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The extremal Kirchhoff index of a class of unicyclic graphs[1]

Qiuzhi GUO, Hanyuan DENG[2], Dandan CHEN

College of Mathematics and Computer Science,

Hunan Normal University, Changsha, Hunan 410081, P. R. China

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Abstract

The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distances between all pairs of vertices. A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle. In this paper, we determine the minimal and maximal Kirchhoff indices among all fully loaded unicyclic graphs with n vertices, and characterize the extremal graphs.

1 Introduction

In 1993, Klein and Randić [1] defined resistance distance on the basis of electrical network theory. They viewed a connected graph G as an electrical

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[2]Corresponding author: hydeng@hunnu.edu.cn

network N by replacing each edge of G with a unit resistor. Let $v_1, v_2, \cdots, v_n$ be labeled vertices of G, 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. The conventional distance between vertices v_i and v_j, denoted by $d(v_i, v_j)$, is the length of a shortest path between them. H. Wiener in [2] defined a famous Wiener index $W(G) = \sum_{i<j} d(v_i, v_j)$. Analogue to Wiener index, the Kirchhoff index $Kf(G)$ is defined in [3]: $Kf(G) = \sum_{i<j} r_G(v_i, v_j)$.

As a useful structure-descriptor, Kirchhoff index is well studied in [4]. Much work has been done to compute Kirchhoff index of some classes of graphs, such as complete graphs [5], cycles [5,6], platonic solids [5,7], distance transitive graphs [11], circulant graphs [12], linear hexagonal chains [13], unicyclic graphs [14,15], and so on [8,9,10,16,17].

A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle.

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 components of $G - E(C_l)$ containing v_i, $1 \leq i \leq l$. 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. If $G = U(C_l; T_1, T_2, \cdots, T_l)$ is a fully loaded unicyclic graph, then $T_1, T_2, \cdots, T_l$ are all nontrivial.

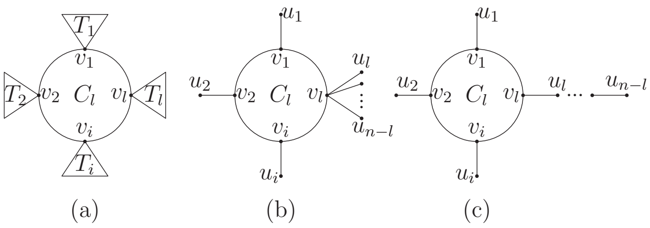

Figure 1. (a) $U(C_l; T_1, T_2, \cdots, T_l)$; (b) $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$; (c) $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$.

Let $\mathcal{U}(n, l)$ $(n \geq 2l)$ be the set of all fully loaded unicyclic graphs with n

vertices and the unique cycle C_l, S_n and P_n be the star and the path on n vertices, respectively.

In this paper, we will show that $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ and $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$ have minimal and maximal Kirchhoff index, respectively, among $\mathcal{U}(n, l)$, where $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ and $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$ are the fully loaded unicyclic graphs shown in Figure 1(b)(c).

2 The extremal Kirchhoff indices among $\mathcal{U}(n, l)$

Lemma 2.1([1]). Let x be a cut-vertex of a graph G, and let a and b be vertices in different components of $G - x$. Then

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

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 Wiener index among all trees with n vertices, respectively. So, we have

Lemma 2.2([18]). Let T be a n-vertex tree different from P_n and S_n. Then

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

Lemma 2.3([15]). 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, $i = 1, 2$.

Lemma 2.4([15]). If G_1, G_2 and G_3 are obtained from a connected graph G by attaching S_t, T_t and P_t to the vertex x of G, respectively, as shown in

Figure 2, where the star S_t, T_t and the path P_t are different trees rooted at x with t vertices. Then

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

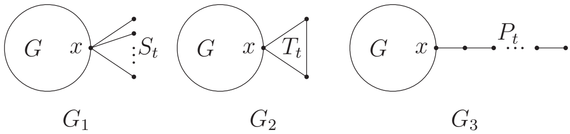

Figure 2.

