sum_{i=1}^{p} \frac{n - \overline{\mu}_i}{n}} \quad \text{by AM and HM inequality} \tag{6} \\
&= n - p - 1 + \frac{p}{1 - 2/n} \quad \text{as } \sum_{i=1}^{p} \overline{\mu}_i = 2p \\
&= n - 1 + \frac{2p}{n - 2}.
\end{aligned}$$

9

First part of the proof is done.

Now suppose that the equality holds in (3). Then all inequalities in the above argument must be equalities. From the equality in (6), we get

$$\frac{n}{n - \overline{\mu}_1} = \frac{n}{n - \overline{\mu}_2} = \cdots = \frac{n}{n - \overline{\mu}_p}\,, \quad \text{that is, } \overline{\mu}_1 = \overline{\mu}_2 = \cdots = \overline{\mu}_p\,.$$

Using (5), from the above, we get

$$\overline{\mu}_1 = \overline{\mu}_2 = \cdots = \overline{\mu}_p = 2.$$

From the above, we conclude that each connected component $(n_i \geq 2)$ is isomorphic to K_2, otherwise, the largest Laplacian eigenvalue in $\overline{G}$ is $\overline{\mu}_1 \geq 3$, a contradiction. Hence $\overline{G} \cong pK_2 \cup (n - 2p)K_1 = pK_2 \cup \overline{K_{n-2p}}$, that is, $G \cong K_n - p\,K_2$.

Conversely, let G be isomorphic to the graph $K_n - p\,K_2$. Then the Laplacian spectrum of G is

$$S(G) = \{n^{(n-p-1)}, (n-2)^{(p)}, 0\}\,.$$

Hence the equality holds in (3). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad\square$

Lemma 3.2. ([21]) *Let G be a simple graph on n vertices which has at least one edge. Then*

$$\mu_1 \geq \Delta + 1\,, \tag{7}$$

where Δ is the maximum degree in G. Moreover, if G is connected, then the equality holds in (7) if and only if $\Delta = n - 1$.

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

$$A_1 = \frac{a_1 + a_2 + \cdots + a_n}{n}$$

$$A_2 = \frac{a_1 a_2 + a_1 a_3 + \cdots + a_1 a_n + a_2 a_3 + \cdots + a_{n-1} a_n}{\frac{1}{2}\,n(n-1)}$$

$$\vdots$$

$$A_{n-1} = \frac{a_2 \ldots a_{n-1}\,a_n + a_1 a_3 \ldots a_{n-1}\,a_n + \cdots + a_1 a_2 \ldots a_{n-2}\,a_n + a_1 a_2 \ldots a_{n-1}}{n}$$

$$A_n = a_1 a_2 \ldots a_n\,.$$

Hence the AM is simply A_1 and the GM is $A_n^{1/n}$. The following result generalize this:

Lemma 3.3. (Maclaurin's Symmetric Mean Inequality [3]) *For positive real numbers $a_1, a_2, \ldots, a_n$,*

$$A_1 \geq A_2^{1/2} \geq A_3^{1/3} \geq \ldots \geq A_{n-1}^{1/(n-1)} \geq A_n^{1/n}.$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_n$.

Theorem 3.3. *For any integer $2 \leq p \leq \lfloor \frac{n}{2} \rfloor$ and any graph G obtained by deleting p edges from K_n, we have*

$$Kf(G) \leq n - 1 - p + \frac{n}{n-p-1} + \frac{(p-1)\,\delta\,n^{n-p-1}\,(n-1)^{p-2}}{t(G)}, \tag{8}$$

where $t(G)$ is the number of spanning trees in G and δ is the minimum degree in G. Moreover, the equality holds in (8) if and only if $G \cong K_n - K_{1,p}$.

Proof. For the sake of consistency, $\overline{\mu}_i$ with $i = 1, 2, \ldots, n$, $\overline{m}$, $\overline{m}_i$ and $\overline{n}_i$ are similarly defined as that in the proof of Theorem 3.2. Then we claim that $\overline{G}$ has exactly $n - p$ components of order n and with p edges. It follows that

$$\overline{\mu}_i = 0, \ i = p+1, p+2, \ldots, n, \ \text{ that is, } \ \mu_i = n, \ i = 1, 2, \ldots, n-p-1. \tag{9}$$

