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Bicyclic graphs with extremal Kirchhoff index*

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Abstract

Let $S_n^{p,q}$ denote the graph obtained from cycles C_p and C_q by attaching $n+1-p-q$ pendent edges to the unique common vertex of them. Let $P_n^{p,q}$ be the graph consisting of two disjoint cycles C_p and C_q and a path of length $n-p-q+1$ joining them (when $n-p-q+1=0$, $P_n^{p,q}$ coincides with $S_n^{p,q}$). In this paper, we show that among all n-vertex bicyclic graphs with exactly two cycles: (a) $P_n^{3,3}$ has the maximal Kirchhoff index, (b) the following graphs have the minimal Kirchhoff indices: $S_5^{3,3}$; $S_6^{3,4}$; $S_7^{4,4}$; $S_8^{4,4}$ and $S_8^{4,5}$; $S_n^{4,4}$ $(9 \leq n \leq 11)$; $S_{12}^{4,4}$, $S_{12}^{3,4}$ and $S_{12}^{3,3}$; $S_n^{3,3}$ $(n > 12)$.

1 Introduction

In 1993, Klein and Randić [1] defined a new distance function named resistance distance on the basis of electrical network theory. Let G be a connected graph with vertices labelled as $v_1, v_2, \cdots, v_n$. They view 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 $r(v_i, v_j)$ (if more than one graphs are considered, we write $r_G(v_i, v_j)$ in order to avoid confusion), is defined to be the effective resistance between them in N. Recall that the conventional distance between vertices v_i and v_j, denoted by $d(v_i, v_j)$, is the length of a shortest path

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between them and the famous Wiener index $W(G)$ [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 $Kf(G)$ [2] is defined as:

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

So far, resistance distance has been studied extensively such as [3, 4, 5, 6]. As a new structure-descriptor [7], Kirchhoff index is well studied. On the one hand, simple closed-form formulae or numerical values of Kirchhoff index of some classes of graphs have been obtained, such as complete graphs [8], cycles [8, 9], platonic solids [8, 10], some fullerenes including buckminsterfullerene [11, 12, 13], distance transitive graphs [14], circulant graphs [15], linear hexagonal chains [16], and so on [13, 14, 17, 18]. On the other hand, sharp bounds for Kirchhoff index of some classes of graphs are obtained and graphs with extremal Kirchhoff index are characterized as well. For instance, for a general connected graph G, Lukovits et al. [9] proved that

$$n - 1 \leq Kf(G) \leq \frac{n^3 - n}{6},$$

the first equality holds if and only if G is a complete graph, while the second does if and only if G is a path. For a circulant graph G, Ref. [15] proved that

$$n - 1 \leq Kf(G) \leq \frac{n^3 - n}{12},$$

the second equality holds if and only if G is a cycle.

Since Kirchhoff index and Wiener index of trees coincide [1] and Wiener indices of graphs are extensively studied, so it is natural to consider Kirchhoff index of graphs with cycles. In Ref. [19], unicyclic graphs with extremal Kirchhoff index are characterized and sharp bounds for Kirchhoff index of such graphs are obtained as well. A bicyclic graph is a connected graph whose edge number is one more than its vertex number; that is, its cyclomatic number is 2. Obviously a bicyclic graph contains either two or three cycles. Through this article we restrict our consideration on bicyclic graphs with exactly two cycles.

For convenience, we employ some notations. We may represent a unicylic graph G by $U(C_l; T_1, T_2, \ldots, T_l)$, where C_l is the unique cycle $v_1 v_2 \ldots v_l v_1$. For each i, T_i is a tree rooted at v_i. Let $\mathcal{G}_n^{p,q}$ be the set of n-vertex bicyclic connected graphs with exactly two cycles C_p and C_q. For $G \in \mathcal{G}_n^{p,q}$, G is represented as follows: $C_p = v_1 v_2 \cdots v_p v_1$ and $C_q = u_1 u_2 \cdots u_q u_1$ are two cycles such that there is a v_1, u_1-path $P = v_1 w_1 \cdots w_{m-1} u_1$ joining them. The trees T_{v_i} $(1 \leq i \leq p)$, T_{u_j} $(1 \leq j \leq q)$ and T_{w_k} $(1 \leq k \leq m-1)$ are rooted at v_i, u_j and w_k, respectively. We say a tree T trivial if $|V(T)| = 1$, i.e., T is an singleton vertex. For example, see Fig. 1. Let $S_n^{p,q}$ denote the graph obtained from cycles C_p and C_q by attaching $n+1-p-q$ pendent edges to the unique common vertex of them. Let $P_n^{p,q}$ be the graph consisting of two disjoint cycles C_p and C_q and a path of length $n-p-q+1$ joining them (when $n-p-q+1=0$, $P_n^{p,q}$ coincides with $S_n^{p,q}$). $S_n^{p,q}$ and $P_n^{p,q}$ are depicted in Fig. 2 .