Lemma 2.5([15]). (i) Let G be a connected graph with two pendent 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 $G' = G - yy_1 + xy_1$.

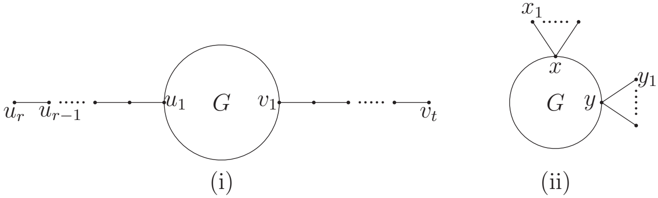

Figure 3.

Theorem 2.6. Let $G \in \mathcal{U}(n,l)$. If G is different from $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ and $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$, then

$$Kf(U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})) < Kf(G) < Kf(U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})).$$

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

For each i, T_i is a star with v_i as its central vertex by Lemma 2.4.

If $n > 2l+1$, then all but one of the T_i are K_2. Otherwise, we suppose that there are two trees T_i and T_j such that they both have more than two vertices. By Lemma 2.4, T_i and T_j are both stars. Let x_1 and y_1 be leaves of T_i and T_j, respectively. Without loss of generality, assume that $Kf_{x_1}(G) \leq Kf_{y_1}(G)$, then $Kf(G') < Kf(G)$ by Lemma 2.5, where $G' = G - v_j y_1 + v_i y_1$. This contradicts the choice of G.

So, $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ is the unique graph with the minimal Kirchhoff index among $\mathcal{U}(n,l)$.

Similarly, $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$ is the unique graph with the maximal Kirchhoff index among $\mathcal{U}(n,l)$.

In the following, we compute the Kirchhoff indices of $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ and $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$.

By the definition of Kirchhoff index and Figure 1(b), we have

$$\begin{aligned} & Kf(U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})) \\ = & \sum_{1\leq i<j\leq n-l} r(u_i,u_j) + \sum_{1\leq i<j\leq l} r(v_i,v_j) + \sum_{i=1}^{l}\sum_{j=1}^{n-l} r(v_i,u_j) \end{aligned}$$

and $Kf(C_l) = \sum_{1\leq i<j\leq l} r(v_i,v_j)$

$$\begin{aligned} & \sum_{1\leq i<j\leq n-l} r(u_i,u_j) \\ = & \sum_{1\leq i<j\leq l} r(v_i,v_j) + (n-2l)\sum_{i=1}^{l-1} r(v_i,v_l) \\ & +2((n-l-1)+(n-l-2)+\cdots+2+1)) \\ = & Kf(C_l) + (n-2l)Kf_{v_l}(C_l) + (n-l)(n-l-1) \end{aligned}$$

$$\sum_{i=1}^{l}\sum_{j=1}^{n-l} r(v_i,u_j)$$
$$= \sum_{i=1}^{l}\sum_{j=1}^{l} r(v_i,v_j) + (n-2l)\sum_{i=1}^{l} r(v_i,v_l) + l(n-l)$$
$$= 2Kf(C_l) + (n-2l)Kf_{v_l}(C_l) + l(n-l)$$

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

$$Kf(U(C_l;K_2,\cdots,K_2,S_{n-2(l-1)}))$$
$$= 4Kf(C_l) + 2(n-2l)Kf_{v_l}(C_l) + (n-l)(n-l-1) + l(n-l)$$
$$= \tfrac{1}{3}(l^3-l) + \tfrac{1}{3}(n-2l)(l^2-1) + (n-1)(n-l)$$
$$= -\tfrac{1}{3}l^3 + \tfrac{1}{3}nl^2 + (\tfrac{4}{3}-n)l + n^2 - \tfrac{4}{3}n \qquad (1)$$