Moreover, we have

$$\sum_{i=1}^{p} \overline{\mu}_i = 2p. \tag{10}$$

Now we assume that $\overline{G} = \bigcup_{i=1}^{n-p} H_i$ and $\overline{\Delta}$ is the maximum degree in $\overline{G}$. Then, by Lemmas 3.1 and 3.2, we have

$$\overline{\Delta} + 1 \leq \overline{\mu}_1 = \max_{1 \leq i \leq n-p} \mu_1(H_i) \leq p + 1. \tag{11}$$

Putting $n = p - 1$ and $a_i = n - \overline{\mu}_{i+1}$, $i = 1, 2, \ldots, p-1$ in Lemma 3.3, we get $A_1 \geq A_{p-2}^{1/(p-2)}$, that is,

$$\frac{\sum_{i=2}^{p} (n - \overline{\mu}_i)}{p - 1} \geq \left[\frac{\prod_{i=2}^{p} (n - \overline{\mu}_i) \sum_{i=2}^{p} \frac{1}{n - \overline{\mu}_i}}{p - 1} \right]^{1/(p-2)}. \tag{12}$$

11

It is well known that

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

Since $n - \mu_{n-1} = \overline{\mu}_1 \geq \overline{\Delta} + 1$ and $n - \overline{\Delta} - 1 = \delta$, we have

$$\prod_{i=2}^{p} (n - \overline{\mu}_i) = \prod_{i=2}^{p} \mu_{n-i} = \frac{\prod_{i=1}^{n-1} \mu_i}{\prod_{i=1}^{n-p-1} \mu_i \cdot \mu_{n-1}} \geq \frac{n \, t(G)}{n^{n-p-1} \, \delta}$$

and

$$\frac{\sum_{i=2}^{p} (n - \overline{\mu}_i)}{p - 1} = \frac{n(p-1) - (2p - \overline{\mu}_1)}{p - 1} \leq n - 1 \quad \text{as } \overline{\mu}_1 \leq p + 1.$$

Using the above result in (12), we get

$$\sum_{i=2}^{p} \frac{1}{n - \overline{\mu}_i} \leq \frac{(p-1)}{\prod_{i=2}^{p} (n - \overline{\mu}_i)} \, (n-1)^{p-2}$$

$$\leq \frac{(p-1)\,(n-1)^{p-2}\,\delta\,n^{n-p-1}}{n\,t(G)} \, . \tag{13}$$

Therefore, we have

$$
\begin{aligned}
Kf(G) &= \sum_{i=1}^{n-1} \frac{n}{\mu_i} \\
&= \sum_{i=1}^{n-1} \frac{n}{n - \overline{\mu}_{n-i}} \quad \text{as } \mu_i = n - \overline{\mu}_{n-i} \\
&= n - 1 - p + \sum_{i=1}^{p} \frac{n}{n - \overline{\mu}_i} \quad \text{by (9)} \\
&\leq n - 1 - p + \frac{n}{n - p - 1} + \sum_{i=2}^{p} \frac{n}{n - \overline{\mu}_i} \quad \text{by (11)} \, .
\end{aligned}
$$

Using (13) in the above, we get the required result in (8). First part of the proof is done.

Now suppose that the equality holds in (8). Then all inequalities in the above argument must be equalities. From the equality in (12), we get $\overline{\mu}_2 = \overline{\mu}_3 = \cdots = \overline{\mu}_p$, by Lemma 3.3.

From the equality in (13), we get $\overline{\mu}_1 = p + 1$. Using (10) with the above results, we get $\overline{\mu}_2 = \overline{\mu}_3 = \cdots = \overline{\mu}_p = 1$. Thus we must have $\overline{G}$ is tree $K_{1,p}$ and all the remaining

12

$n - p - 1$ components are trivially K_1's. Equivalently, we deduce that $G = K_n - K_{1,p}$.

Conversely, let $G \cong K_n - K_{1,p}$. Then we have $\mu_1 = \mu_2 = \cdots = \mu_{n-p-1} = n$, $\mu_{n-p} = \mu_{n-p+1} = \cdots = \mu_{n-2} = n - 1$ and $\mu_{n-1} = n - p - 1$. Also we have $t(G) = (n - p - 1) n^{n-p-2} (n - 1)^{p-1}$ and $\delta = n - p - 1$. Now,

$$n - 1 - p + \frac{n}{n - p - 1} + \frac{(p - 1)\delta n^{n-p-1}(n - 1)^{p-2}}{t(G)}$$

$$= n - p - 1 + \frac{n}{n - 1}(p - 1) + \frac{n}{n - p - 1}$$

$$= Kf(K_n - K_{1,p}).$$

This completes the proof. $\square$

The following lemma was implicitly proved in [16].

