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The second maximal and minimal Kirchhoff indices of unicyclic graphs[1]

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Abstract

Resistance distance was introduced by Klein and Randić. The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distances between all pairs of vertices. In this paper, we give the second maximal and minimal Kirchhoff indices of unicyclic graphs and characterize the extremal graphs.

1 Introduction

In 1993, Klein and Randić [1] defined a new distance function named resistance distance on the basis of electrical network theory. The term resistance distance was used because of the physical interpretation: one imagines unit

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resistors on each edge of a connected graph G with vertices $v_1, v_2, \cdots, v_n$ and takes the resistance distance between vertices v_i and v_j of G to be the effective resistance between vertices v_i and v_j, denoted by $r_G(v_i, v_j)$. Recall that the conventional 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 and the famous Wiener index [2] is the sum of distances between all pairs of vertices; that is,

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

Analogue to Wiener index, the Kirchhoff index [3] is defined as

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

Similar to the conventional distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical and physical interpretations [4,5], but with a substantial potential for chemical applications. In fact, for those two distance functions, 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 that chemical communication in molecules is rather wavelike suggests the utility of this concept in chemistry. So in recent years, the resistance distance was much studied in the chemical literature [6-17]. It is found that the resistance distance is closely related with many well known graph invariants, such as the connectivity index, the Balaban index, etc. This further suggests the resistance distance is worthy of study.

The resistance distance is also well studied in mathematical literatures. Much work has been done to compute Kirchhoff index of some classes of graphs, or give some bounds for Kirchhoff index of graphs and characterize extremal graphs [10,15,18].

For instance, unicyclic graphs with extremal Kirchhoff index are characterized and sharp bounds for Kirchhoff index of such graphs are obtained [19].

In this paper, we give the second maximal Kirchhoff index among n-vertex unicyclic graphs and characterize extremal graphs as well.

2 Some Lemmas

For convenience, we represent a unicyclic graph G with the unique cycle $C_l = v_1v_2\cdots v_lv_1$ as $G = U(C_l; T_1, T_2, \cdots, T_l)$, where T_i is the component of $G - E(C_l)$ containing v_i, $1 \le i \le l$. Obviously, T_i is a tree rooted at v_i, see Figure 1(a). We say T_i trivial if it is an isolated vertex.

Let $\mathcal{U}(n, l)$ be the set of all unicyclic graphs with n vertices and the unique cycle C_l, S_n^l the unicyclic graph obtained from cycle C_l by adding $n - l$ pendant edges to a vertex of C_l and P_n^l the unicyclic graph obtained by identifying one end vertex of path P_{n-l+1} with any vertex of C_l, see Figure 1(b)(c). It is obvious that $S_n^n = P_n^n = C_n$.

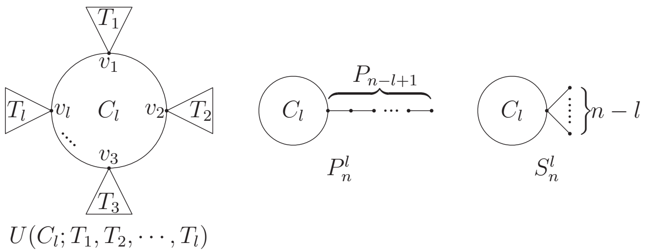


Figure 1. The graphs $U(C_l; T_1, T_2, \cdots, T_l)$, P_n^l and S_n^l.

For a tree, the Kirchhoff index coincides with the Wiener index. It was shown that P_n and S_n have the maximal and minimal Kirchhoff index among all trees with n vertices, respectively.

Lemma 2.1([20]). Let T be a n-tree different from P_n and S_n. Then

$$Kf(S_n) < Kf(T) < Kf(P_n).$$

In [19], it was shown that P_n^l and S_n^l have the maximal and minimal Kirchhoff index among $\mathcal{U}(n,l)$, respectively.

Lemma 2.2([19]). Let $G \in \mathcal{U}(n,l)$.
(i) If $G \neq P_n^l$, then $Kf(G) < Kf(P_n^l)$;
(ii) If $G \neq S_n^l$, then $Kf(G) > Kf(S_n^l)$.