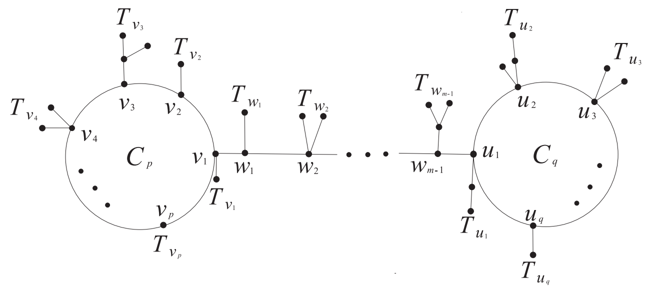

Fig. 1. Illustration for a graph in $\mathcal{G}_n^{p,q}$.

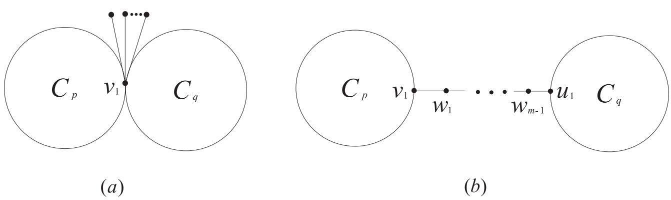

Fig. 2. (a) $S_n^{p,q}$, and (b) $P_n^{p,q}$.

In the present work, we first prove that for each $G \in \mathcal{G}_n^{p,q}$, $Kf(S_n^{p,q}) \leq Kf(G) \leq Kf(P_n^{p,q})$ with the first equality holds if and only if $G = S_n^{p,q}$ (Theorem 2.6) and the second does if and only if $G = P_n^{p,q}$ (Theorem 2.7). Bounds on Kirchhoff indices of graphs in $\mathcal{G}_n^{p,q}$ are obtained accordingly. According to the above results, we can investigate n-vertex bicyclic graphs with minimal and maximal Kirchhoff index only among $S_n^{p,q}$ and $P_n^{p,q}$ $(3 \leq p \leq n-2,\ 3 \leq q \leq n-2)$. In the last section, bicyclic graphs with extremal Kirchhoff index are characterized. We obtain that among bicyclic graphs with exactly two cycles: (a) $P_n^{3,3}$ has the maximal Kirchhoff index, (b) if $n = 5$, $S_5^{3,3}$ has the minimal Kirchhoff index; if $n = 6$, $S_6^{3,4}$ has the minimal Kirchhoff index; if $n = 7$, $S_7^{4,4}$ has the minimal Kirchhoff index; if $n = 8$, $S_8^{4,4}$ and $S_8^{4,5}$ have the minimal Kirchhoff index; if $9 \leq n \leq 11$, $S_n^{4,4}$ has the minimal Kirchhoff index; if $n = 12$, $S_{12}^{4,4}$, $S_{12}^{3,4}$ and $S_{12}^{3,3}$ have the minimal Kirchhoff index; if $n > 12$, $S_n^{3,3}$ has the minimal Kirchhoff index.

2 Bounds for Kirchhoff indices

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

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

Lemma 2.2. *[1] Let x be a cut-vertex of a connected graph, and let a and b be vertices occurring in different components which arise upon deletion of x. Then*

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

For $v_i \in V(G)$, define $Kf_{v_i}(G)$ as the sum of resistance distances between v_i and other vertices of G; that is,

$$Kf_{v_i}(G) = \sum_{v_j \in V(G)} r_G(v_i, v_j).$$

Theorem 2.3. *Let x be a cut-vertex of a connected graph G such that $G - x$ has exactly two components G_1 and G_2. Let G_i' be the subgraph of G induced by $V(G_i) \bigcup \{x\}$ $(i = 1, 2)$. Then*