$$Kf(U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)}))$$
$$= \sum_{1\le i<j\le n-l} r(u_i,u_j) + \sum_{1\le i<j\le l} r(v_i,v_j) + \sum_{i=1}^{l}\sum_{j=1}^{n-l} r(v_i,u_j)$$

and

$$\sum_{1\le i<j\le n-l} r(u_i,u_j)$$
$$= \sum_{1\le i<j\le l} r(v_i,v_j) + (n-2l)\sum_{i=1}^{l-1} r(v_i,v_l)$$
$$+l(l-1) + \tfrac{1}{2}(l-1)(n-2l)(n-2l+5) + \sum_{l\le i<j\le n-l} r(u_i,u_j)$$
$$= Kf(C_l) + (n-2l)Kf_{v_l}(C_l) + l(l-1)$$
$$+\tfrac{1}{2}(l-1)(n-2l)(n-2l+5) + Kf(P_{n-2l+1})$$

$$\sum_{i=1}^{l}\sum_{j=1}^{n-l} r(v_i,u_j)$$
$$= \sum_{i=1}^{l}\sum_{j=1}^{l} r(v_i,v_j) + (n-2l)\sum_{i=1}^{l} r(v_i,v_l) + l(l + \tfrac{1}{2}(n-2l)(n-2l+3))$$
$$= 2Kf(C_l) + (n-2l)Kf_{v_l}(C_l) + l^2 + \tfrac{1}{2}l(n-2l)(n-2l+3))$$

Note that $Kf(P_{n-2l+1}) = \frac{1}{6}((n-2l+1)^3 - (n-2l+1))$,

$$
\begin{aligned}
& Kf(U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})) \\
= \; & 4Kf(C_l) + 2(n-2l)Kf_{v_l}(C_l) + Kf(P_{n-2l+1}) + 2l^2 - l \\
& + \tfrac{1}{2}(l-1)(n-2l)(n-2l+5) + \tfrac{1}{2}l(n-2l)(n-2l+3) \\
= \; & \tfrac{7}{3}l^3 - (\tfrac{5}{3}n+6)l^2 + (4n+\tfrac{11}{3})l + \tfrac{1}{6}n^3 - \tfrac{5}{2}n \qquad (2)
\end{aligned}
$$

Combining the two equations (1) and (2) with Theorems 2.6, we have

Theorem 2.7. Let $G \in \mathcal{U}(n,l)$. If G is different from $U(C_l; K_2, \cdots, K_2, S_{n-2(l-1)})$ and $U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)})$, then

$-\frac{1}{3}l^3 + \frac{1}{3}nl^2 + (\frac{4}{3}-n)l + n^2 - \frac{4}{3}n < Kf(G) < \frac{7}{3}l^3 - (\frac{5}{3}n+6)l^2 + (4n + \frac{11}{3})l + \frac{1}{6}n^3 - \frac{5}{2}n$.

3 The extremal Kirchhoff indices among all loaded unicyclic graphs

In this section, we will determine the smallest and largest Kirchhoff indices among all loaded unicyclic graphs with $n \geq 6$ vertices and characterize the extremal graphs. By Theorem 2.7, we only need to find $Kf_{min} = \min\{f(l) | 3 \leq l \leq [\frac{n}{2}]\}$ and $Kf_{max} = \max\{g(l) | 3 \leq l \leq [\frac{n}{2}]\}$, where $f(l) = -\frac{1}{3}l^3 + \frac{1}{3}nl^2 + (\frac{4}{3}-n)l + n^2 - \frac{4}{3}n$ and $g(l) = \frac{7}{3}l^3 - (\frac{5}{3}n+6)l^2 + (4n+\frac{11}{3})l + \frac{1}{6}n^3 - \frac{5}{2}n$.

Firstly, the derivative of $f(l)$ is

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

Case 1. If $6 \leq n \leq 7$, then $[\frac{n}{2}] = 3$ and $l = 3$. $Kf_{min} = f(3) = Kf(G(C_3; K_2, K_2, S_{n-4}))$.