Lemma 3.4. ([16]) *Let G be a connected graph obtained by deleting $p \leq n - 1$ edges from the complete graph K_n. Then we have*

$$t(G) \geq n^{n-p-2}(n - 1)^{p-1}(n - p - 1), \tag{14}$$

with equality holding if and only if $G \cong K_n - K_{1,p}$.

Combining Lemma 3.4 and Theorem 3.3, we can easily deduce the following corollary.

Corollary 3.1. *For any integer $2 \leq p \leq \lfloor \frac{n}{2} \rfloor$ and any graph G obtained by deleting p edges from K_n, we have*

$$Kf(G) \leq n - 1 - p + \frac{n}{n - p - 1} + \frac{n(p - 1)\delta}{(n - 1)(n - p - 1)}, \tag{15}$$

where δ is the minimum degree in G. Moreover, the equality holds in (8) if and only if $G \cong K_n - K_{1,p}$.

3.2 The ordering of connected graphs with larger Kirchoff indices

In this subsection we will determine the graphs from $\mathcal{G}(n)$ $(n > 27)$ with first to ninth largest Kirchhoff indices. Considering Lemma 2.2 (1) and Corollary 2.2, we find that the

path P_n has the largest Kirchhoff index among all graphs from $\mathcal{G}(n)$. Before stating our main result, we first prove a lemma below.

Lemma 3.5. *For any connected graph G of order n and with $m > n + 1$ edges, there exists a connected graph G_1 of order n and with $n + 1$ edges such that $Kf(G_1) > Kf(G)$.*

Proof. For any connected graph G of order n with $m > n+1$ edges, choosing and deleting one non-cut edge from G, we can get a connected graph G' of order n with $m - 1$ edges and $Kf(G') > Kf(G)$ by Lemma 2.2 (1). Repeating the above process by $m-n-1$ times, we can obtain a connected graph G_1 of order n with $n + 1$ edges and $Kf(G_1) > Kf(G)$, completing the proof of this lemma. $\qquad\square$

Now we denote by Q_n^k (see Figure 3 for the case when $k = 3$) the graph obtained by attaching a pendent edge to the unique neighbor of the pendent vertex in P_{n-1}^k. Let R_n^3 be a graph, shown in Figure 3, which is obtained by attaching a pendent edge to the vertex with the distance 2 from the pendent vertex in P_{n-1}^3. A graph CQ_n^3 is obtained by attaching a pendent edge to a vertex of C_3 in Q_{n-1}^3 with degree 2. Let $C_3(k_1, k_2)$ be a graph obtained attaching a path of length k_1 to one vertex of C_3 and a path of length k_2 to another vertex in C_3. Denote by $C_3(k_1, k_2, k_3)$ a graph obtained by attaching three paths of lengths k_1, k_2 and k_3, respectively, to three vertices of C_3. In the following we define two sets of graphs:

$$\mathcal{H}(n) = \left\{ P_n^3, Q_n^3, R_n^3, C_3(1, n - 4), C_3(2, n - 5), CQ_n^3 \right\},$$

$$\mathcal{T}^0(n) = \left\{ P_n, T_n(n - 3, 1^2), T_n(n - 4, 2, 1), T_n(1^2; 1^2), T_n(n - 5, 3, 1), T_n(1^2; 2, 1) \right\}.$$
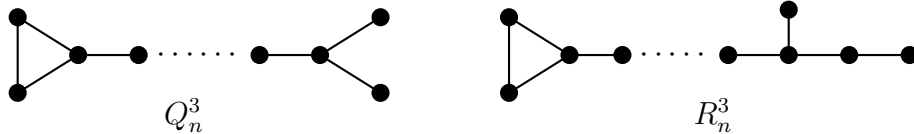

Figure 3: The graphs Q_n^3 and R_n^3

It is not difficult to verify that any spanning tree of the graphs $C_3(1, 1)$ and $C_3(1, 1, 1)$ must be in the set $\mathcal{T}^0(n)$.

Lemma 3.6. *Let G be a connected graph of order n ($n \geq 10$) with n edges and maximum degree $\Delta \geq 3$, cycle length $k > 4$. Then G has a spanning tree T with $T \notin \mathcal{T}^0(n)$.*

Proof. Assume that G contains a cycle C_k as a subgraph. According to the value of Δ, we divide into the following two cases.