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

Proof. By Lemma 2.2,

$$\begin{aligned}
Kf(G) =& \sum_{i<j} r_G(v_i, v_j) \\
=& \frac{1}{2} \sum_{v_i,v_j \in V(G_1')} r_G(v_i, v_j) + \frac{1}{2} \sum_{v_i,v_j \in V(G_2')} r_G(v_i, v_j) + \sum_{v_i \in V(G_1), v_j \in V(G_2)} r_G(v_i, v_j) \\
=& \frac{1}{2} \sum_{v_i,v_j \in V(G_1')} r_{G_1'}(v_i, v_j) + \frac{1}{2} \sum_{v_i,v_j \in V(G_2')} r_{G_2'}(v_i, v_j) \\
&+ \sum_{v_i \in V(G_1), v_j \in V(G_2)} (r_{G_1'}(v_i, x) + r_{G_2'}(x, v_j)) \\
=& Kf(G_1') + Kf(G_2') + \sum_{v_j \in V(G_2)} (Kf_x(G_1') + (|V(G_1')| - 1) r_{G_2'}(x, v_j)) \\
=& Kf(G_1') + Kf(G_2') + (|V(G_1')| - 1) Kf_x(G_2') + (|V(G_2')| - 1) Kf_x(G_1').
\end{aligned}$$

□

Lemma 2.4. *Let $G = U(C_l; T_1, T_2, \ldots, T_l)$. Assume that trees T_i and T_j are nontrivial stars with their centers at v_i and v_j and leaves u_i and u_j different from v_i and v_j, respectively. If $Kf_{u_i}(G) \leq Kf_{u_j}(G)$, let $G' = G - v_j u_j + v_i u_j$. Then*

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

Proof. For any two vertices $v_k, v_l \in V(G) \backslash \{u_j\}, r_G(v_k, v_l) = r_{G'}(v_k, v_l)$. While

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

Therefore,

$$Kf(G') = Kf(G) - Kf_{u_j}(G) + Kf_{u_j}(G') < Kf(G).$$

□

Lemma 2.5. *Let $G = U(C_l; T_1, T_2, \ldots, T_l)$. Assume that T_i and T_j are nontrivial paths with end vertices v_i and u_i, and v_j and u_j, respectively, and the neighbor of u_j is a. If $Kf_{u_i}(G) \geq Kf_{u_j}(G)$, let $G' = G - a u_j + u_i u_j$. Then*

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

Proof. For any two vertices $v_k, v_l \in V(G) \backslash \{u_j\}, r_G(v_k, v_l) = r_{G'}(v_k, v_l)$. While

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

Therefore,

$$Kf(G') = Kf(G) - Kf_{u_j}(G) + Kf_{u_j}(G') > Kf(G).$$

□

Theorem 2.6. *Let $G \in \mathcal{G}_n^{p,q}$ and $G \neq S_n^{p,q}$. Then $Kf(G) > Kf(S_n^{p,q})$.*

Proof. Suppose that a bicyclic graph G_0 has minimal Kirchhoff index among graphs in $\mathcal{G}_n^{p,q}$. For G_0, we prove the following Claims.

Claim 1. T_{v_i}, T_{u_j} and T_{w_k} are all stars with their centers at v_i, u_j and w_k for each i, j and k.

Without loss of generality, suppose that tree T_{v_i} is not a star. Let G_1 be constructed from G_0 by deleting all the edges of T_{v_i} and connecting all the isolated vertices to v_i; that is, T_{v_i} is a star in G_1 with its center at v_i and denote it by S_{v_i}. For G_0, v_i is a cut vertex, T_{v_i} and $G_0-(V(T_{v_i})-v_i)$ are two induced subgraphs. By Lemma 2.1, $Kf(S_{v_i}) < Kf(T_{v_i})$. On the other hand, $Kf_{v_i}(S_{v_i}) < Kf_{v_i}(T_{v_i})$. Then by Theorem 2.3, $Kf(G_1) < Kf(G_0)$, which contradicts the choice of G_0. Hence Claim 1 holds.

Claim 2. The length of P is 0.

Suppose to the contrary that the length of P is k ($k \geq 1$). Assume that $v_1 = w_0, u_1 = w_k$. Let $e = w_iw_{i+1}$ be an edge of P. Let G_2 be the graph obtained from G_0 by first contracting e and then attaching a pendent edge w_ia to w_i. Assume that G_{01} and G_{02} are two components of $G_0 - e$ and G_{21} and G_{22} are copies of G_{01} and G_{02} in G_2, respectively. See Fig. 3.