Case 2. If $n \geq 11$, then $f'(l) > 0$ for $3 \leq l \leq [\frac{n}{2}]$ since $l_1 < 3$ and $l_2 > [\frac{n}{2}]$, where $l_1 < l_2$ are the real roots of $f'(l) = 0$. So, $Kf_{min} = f(3) = Kf(G(C_3; K_2, K_2, S_{n-4}))$.

Case 3. If $8 \leq n \leq 10$, computing indirectly,

(i) $f(3) = \frac{145}{3} > f(4) = 48$ for $n = 8$;

(ii) $f(3) = 64 < f(4) = 65$ for $n = 9$;

(iii) $f(3) = \frac{245}{3} < f(4) = 84 < f(5) = 85$ for $n = 10$.

$$Kf_{min} = \begin{cases} f(4), & n = 8; \\ f(3), & n = 9, 10. \end{cases}$$

So, we have

Theorem 3.1. Let G be a loaded unicyclic graph with $n \geq 6$ vertices. Then

$$Kf(G) \geq \begin{cases} n^2 - 16 = 48, & n = 8; \\ n^2 - \frac{4}{3}n - 5, & n \neq 8 \end{cases}$$

with equation if and only if $G = U(C_4; K_2, K_2, K_2, K_2)$ for $n = 8$ and $G = U(C_3; K_2, K_2, S_{n-4})$ for $n \neq 8$.

Secondly, the derivative of $g(l)$ is

$$g'(l) = 7l^2 - (\frac{10}{3}n + 12)l + 4n + \frac{11}{3}.$$

The two real roots of $g'(l) = 0$ are

$$l_1 = \frac{(10n + 36) - \sqrt{100n^2 - 288n + 372}}{42}$$

$$l_2 = \frac{(10n + 36) + \sqrt{100n^2 - 288n + 372}}{42}.$$

It is obvious that $l_1 < 3$ and $l_2 > 3$ for $n \geq 6$.

Case 1. If $l_2 \geq [\frac{n}{2}]$, then $g'(l) < 0$ for $3 \leq l \leq [\frac{n}{2}]$, and $Kf_{max} = g(3)$.

Case 2. If $l_2 < [\frac{n}{2}]$, then $g'(l) < 0$ for $3 \leq l < l_2$ and $g'(l) > 0$ for $l_2 < l \leq [\frac{n}{2}]$, and $Kf_{max} = \max\{g(3), g([\frac{n}{2}])\}$.

Now, we compare $g(3)$ with $g([\frac{n}{2}])$. Let $h(n) = g(3) - g([\frac{n}{2}])$.

If n is even, then $h(n) = g(3) - g(\frac{n}{2}) = \frac{1}{8}n^3 - \frac{1}{2}n^2 - \frac{29}{6}n + 20$. $h(n) \geq h(6) = 0$ since $h'(n) = \frac{3}{8}(n - \frac{4}{3})^2 - \frac{11}{2} > 0$ for $n \geq 6$. So, $g(3) \geq g(\frac{n}{2})$ and $Kf_{max} = g(3)$ with equation if and only if $n = 6$ (i.e.,$l = 3$).

If n is odd, then $h(n) = g(3) - g(\frac{n-1}{2}) = \frac{1}{8}n^3 - \frac{11}{24}n^2 - \frac{151}{24}n + \frac{189}{8}$. $h(n) \geq h(7) = 0$ since $h'(n) = \frac{3}{8}(n - \frac{11}{9})^2 - \frac{185}{27} > 0$ for $n \geq 7$. So, $g(3) \geq g(\frac{n-1}{2})$, and $Kf_{max} = g(3)$ with equation if and only if $n = 7$ (i.e., $l = 3$).

So, we have

Theorem 3.2. Let G be a loaded unicyclic graph with $n \geq 6$ vertices. Then

$$Kf(G) \leq \frac{1}{6}n^3 - \frac{11}{2}n + 20.$$

with equation if and only if $G = U(C_3; K_2, K_2, P_{n-4})$.

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