Case 1. $\Delta \geq 4$.

In this case, we choose $G - e$ where e is on the cycle in G but not incident with the vertex of degree Δ in it. Then $G - e$ is a spanning tree of G with maximum degree $\Delta \geq 4$. Then $G - e \notin \mathcal{T}^0(n)$, since any tree in $\mathcal{T}^0(n)$ has maximum degree 3.

Case 2. $\Delta = 3$.

Assume that v is a vertex in C_k of degree 3 in G. Note that $k \geq 5$ from the condition in this lemma. Now we choose an edge $e = v_1 v_2$ on the cycle C_k in G such that v_1 and v_2 are all in the distance as large as possible from the vertex v. Since $k \geq 5$, we have $d_G(v, v_1) \geq 2$ and $d_G(v, v_2) \geq 2$. Then $G - e$ is a spanning tree of G with $G - e \notin \mathcal{T}^0(n)$, since neither of neighbors of v are pendent vertices. $\qquad \square$

Lemma 3.7. *Let $G \notin \mathcal{H}(n)$ be a connected graph of order n ($n \geq 8$) with n edges and maximum degree $\Delta \geq 3$, cycle length $k = 3$. Then G has a spanning tree T with $T \notin \mathcal{T}^0(n)$.*

Proof. For the case $\Delta > 3$, from a similar reasoning as that in Case 1 in the proof of Lemma 3.6, our result follows immediately. Therefore it suffices to consider the case $\Delta = 3$. Assume that $C_3 = v_1 v_2 v_3 v_1$ in G. Next we deal with the following three cases.

Case 1. There is only one vertex, say v_1, of C_3 in G with degree 3.

In this case, we choose the edge $e = v_2 v_3$ in C_3. Then $G - e$ is a spanning tree of G, in which the vertex v_1 is still of degree 3. Thus we have $G - e \not\cong P_n$. If $G - e \cong T_n(n - 3, 1^2)$, then the super graph G obtained by inserting the edge e into $T_n(n - 3, 1^2)$ is just P_n^3, contradicting the fact that $G \notin \mathcal{H}(n)$. Therefore $G - e \not\cong T_n(n - 3, 1^2)$. By a similar reasoning, we can conclude that $G - e \not\cong T_n(1^2; 1^2)$ for the edge $e \in E(G)$ defined as above from the condition that $G \not\cong Q_n^3$. Moreover, if $G - e \cong T_n(1^2; 2, 1)$ for the edge e in the triangle in G and not incident with the vertex v in it, then we claim that $G \cong R_n^3$. This is impossible because of the fact that $G \notin \mathcal{H}(n)$. Therefore, we have $G - e \notin \mathcal{T}^0(n)$.

Case 2. There are exactly two vertices, say v_1 and v_2, of C_3 in G with degree 3.

In this case, without loss of generality, we assume that the eccentricity of v_1 is not more than that of v_2 in G. Let $e = v_2 v_3$. Then $G - e$ is a spanning tree in G. Since $G \not\cong C_3(1, n-4)$, we deduce that $G - e \not\cong T_n(n-4, 2, 1)$. Similarly, we have $G - e \not\cong T_n(n-5, 3, 1)$ from the condition $G \not\cong C_3(2, n-5)$. Moreover, $G - e \not\cong T_n(1^2; 2, 1)$, since $G \not\cong CQ_n^3$. Note that, in $G - e$, there are at least two pendent vertices at the distance $d \geq 2$ to v_1 with degree 3. Therefore we have $G - e \notin \mathcal{T}^0(n)$ as desired.

Case 3. All the vertices of C_3 in G are of degree 3.

Assume that v_1 has the smallest eccentricity among all the vertices of C_3 in G. Let $e = v_2 v_3$. Then $G - e$ is a spanning tree of G such that v_1 is of degree 3 in it. Moreover, $G - e \notin \mathcal{T}^0(n)$, since there are at least three pendent vertices at the distance at least 2 to v_1 in $G - e$. This completes the proof for this case, ending the proof of this lemma. $\square$

Theorem 3.4. *Let $n > 27$. Then we have*

$$Kf(P_n) > Kf(T_n(n-3, 1^2)) > Kf(P_n^3) > Kf(T_n(n-4, 2, 1)) > Kf(T_n(1^2; 1^2)) > Kf(Q_n^3)$$
$$> Kf(T_n(n-5, 3, 1)) > Kf(T_n(n-4, 1^3)) = Kf(T_n(1^2; 2, 1)) > Kf(C_{3,3}^{n-5}).$$