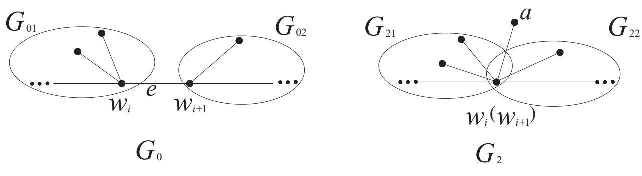

Fig. 3. Graphs G_0 and G_2.

In the following, we prove $Kf(G_2) < Kf(G_0)$.

For $x, y \in V(G_{01})\backslash\{w_i\}$ or $x, y \in V(G_{02})\backslash\{w_{i+1}\}$, $r_{G_2}(x, y) = r_{G_0}(x, y)$; and for $x \in V(G_{01})\backslash\{w_i\}, y \in V(G_{02})\backslash\{w_{i+1}\}$, $r_{G_2}(x, y) = r_{G_0}(x, y) - 1 < r_{G_0}(x, y)$. On the other hand,

$$\sum_{x\in V(G_{01})} r_{G_0}(x, w_{i+1}) = \sum_{x\in V(G_{21})} r_{G_2}(x, a) \text{ and } \sum_{x\in V(G_{02})} r_{G_0}(x, w_i) = \sum_{x\in V(G_{22})} r_{G_2}(x, a).$$

So

$$\begin{aligned}
&Kf_{w_i}(G_0) + Kf_{w_{i+1}}(G_0)\\
=&Kf_{w_i}(G_{01}) + \sum_{x\in V(G_{02})} r_{G_0}(x, w_i) + Kf_{w_{i+1}}(G_{02}) + \sum_{x\in V(G_{01})} r_{G_0}(x, w_{i+1})\\
=&Kf_{w_i}(G_{21}) + \sum_{x\in V(G_{22})} r_{G_2}(x, a) + Kf_{w_{i+1}}(G_{22}) + \sum_{x\in V(G_{21})} r_{G_2}(x, a)\\
=&(Kf_{w_i}(G_{21}) + Kf_{w_i}(G_{22}) + r_{G_2}(a, w_i))\\
&+ (\sum_{x\in V(G_{22})} r_{G_2}(x, a) + \sum_{x\in V(G_{21})} r_{G_2}(x, a) - r_{G_2}(a, w_i))\\
=&Kf_{w_i}(G_2) + Kf_a(G_2).
\end{aligned}$$

By the definition of Kirchhoff index, we obtain $Kf(G_2) < Kf(G_0)$. This contradicts the hypothesis. Hence Claim 2 holds.

Claim 3. If $p + q \le n$, then only T_{v_1} ($T_{v_1} = T_{u_1}$) is nontrivial.

Without losing generality, suppose to the contrary that tree T_{v_i} ($i \neq 1$) is nontrivial. By Claim 1, we know that T_{v_1} and T_{v_i} are both stars. Let G_{01} and G_{02} be the subgraphs of G_0 induced by $V(T_{v_1}) \bigcup \ldots \bigcup V(T_{v_p})$ and $V(G_0) \backslash V(G_{01}) \bigcup \{u_1\}$, respectively.

If $Kf_{v_i}(G_{01}) < Kf_{v_1}(G_{01})$, construct G_0' by identifying v_i of G_{01} with u_1 of G_{02}. See Fig. 4. Then by Theorem 2.3, $Kf(G_0') < Kf(G_0)$, a contradiction. If $Kf_{v_i}(G_{01}) \geq$

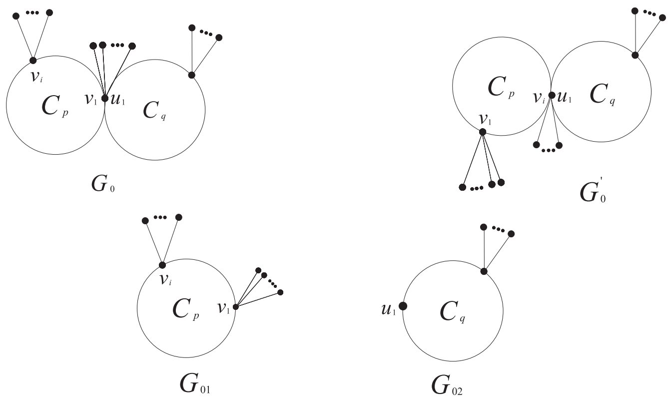

Fig. 4. Four graphs G_0, G_{01}, G_{02} and G_0'.