Lemma 2.3([1]). Let x be a cut vertex of a connected graph and a and b be vertices occurring in different components which arise upon deletion of x. Then

$$r_G(a,b) = r_G(a,x) + r_G(x,b).$$

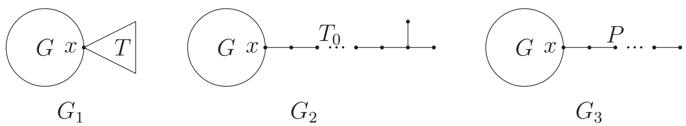
Lemma 2.4. Let G_1 and G_2 be two connected graphs with exactly one common vertex x, and $G = G_1 \cup G_2$. Then

$$Kf(G) = Kf(G_1) + Kf(G_2) + (|V(G_1)|-1)Kf_x(G_2) + (|V(G_2)|-1)Kf_x(G_1)$$

where $Kf_x(G_i) = \sum\limits_{y \in V(G_i)} r_{G_i}(x,y)$ is the sum of resistance distances between x and other vertices of G_i, $i = 1, 2$.

Proof. From the definition of Kirchhoff index and Lemma 2.3, we have

$$\begin{aligned} & Kf(G) \\ = & \sum_{i<j} r_G(v_i, v_j) \\ = & Kf(G_1) + Kf(G_2) + \sum_{a \in V(G_1)-\{x\}} \sum_{b \in V(G_2)-\{x\}} r_G(a,b) \\ = & Kf(G_1) + Kf(G_2) + \sum_{a \in V(G_1)-\{x\}} \sum_{b \in V(G_2)\{x\}} (r_G(a,x) + r_G(x,b)) \\ = & Kf(G_1) + Kf(G_2) + (|V(G_1)|-1)Kf_x(G_2) + (|V(G_2)|-1)Kf_x(G_1). \end{aligned}$$



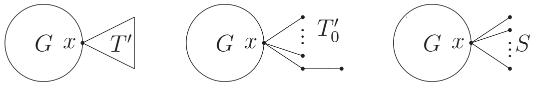


Figure 2.

Lemma 2.5. (i) If G_1, G_2 and G_3 are obtained from a connected graph G by attaching T, T_0 and P to the vertex x of G, respectively, as shown in Figure 2, where T, T_0 and the path P are different trees rooted at x with the same size. Then

$$Kf(G_1) < Kf(G_2) < Kf(G_3).$$

(ii) If G'_1, G'_2 and G'_3 are obtained from a connected graph G by attaching T', T'_0 and S to the vertex x of G, respectively, as shown in Figure 2, where T', T'_0 and the star S are different trees rooted at x with the same size. Then

$$Kf(G'_1) > Kf(G'_2) > Kf(G'_3).$$

Proof. Since Kirchhoff index and Wiener index of trees coincide, we have (i) $Kf_x(T) < Kf_x(T_0) < Kf_x(P)$ and $Kf(T) < Kf(T_0) < Kf(P)$; (ii) $Kf_x(T') > Kf_x(T'_0) > Kf_x(S)$ and $Kf(T') > Kf(T'_0) > Kf(S)$. Lemma 2.5 is a immediate result of Lemma 2.4.

Lemma 2.6. (i) Let G be a connected graph with two pendant paths $P_1 = u_1u_2\cdots u_r$ and $P_2 = v_1v_2\cdots v_t$, and $r \geq 2$, $t \geq 2$, depicted in Figure 3(i). If $Kf_{v_t}(G) \geq Kf_{u_r}(G)$, then

$$Kf(G') > Kf(G)$$

where $G' = G - u_ru_{r-1} + v_tu_r$.

(ii) Let G be a connected graph with two nontrivial stars S_1 and S_2 attached at their centers x and y, and x_1 and y_1 are leaves of S_1 and S_2, respectively, depicted in Figure 3(ii). If $Kf_{x_1}(G) \leq Kf_{y_1}(G)$, then

$$Kf(G') < Kf(G)$$

where $G' = G - yy_1 + xy_1$.

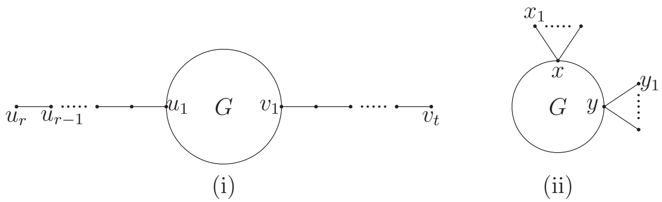


Figure 3.