Proof. In view of Corollary 2.2 and Lemma 2.6, considering Lemma 2.2 (2), we claim that the remaining is only to prove the following inequalities:

$$Kf(P_n^3) > Kf(T_n(n-4, 2, 1)), \tag{16}$$

$$Kf(Q_n^3) > Kf(T_n(n-5, 3, 1)), \tag{17}$$

$$Kf(T_n(1^2; 2, 1)) > Kf(C_{3,3}^{n-5}). \tag{18}$$

From Lemma 2.4 and the results in [19], we have

$$Kf(T_n(n-4, 2, 1)) = \binom{n+1}{3} - 2n + 8 = \frac{n^3 - 13n + 48}{6},$$

$$Kf(T_n(n-5, 3, 1)) = \binom{n+1}{3} - 3n + 15 = \frac{n^3 - 19n + 90}{6},$$

$$Kf(T_n(1^2; 2, 1)) = \binom{n+1}{3} - 3n + 11 = \frac{n^3 - 19n + 66}{6}.$$

16

By Lemmas 2.6 and 2.7, we arrive at the following results:

$$Kf(P_n^3) = \frac{n^3 - 11n + 18}{6}, \quad Kf(C_{3,3}^{n-5}) = \frac{n^3 - 21n + 36}{6}.$$

Some straightforward calculations show the validity of inequalities (16) and (18) for $n > 27$.

Setting $T' = T_{n-2}(n - 5, 1^2)$ and applying Lemma 2.8 to the vertex of degree 3 in C_3 of Q_n^3, we have

$$
\begin{aligned}
Kf(Q_n^3) &= Kf(C_3) + Kf(T') + 2Kf_x(T') + (n - 2)Kf_x(C_3) \\[2mm]
&= 2 + \frac{(n-2)^3 - 7(n-2) + 18}{6} \\[2mm]
&\quad + 2\left[1 + 2 + 3 + \cdots\cdots + (n - 5) + 2(n - 4)\right] + \frac{4}{3}(n - 3) \\[2mm]
&= \frac{n^3 - 17n + 36}{6}.
\end{aligned}
$$

It can be easily checked that $\dfrac{n^3 - 17n + 36}{6} > \dfrac{n^3 - 19n + 90}{6}$ when $n > 27$, i.e., the inequality (17) holds if $n > 27$. This completes the proof of this theorem. $\square$

Now we define a new set of graphs as follows:

$$\mathcal{G}^0(n) = \mathcal{T}^0(n) \bigcup \left\{T_n(n - 4, 1^3), P_n^3, Q_n^3, C_{3,3}^{n-5}\right\}.$$

In the following theorem we order the graphs from $\mathcal{G}(n)$ with first to tenth largest Kirchhoff indices.

Theorem 3.5. *Let G be any graph from $\mathcal{G}(n) \setminus \mathcal{G}^0(n)$ with $n > 27$. Then we have*

$$Kf(P_n) > Kf(T_n(n - 3, 1^2)) > Kf(P_n^3) > Kf(T_n(n - 4, 2, 1)) > Kf(T_n(1^2; 1^2)) > Kf(Q_n^3)$$

$$> Kf(T_n(n - 5, 3, 1)) > Kf(T_n(n - 4, 1^3)) = Kf(T_n(1^2; 2, 1)) > Kf(C_{3,3}^{n-5}) > Kf(G).$$

Proof. By Theorem 3.4, it suffices to prove that $Kf(G) < Kf(C_{3,3}^{n-5})$ for any graph $G \in \mathcal{G}(n) \setminus \mathcal{G}^0(n)$ with $n > 27$.

If $G \in \mathcal{G}(n) \setminus \mathcal{G}^0(n)$ has $m > n + 1$ edges, by Lemma 3.5, we conclude that there exists a connected graph G_1 of order n and with $n + 1$ edges such that $Kf(G) < Kf(G_1)$. By

17

Lemma 2.7, we have $Kf(G) < Kf(G_1) \le Kf(C_{3,3}^{n-5})$. Clearly, for any connected graph G of order n and with $n+1$ edges, $Kf(G) < Kf(C_{3,3}^{n-5})$ from Lemma 2.7, again.