$Kf_{v_1}(G_{01})$, assume that a and b are leaves of T_{v_1} and T_{v_i}, respectively. Then

$$Kf_a(G_{01}) = Kf_{v_1}(G_{01}) - 1 + |V(G_{01})| - 1,$$

$$Kf_b(G_{01}) = Kf_{v_i}(G_{01}) - 1 + |V(G_{01})| - 1,$$

so $Kf_b(G_{01}) \geq Kf_a(G_{01})$. Let $G_0' = G_0 - v_i b + v_1 b$, and let G_{02}' be the copy of G_{02} in G_0' and G_{01}' be the subgraph of G_0' induced by $V(G_0') \backslash V(G_{02}') \bigcup \{v_1\}$. By Lemma 2.4, $Kf(G_{01}') < Kf(G_{01})$. Also $Kf_{v_1}(G_{01}') < Kf_{v_1}(G_{01})$, since $Kf_{v_1}(G_{01}') = Kf_{v_1}(G_{01}) - r_{G_{01}}(b, v_1) + 1$. By Theorem 2.3, we obtain $Kf(G_0') < Kf(G_0)$, a contradiction. Hence Claim 3 holds.

Claims 1, 2 and 3 yield Theorem 2.6. □

Theorem 2.7. *Let $G_0 \in \mathcal{G}_n^{p,q}$ and $G \neq P_n^{p,q}$. Then $Kf(G) < Kf(P_n^{p,q})$.*

Proof. Suppose that a bicyclic graph G_0 has maximal Kirchhoff index among graphs in $\mathcal{G}_n^{p,q}$. For G_0, we prove the following Claims.

Claim 1. T_{v_i}, T_{u_j} and T_{w_k} are all paths with their end vertices v_i, u_j and w_k for each i, j and k.

Without loss of generality, suppose that T_{v_i} is not a path. Let G_1 be the graph constructed from G_0 by deleting all the edges of T_{v_i} and connecting v_i and all the isolated vertices into a path; that is, T_{v_i} is a path with end vertex v_i in G_1 and denote it by P_{v_i}. For G_0, v_i is a cut vertex, T_{v_i} and $G_0 - (V(T_{v_i}) - v_i)$ are two induced subgraphs. By Lemma 2.1, we obtain $Kf(P_{v_i}) > Kf(T_{v_i})$. On the other hand, $Kf_{v_i}(P_{v_i}) > Kf_{v_i}(T_{v_i})$. By Theorem 2.3, $Kf(G_1) > Kf(G_0)$, which contradicts the choice of G_0. Hence Claim 1 holds.

Claim 2. Assume that $T_{w_0} = T_{v_1}$ and $T_{w_m} = T_{u_1}$, then T_{w_i} is trivial $(0 \leq i \leq m)$.

If not, without losing generality, suppose that there is nontrivial T_{w_j}. By Claim 1, we know that T_{w_j} is a path with w_j as its end vertex and assume that u is the other end vertex. Let $G_2 = G_0 - w_j w_{j+1} + u w_{j+1}$ (if $j = m$, $G_2 = G_0 - w_{j-1} w_j + u w_{j-1}$). Assume that G_{01} and G_{02} are two components of $G_0 - w_j w_{j+1}$ and G_{21} and G_{22} are two components of $G_2 - u w_{j+1}$. See Fig. 5.

In the following, we prove $Kf(G_2) > Kf(G_0)$.

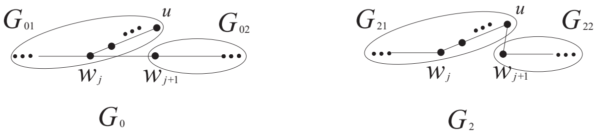

Fig. 5. Graphs G_0 and G_2.

Since $Kf(G_{01}) = Kf(G_{21})$ and $Kf(G_{02}) = Kf(G_{22})$, we have

$$\begin{aligned} Kf(G_2) - Kf(G_0) =& (Kf(G_{21}) + Kf(G_{22}) + \sum_{x\in V(G_{21}), y\in V(G_{22})} r_{G_2}(x,y)) \\ &- (Kf(G_{01}) + Kf(G_{02}) + \sum_{x\in V(G_{01}), y\in V(G_{02})} r_{G_0}(x,y)) \\ =& \sum_{x\in V(G_{21}), y\in V(G_{22})} r_{G_2}(x,y) - \sum_{x\in V(G_{01}), y\in V(G_{02})} r_{G_0}(x,y) \\ =& k|V(G_{02})|(|V(G_{01})| - k - 1) > 0, \end{aligned}$$

where k is the length of the path T_{w_j}. So $Kf(G_2) > Kf(G_0)$, a contradiction. Hence Claim 2 holds.