Proof. (i) For $u, v \in V(G) - \{u_r\}$, we have $r_G(u,v) = r_{G'}(u,v)$, and

$$Kf_{u_r}(G') = Kf_{v_t}(G) - r_G(u_r, v_t) + |V(G)| - 1 > Kf_{v_t}(G) \geq Kf_{u_r}(G).$$

So, $Kf(G') = Kf(G) - Kf_{u_r}(G) + Kf_{u_r}(G') > Kf(G)$.

(ii) For any $u, v \in V(G) - \{y_1\}$, $r_G(u,v) = r_{G'}(u,v)$. And $r_G(x_1, y_1) > 2$,

$$Kf_{y_1}(G') = Kf_{x_1}(G') = Kf_{x_1}(G) - r_G(x_1, y_1) + 2 < Kf_{x_1}(G) \leq Kf_{y_1}(G).$$

So, $Kf(G') = Kf(G) - Kf_{y_1}(G) + Kf_{y_1}(G') < Kf(G)$.

3 The second maximal Kirchhoff index of unicyclic graphs

Theorem 3.1. Let $G \in \mathcal{U}(n,l)$, $3 \leq l \leq n-3$ and $G \neq P_n^l$.

(i) If $n \geq 8$, then $Kf(G) \leq Kf(H_0)$ with the equality if and only if $G \cong H_0$ (see Figure 4(3));

(ii) If $n = 7$, then $Kf(G) \leq Kf(H_0) = Kf(H_{[\frac{l}{2}]+1})$ with the equality if and only if $G \cong H_0$ or $G \cong H_{[\frac{l}{2}]+1}$;

(iii) If $n = 6$, then $Kf(G) \leq Kf(H_1)$ with the equality if and only if $G \cong H_1$.

Proof. Suppose that $G = U(C_l; T_1, T_2, \cdots, T_l)$ has the second maximal Kirchhoff index among $\mathcal{U}(n,l)$.

First, at most two of $T_1, T_2, \cdots, T_l$ are not trivial.

Otherwise, without loss of generality, we assume that T_1, T_2, T_3 are not trivial. They must be paths from Lemmas 2.4, 2.2(i) and 2.1. Let $T_1 = v_1 a_2 a_3 \cdots a_r$, $T_2 = v_2 b_2 b_3 \cdots b_s$, $T_3 = v_3 c_2 c_3 \cdots c_t$. If $Kf_{a_r}(G) \geq Kf_{b_s}(G)$, then

$$Kf(G) < Kf(G - b_{s-1}b_s + a_r b_s) < Kf(P_n^l)$$

by Lemma 2.6. If $Kf_{a_r}(G) < Kf_{b_s}(G)$, we also have from Lemma 2.6

$$Kf(G) < Kf(G - a_{r-1}a_r + b_s a_r) < Kf(P_n^l).$$

This contradicts the choice of G.

Next, if exactly two of $T_1, T_2, \cdots, T_l$ are not trivial, without loss of generality, we assume that T_1 and T_i are not trivial, $1 < i \leq l$. Then they are paths from Lemmas 2.4, 2.2(i) and 2.1, i.e., G is the graph shown in Figure 4(1). Let $T_1 = v_1 a_2 \cdots a_r$ and $T_i = v_i b_2 \cdots b_s$, where $r + s + l = n + 2$, $r \geq 2$ and $s \geq 2$. From Lemma 2.6(i), we have $r = 2$ or $s = 2$. Without loss of generality, assume that $s = 2$, i.e., $G = H_i$ is the graph shown in Figure 4(2). Then $r + l = n$. Calculating immediately by Lemma 2.4, we have

$$\begin{aligned} Kf(H_i) = \;& Kf(C_l) + Kf(P_r) + Kf(P_2) + (n-l)Kf_{v_1}(C_l) \\ & +(n-r)Kf_{v_1}(P_r) + (n-2)Kf_{v_i}(P_2) + (r-1)r_{C_l}(v_1, v_i) \\ = \;& Kf(C_l) + Kf(P_{n-l}) + 1 + (n-l)Kf_{v_1}(C_l) \\ & +\tfrac{1}{2}r(r-1)(n-r) + (n-2) + (r-1)r_{C_l}(v_1, v_i) \\ = \;& Kf(C_l) + (n-l)Kf_{v_1}(C_l) + Kf(P_{n-l}) + (n-1) \\ & +\tfrac{1}{2}(n-l)(n-l-1)l + (n-l-1)r_{C_l}(v_1, v_i) \end{aligned}$$