Now we only need to consider the connected graphs of order n and with $m \le n$ edges. In the case when $m = n-1$ with $n > 27$, for any graph $G \notin \mathcal{T}^0(n) \bigcup \{T_n(n-4,1^3)\}$ of order n and with $n-1$ edges, i.e., G is a tree, by Corollary 2.2 and Lemma 2.8, we have

$$
\begin{aligned}
Kf(G) &\le Kf(T_n(n-6,4,1)) \\
&= \binom{n+1}{3} - 4n + 24 \\
&= \frac{n^3 - 25n + 144}{6} \\
&< \frac{n^3 - 21n + 36}{6} \\
&= Kf(C_{3,3}^{n-5}).
\end{aligned}
$$

Now we focus on the case when $m = n$. Combining Lemma 3.6 and Corollaries 2.1 and 2.2, we find that, when $n > 27$, for any connected graph G of order n and with n edges, maximum degree $\Delta \ge 3$ and cycle length $k > 4$, we have $Kf(G) \le Kf(T_n(n-6,4,1)) < Kf(C_{3,3}^{n-5})$. By Lemma 2.9, we have $Kf(G) \le Kf(P_n^4)$ for any connected graph G of order n and with n edges and cycle length 4. From Lemma 3.7, Corollaries 2.1 and 2.2, we have $Kf(G) \le Kf(T_n(n-6,4,1)) < Kf(C_{3,3}^{n-5})$ for any graph $G \notin \mathcal{H}(n)$ of order n with n edges, cycle length 3 and maximum degree Δ. Thus the remaining for this case is to show that $Kf(G) < Kf(C_{3,3}^{n-5})$ for any graph G from the set $\{R_n^3, P_n^4, C_n, C_3(1, n-4), C_3(2, n-5), CQ_n^3\}$. From Corollary 2.3, $Kf(CQ_n^3) < Kf(C_3(1, n-4))$. Note that $Kf(P_n^3) = \dfrac{n^3 - 11n + 18}{6}$ and $Kf(P_n) = \dfrac{n^3 - n}{6}$ ([19]). Applying Lemma 2.8 to the vertices in C_3 of $C_3(1, n-4), C_3(2, n-5)$, respectively, with degree 3 and a smaller eccentricity, we have

$$
Kf(C_3(1, n-4)) = \frac{n^3 - 27n + 82}{6}, \quad Kf(C_3(2, n-5)) = \frac{n^3 - 25n + 88}{6},
$$

both of them is less than $\dfrac{n^3 - 21n + 36}{6} = Kf(C_{3,3}^{n-5})$. Moreover, we have $Kf(CQ_n^3) < Kf(C_{3,3}^{n-5})$. By the formula

$$
Kf(P_n^l) = \frac{n^3 - 2n}{6} + \frac{(1+2n)l}{4} + \frac{l^3}{4} - \frac{(3+2n)l^2}{6}
$$

18

in [24], we can get

$$Kf(P_n^4) = \frac{n^3 - 22n + 54}{6} < \frac{n^3 - 21n + 36}{6} = Kf(C_{3,3}^{n-5}) \quad \text{when} \quad n > 27.$$

Also from [24], we have $Kf(C_n) = \dfrac{n^3 - n}{12}$. Therefore it follows that

$$
\begin{aligned}
Kf(C_n) &= \frac{n^3 - n}{12} \\
&< \frac{n^3 - 21n + 36}{6} \\
&= Kf(C_{3,3}^{n-5}) \quad as \quad n^3 - 41n + 72 > 0 \quad \text{when} \quad n > 27.
\end{aligned}
$$

Finally, setting $T'' = T_{n-2}(n-6, 2, 1)$, by the application of Lemma 2.8 to the vertex, say x, of degree 3 on the triangle C_3 of R_n^3, we have

$$
\begin{aligned}
Kf(R_n^3) &= Kf(C_3) + Kf(T'') + (n-3)Kf_x(C_3) + 2Kf_x(T'') \\
&= 2 + \frac{(n-2)^2 - 13(n-2) + 48}{6} + \frac{4}{3}(n-3) \\
&\quad + 2\Big[1 + 2 + \cdots + (n-5) + (n-4) + (n-5)\Big] \\
&= \frac{n^3 - 23n + 66}{6}.
\end{aligned}
$$

Obviously, we conclude that

$$Kf(R_n^3) = \frac{n^3 - 23n + 66}{6} < \frac{n^3 - 21n + 36}{6} = Kf(C_{3,3}^{n-5}) \quad \text{if} \quad n > 27.$$

Thus we complete the proof of this theorem. $\qquad\square$

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