Claim 3. If $p + q \leq n$, then T_{v_i} and T_{u_j} are trivial for each i and j.

Without loss of generality, suppose to the contrary that T_{v_i} is nontrivial ($i \neq 1$, since T_{v_1} is trivial by Claim 2). By Claim 1, we know that T_{v_i} is a path. Assume that a ($a \neq v_i$) is the endvertex of T_{v_i} and b is the neighbor of a. Let G_{01} and G_{02} be two components of $G_0 - u_1$, and let G^*_{0k} be the subgraph of G_0 induced by $V(G_{0k})\bigcup\{u_1\}$ ($k = 1, 2$).

If $Kf_a(G^*_{01}) > Kf_{u_1}(G^*_{01})$, construct G'_0 by identifying a of G^*_{01} with u_1 of G^*_{02} in the same way as in Theorem 2.6. By Theorem 2.3, $Kf(G'_0) > Kf(G_0)$, a contradiction. If $Kf_a(G^*_{01}) \leq Kf_{u_1}(G^*_{01})$, let $G'_0 = G_0 - ab - w_{m-1}u_1 + w_{m-1}a + au_1$. Assume that G'_{01} and G'_{02} are two components of $G'_0 - u_1$ and G''_{0k} is the subgraph of G'_0 induced by $V(G'_{0k})\bigcup\{u_1\}$ ($k = 1, 2$). By Lemma 2.5, $Kf(G''_{01}) > Kf(G^*_{01})$. Also $Kf_{u_1}(G''_{01}) > Kf_{u_1}(G^*_{01})$, since $Kf_{u_1}(G''_{01}) = Kf_{u_1}(G^*_{01}) - r_{G^*_{01}}(a, u_1) + |G^*_{01}| - 1$. Then by Theorem 2.3, we obtain $Kf(G'_0) > Kf(G_0)$, a contradiction. So T_{v_i} ($i \neq 1$) is trivial. Similarly, we can prove that T_{u_j} ($j \neq 1$) is trivial. Hence Claim 3 holds.

Claims 1, 2 and 3 yield Theorem 2.7. □

We now compute $Kf(S^{p,q}_n)$ and $Kf(P^{p,q}_n)$.

For $S_n^{p,q}$, since v_1 is a cut vertex, let G_1 and G_2 be the subgraphs of $S_n^{p,q}$ induced by $V(S_n^{p,q})\backslash V(C_q)\bigcup\{v_1\}$ and $V(C_q)$, respectively. Then

$$Kf(G_1) = \tfrac{p^3-p}{12} + (n-p-q+1)^2 + \tfrac{p^2-1}{6}(n-p-q+1) + (n-p-q+1)(p-1);$$

$$Kf(G_2) = \tfrac{q^3-q}{12};$$

$$Kf_{v_1}(G_1) = \tfrac{p^2-1}{6} + n - p - q + 1;$$

$$Kf_{v_1}(G_2) = \tfrac{q^2-1}{6}.$$

By Theorem 2.3,

$$Kf(S_n^{p,q}) = \frac{1}{12}[-p^3 - q^3 + 2n(p^2+q^2) + (-12n+13)(p+q) + 12n^2 - 4n - 12]. \quad (1)$$

For $P_n^{p,q}$, since u_1 is a cut vertex, let G_1' and G_2' be the subgraphs of $P_n^{p,q}$ induced by $V(P_n^{p,q})\backslash V(C_q)\bigcup\{u_1\}$ and $V(C_q)$, respectively. Then

$$Kf(G_1') = \tfrac{p^3-p}{12} + \tfrac{(n-p-q+1)^2-(n-p-q+1)}{6} + \tfrac{p^2-1}{6}(n-p-q+1) + \tfrac{(n-p-q+2)(n-p-q+1)(p-1)}{2};$$

$$Kf(G_2') = \tfrac{q^3-q}{12};$$

$$Kf_{u_1}(G_1') = \tfrac{(n-p-q+2)(n-p-q+1)}{2} + \tfrac{p^2-1}{6} + (p-1)(n-p-q+1);$$

$$Kf_{u_1}(G_2') = \tfrac{q^2-1}{6}.$$

By Theorem 2.3, we have

$$Kf(P_n^{p,q}) = \frac{1}{12}[3p^3 + 3q^3 + (-4n-6)(p^2+q^2) + (6n+3)(p+q) + 2n^3 - 6n]. \quad (2)$$

Combining Eqs. (1) and (2) with Theorems 2.6 and 2.7, we obtain bounds for kirchhoff indices of graphs in $\mathcal{G}_n^{p,q}$ in the following result.