where

$$r_{C_l}(v_1, v_i) = \frac{(i-1)(l-i+1)}{l} \leq \begin{cases} \frac{l}{4}, & \text{if } l \text{ is even;} \\ \frac{(l-1)(l+1)}{4l}, & \text{if } l \text{ is odd} \end{cases}$$

with the equality if and only if $i = [\frac{l}{2}] + 1$ or $i = [\frac{l+1}{2}] + 1$.

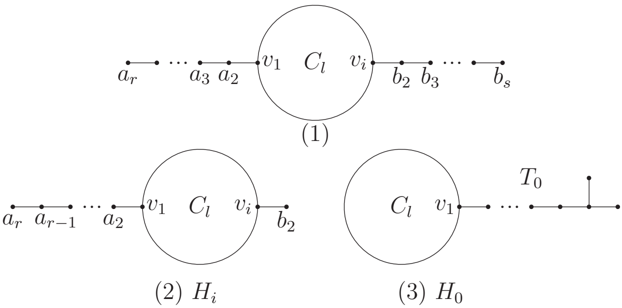


Figure 4.

If exactly one of $T_1, T_2, \cdots, T_l$ is not trivial, without loss of generality, we assume that T_1 is not trivial. Since $G \neq P_n^l$, $T_1 \neq P_{n-l+1}$. From Lemma 2.4 and $Kf_{v_1}(T_1) \leq Kf_{v_1}(T_0)$, we know that G is the graph H_0 shown in Figure 4(3).

$$\begin{aligned} Kf(H_0) = \;& Kf(C_l) + Kf(T_0) + (n-l)Kf_{v_1}(C_l) + (l-1)Kf_{v_1}(T_0) \\ = \;& Kf(C_l) + Kf(P_{n-l}) + \tfrac{1}{2}(n-l-1)(n-l-2) + (n-l+1) \\ & +(n-l)Kf_{v_1}(C_l) + \tfrac{1}{2}(n-l+2)(n-l-1)(l-1). \end{aligned}$$

So, we only need to compare the Kirchhoff indices of H_i and H_0.

I. If l is even, then $l \geq 4$, $r_{C_l}(v_1, v_i) \leq r_{C_l}(v_1, v_{\frac{l}{2}+1}) = \frac{1}{4}l$ and

$$\begin{aligned} & Kf(H_i) - Kf(H_0) \\ \leq \;& Kf(H_{[\frac{l}{2}]+1}) - Kf(H_0) \\ = \;& -4 + 2n - nl + l^2 + (n-l-1)r_{C_l}(v_1, v_{\frac{l}{2}+1}) \\ = \;& -4 + 2n - \tfrac{l}{4} - \tfrac{3nl}{4} + \tfrac{3l^2}{4}. \end{aligned}$$

Let $f(l) = -4 + 2n - \frac{l}{4} - \frac{3nl}{4} + \frac{3l^2}{4}$. We have

$$f(4) = 7 - n \quad \text{and} \quad f(n-3) = \frac{7}{2} - \frac{n}{2}.$$

It follows that

(i) $Kf(H_i) < Kf(H_0)$ for $n \geq 8$;

(ii) $Kf(H_i) \leq Kf(H_0) = Kf(H_{\frac{l}{2}+1})$ for $n = 7$.

II. If l is odd and $n \geq 8$, then

$r_{C_l}(v_1, v_i) \leq r_{C_l}(v_1, v_{[\frac{l}{2}]+1}) = r_{C_l}(v_1, v_{[\frac{l+1}{2}]+1}) = \frac{(l-1)(l+1)}{4l} < \frac{l+1}{4}$.