Theorem 2.8. *For $G \in \mathcal{G}_n^{p,q}$,*

$$\frac{1}{12}[-p^3 - q^3 + 2n(p^2+q^2) + (-12n+13)(p+q) + 12n^2 - 4n - 12] \leq \; Kf(G) \leq$$
$$\frac{1}{12}[3p^3 + 3q^3 + (-4n-6)(p^2+q^2) + (6n+3)(p+q) + 2n^3 - 6n].$$

3 Bicyclic graphs with extremal Kirchhoff index

By Theorems 2.6 and 2.7, n-vertex bicyclic graphs in $\mathcal{G}_n^{p,q}$ with minimal and maximal Kirchhoff index must belong to the classes of $S_n^{p,q}$ and $P_n^{p,q}$ $(3 \leq p \leq n-2, 3 \leq q \leq n-2)$, respectively. In what follows, we will determine which has the extremal Kirchhoff index among graphs in $\mathcal{G}_n^{p,q}$. Since $S_n^{p,q} \cong S_n^{q,p}$ and $P_n^{p,q} \cong P_n^{q,p}$, without loss of generality, we assume that $p \leq q$. In the following, let

$$\mathcal{H} := \{(p,q)|3 \leq p \leq q \leq n-2, p+q \leq n+1\}.$$

Theorem 3.1. $\max\limits_{(p,q)\in\mathcal{H}}\{Kf(P_n^{p,q})\} = Kf(P_n^{3,3})$.

Proof. By Eq. (2),

$$Kf(P_n^{p,q}) - Kf(P_n^{p-1,q}) = \frac{9p^2 - (8n+21)p + (10n+12)}{12}.$$

Let

$$f(p) := 9p^2 - (8n+21)p + (10n+12) \quad (4 \leq p \leq n-2).$$

Then the two roots of $f(p)$ are

$$p_1 = \frac{8n+21-\sqrt{(8n-\frac{3}{2})^2+\frac{27}{4}}}{18},$$

and

$$p_2 = \frac{8n+21+\sqrt{(8n-\frac{3}{2})^2+\frac{27}{4}}}{18}.$$

Simple calculations show that for $n \geq 5$, $p_1 < 3$ and $p_2 > n/2+1$. Since $p+q \leq n+1$, we have $p+q < 2p_2 = n+2$, and $p < p_2$. For $4 \leq p \leq n-2$, $f(p) < 0$, which implies that $Kf(P_n^{p,q}) < Kf(P_n^{p-1,q})$. So $P_n^{3,q}$ has the maximal Kirchhoff index. For q, $Kf(P_n^{3,q}) = Kf(P_n^{q,3})$ and

$$f(q) = 9q^2 - (8n+21)q + (10n+12) \quad (4 \leq q \leq n-2).$$

Clearly, the two roots of $f(q)$ are also p_1 and p_2.

Case 1. $5 \leq n \leq 27$. Then $p_2 > n-2$. Hence for $4 \leq q \leq n-2$, $f(q) < 0$, which implies that $Kf(P_n^{3,q}) < Kf(P_n^{3,q-1})$. So $P_n^{3,3}$ has the maximal Kirchhoff index.

Case 2. $n > 27$. Then $p_2 < n-2$.

For $4 \le q < \lfloor p_2 \rfloor$, $f(q) < 0$. That is, $Kf(P_n^{3,q}) < Kf(P_n^{3,q-1})$. So $P_n^{3,3}$ has the maximal Kirchhoff index. For $\lceil p_2 \rceil < q \le n-2$, $f(q) > 0$. That is, $Kf(P_n^{3,q}) > Kf(P_n^{3,q-1})$. So $P_n^{3,n-2}$ has the maximal Kirchhoff index. For $q = p_2$, that is, p_2 is integer, $f(q) = 0$ and $Kf(P_n^{3,q}) = Kf(P_n^{3,q-1})$; for $4 \le q < p_2$, $f(q) < 0$ and $Kf(P_n^{3,q}) < Kf(P_n^{3,q-1})$; for $p_2 < q \le n-2$, $f(q) > 0$ and $Kf(P_n^{3,q}) > Kf(P_n^{3,q-1})$. So when $q = p_2$, either $Kf(P_n^{3,3})$ or $Kf(P_n^{3,n-2})$ has maximal Kirchhoff index. Now we compare $Kf(P_n^{3,3})$ with $Kf(P_n^{3,n-2})$. By Eq. (2),