For $l = 3$, we have

$$\begin{aligned} & Kf(H_i) - Kf(H_0) \\ \leq\ & Kf(H_{[\frac{l}{2}]+1}) - Kf(H_0) = Kf(H_{[\frac{l+1}{2}]+1}) - Kf(H_0) \\ =\ & -4 + 2n - nl + l^2 + (n-l-1) r_{C_l}(v_1, v_{[\frac{l}{2}]+1}) \\ =\ & -4 + 2n - nl + l^2 + \tfrac{(l+1)(l-1)}{4l}(n-l-1) \\ =\ & \tfrac{7}{3} - \tfrac{n}{3}. \end{aligned}$$

For $l > 3$, we have

$$\begin{aligned} & Kf(H_i) - Kf(H_0) \\ \leq\ & Kf(H_{[\frac{l}{2}]+1}) - Kf(H_0) = Kf(H_{[\frac{l+1}{2}]+1}) - Kf(H_0) \\ =\ & -4 + 2n - nl + l^2 + (n-l-1) r_{C_l}(v_1, v_{[\frac{l}{2}]+1}) \\ <\ & -4 + 2n - nl + l^2 + \tfrac{l+1}{4}(n-l-1) \\ =\ & -\tfrac{17}{4} + \tfrac{9n}{4} - \tfrac{l}{2} - \tfrac{3nl}{4} + \tfrac{3l^2}{4}. \end{aligned}$$

Let $g(l) = -\frac{17}{4} + \frac{9n}{4} - \frac{l}{2} - \frac{3nl}{4} + \frac{3l^2}{4}$. Then $g(5) = 12 - \frac{3n}{2}$ and $g(n-3) = 4 - \frac{n}{2}$. Therefore, $Kf(H_i) < Kf(H_0)$ for $n \geq 8$.

III. If l is odd, and $n = 6, 7$, then $l = 3$ since $3 \leq l \leq n-3$. We have

$$\begin{aligned} & Kf(H_{[\frac{l}{2}]+1}) - Kf(H_0) = Kf(H_{[\frac{l+1}{2}]+1}) - Kf(H_0) \\ =\ & -4 + 2n - nl + l^2 + (n-l-1) r_{C_l}(v_1, v_{[\frac{l}{2}]+1}) \\ =\ & -4 + 2n - nl + l^2 + \tfrac{(l+1)(l-1)}{4l}(n-l-1) \\ =\ & \tfrac{7}{3} - \tfrac{n}{3}. \end{aligned}$$

It follows that (i) $Kf(H_i) \leq Kf(H_0) = Kf(H_{[\frac{l}{2}]+1})$ for $n = 7$ and $l = 3$; (ii) $Kf(H_0) < Kf(H_{[\frac{l}{2}]+1})$ for $n = 6$ and $l = 3$.

Corollary 3.2. For $n \geq 7$, the second maximal Kirchhoff index among $\mathcal{U}(n, l)$ is

$$Kf(H_0) = 3 - \frac{4n}{3} + \frac{n^3}{6} + \frac{l}{4} + \frac{nl}{2} - \frac{l^2}{2} - \frac{nl^2}{3} + \frac{l^3}{4}$$

Proof. From Theorem 3.1 and Lemma 2.5(i), we know that the second maximal Kirchhoff index among $\mathcal{U}(n, l)$ is $Kf(H_0)$ for $n \geq 7$.

Note that $Kf(C_l) = \frac{l^3-l}{12}$, $Kf_{v_1}(C_l) = \frac{l^2-1}{6}$ and $Kf(P_{n-l}) = \frac{1}{6}((n-l)^3 - (n-l))$.

From the proof of Theorem 3.1, we have

$$\begin{aligned} Kf(H_0) = &\ Kf(C_l) + Kf(P_{n-l}) + \tfrac{1}{2}(n-l-1)(n-l-2) + (n-l+1) \\ &+(n-l)Kf_{v_1}(C_l) + \tfrac{1}{2}(n-l+2)(n-l-1)(l-1) \\ = &\ 3 - \tfrac{4n}{3} + \tfrac{n^3}{6} + \tfrac{l}{4} + \tfrac{nl}{2} - \tfrac{l^2}{2} - \tfrac{nl^2}{3} + \tfrac{l^3}{4}. \end{aligned}$$

4 The second minimal Kirchhoff index of unicyclic graphs

Theorem 4.1. If $G \in \mathcal{U}(n,l)$, $3 \le l \le n-3$ and $G \ne S_n^l$, then $Kf(G) \ge Kf(F_2)$ with the equality if and only if $G = F_2$ (see Figure 5).

Proof. Suppose that $G = U(C_l; T_1, T_2, \cdots, T_l)$ has the second maximal Kirchhoff index among $\mathcal{U}(n,l)$.

First, at most two of $T_1, T_2, \cdots, T_l$ are not trivial.

Otherwise, we may assume that T_1, T_2, T_3 are not trivial. They must be stars with centers v_1, v_2, v_3, respectively, from Lemmas 2.4, 2.2(ii) and 2.1. Let $V(T_1) = \{v_1, a_2, a_3, \cdots, a_r\}$, $V(T_2) = \{v_2, b_2, b_3, \cdots, b_s\}$, $V(T_3) = \{v_3, c_2, c_3, \cdots, c_t\}$. Without loss of generality, we assume that $Kf_{a_2}(G) \le Kf_{b_2}(G)$, then

$$Kf(G) > Kf(G - v_2b_2 + v_1b_2) > Kf(S_n^l)$$

by Lemma 2.6(ii). This contradicts the choice of G.

Next, if exactly two of $T_1, T_2, \cdots, T_l$ are not trivial, without loss of generality, we assume that T_1 and T_i are not trivial, $1 < i \le l$. Then they are stars with centers v_1, v_i, respectively, from Lemmas 2.4, 2.2(ii) and 2.1, i.e., G is the graph shown in Figure 5(1). Let $V(T_1) = \{v_1, a_2, a_3, \cdots, a_r\}$, $V(T_i) = \{v_i, b_2, b_3, \cdots, b_s\}$, where $r + s + l = n + 2$, $r \ge 2$ and $s \ge 2$. From Lemma 2.6, we have $r = 2$ or $s = 2$. Without loss of generality, assume that $s = 2$, i.e., $G = F_i$ is the graph shown in Figure 5(2). Then $r + l = n$. Calculating immediately by Lemma 2.4, we have

$$\begin{aligned} Kf(F_i) = &\ Kf(C_l) + (n-l)Kf_{v_1}(C_l) + (n-l-1)r_{C_l}(v_1, v_i) \\ &+(n-1)(n-l) \end{aligned}$$

where

$$r_{C_l}(v_1, v_i) = \frac{(i-1)(l-i+1)}{l} \ge \frac{l-1}{l}$$

and $Kf(F_i) \geq Kf(F_2)$ with the equality if and only if $i = 2$ or $i = l$.

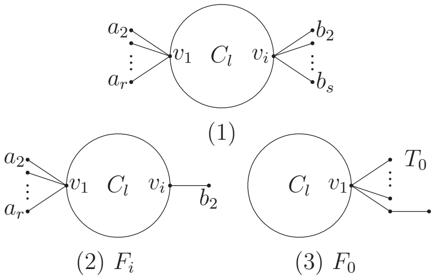


Figure 5.

If exactly one of $T_1, T_2, \cdots, T_l$ is not trivial, without loss of generality, we assume that T_1 is not trivial. Since $G \neq S_n^l$, $T_1 \neq S_{n-l+1}$. From Lemma 2.4 and $Kf_{v_1}(T_1) \geq Kf_{v_1}(T_0)$, we know that G is the graph F_0 shown in Figure 5(3).

$$Kf(F_0) = Kf(C_l) + (n-l)Kf_{v_1}(C_l) + n(n-l) + l - 3.$$

Note that $F_2 \cong F_l$, we only need to compare $Kf(F_2)$ and $Kf(F_0)$.

$$Kf(F_2) - Kf(F_0) = -\frac{1}{l} - \frac{n}{l} - l + 4 < 0$$

since $3 \leq l < n$.

So, F_2 is the unique graph with the second minimal Kirchhoff index among $\mathcal{U}(n, l)$ from Lemma 2.5(ii).

Using $Kf(C_l) = \frac{l^3 - l}{12}$ and $Kf_{v_1}(C_l) = \frac{l^2 - 1}{6}$, we have

Corollary 4.2. For $n \geq 6$, the second minimal Kirchhoff index among $\mathcal{U}(n, l)$ is

$$Kf(F_2) = -\frac{1}{12}l^3 + \frac{1}{6}nl^2 - nl + \frac{1}{12}l - \frac{n}{l} + \frac{1}{l} + n^2 - \frac{1}{6}n.$$

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