$$Kf(P_n^{3,3}) - Kf(P_n^{3,n-2}) = \frac{n^3 + 2n^2 - 53n + 90}{12}.$$

Let

$$c(n) := n^3 + 2n^2 - 53n + 90.$$

The derivative of $c(n)$ is

$$c'(n) = 3n^2 + 4n - 53.$$

It is easy to verify that for $n \ge 5$, $c'(n) > 0$; that is, $c(n)$ is increasing on $[5, +\infty)$. For $n = 5$, $Kf(P_n^{3,3}) = Kf(P_n^{3,n-2})$, so $c(5) = 0$. Hence for $n \ge 6$, $c(n) = Kf(P_n^{3,3}) - Kf(P_n^{3,n-2}) > c(5) = 0$, namely, $Kf(P_n^{3,3}) > Kf(P_n^{3,n-2})$.

Therefore, $Kf(P_n^{3,3})$ has the maximal Kirchhoff index. □

Theorem 3.2.

$$\min_{(p,q)\in\mathcal{H}} \{Kf(S_n^{p,q})\} = \begin{cases} Kf(S_5^{3,3}) & \textit{if } n = 5, \\ Kf(S_6^{3,4}) & \textit{if } n = 6, \\ Kf(S_7^{4,4}) & \textit{if } n = 7, \\ Kf(S_8^{4,4}) = Kf(S_8^{4,5}) & \textit{if } n = 8, \\ Kf(S_n^{4,4}) & \textit{if } 8 < n < 12, \\ Kf(S_{12}^{4,4}) = Kf(S_{12}^{3,4}) = Kf(S_{12}^{3,3}) & \textit{if } n = 12, \\ Kf(S_n^{3,3}) & \textit{otherwise.} \end{cases}$$

Proof. By Eq. (1),

$$Kf(S_n^{p,q}) - Kf(S_n^{p-1,q}) = \frac{-3p^2 + (4n+3)p + (12 - 14n)}{12}.$$

Let

$$g(p) := -3p^2 + (4n+3)p + (12 - 14n) \quad (4 \le p \le n-2),$$

and

$$h(n) := \triangle_{g(p)} = 16n^2 - 144n + 153 \quad (n \ge 5).$$

Case 1. $5 \le n \le 7$. For $n = 5$, $S_5^{3,3}$ is the unique graph, so it has the minimal Kirchhoff index. For $6 \le n \le 7$, $h(n) < 0$. Hence for $4 \le p \le n-2$, $g(p) < 0$. That is, $Kf(S_n^{p,q}) < Kf(S_n^{p-1,q})$. So $Kf(S_6^{4,3}) < Kf(S_6^{3,3})$ and $S_6^{4,3}$ have the minimal Kirchhoff index. For $n = 7$, $Kf(S_7^{4,4}) = 25$ and $Kf(S_7^{3,5}) = \frac{79}{3}$, so $S_7^{4,4}$ has the minimal Kirchhoff index.

Case 2. $n \ge 8$. Then $h(n) > 0$. The two roots of $g(p)$ are

$$p_1 = \frac{3 + 4n - \sqrt{(4n-18)^2 - 171}}{6},$$

and

$$p_2 = \frac{3 + 4n + \sqrt{(4n-18)^2 - 171}}{6}.$$

Simple calculations show that $p_2 > n - 2$, hence $p < p_2$.

Subcase 2.1. $n = 8$. Then $p_1 = 5$, namely, $g(5) = 0$. So $Kf(S_8^{5,q}) = Kf(S_8^{4,q})$. On the one hand, $g(6) > 0$, namely, $Kf(S_8^{6,q}) > Kf(S_8^{5,q})$. On the other hand, $g(4) < 0$, namely, $Kf(S_8^{4,q}) < Kf(S_8^{3,q})$. So when the length of the cycle is 4 or 5, the Kirchhoff index is minimal. Hence $S_8^{4,4}$ and $S_8^{4,5}$ have the minimal Kirchhoff index.

Subcase 2.2. $9 \le n \le 11$. Then $4 < p_1 < 5$. This indicates that for $p \ge 5$, $g(p) > 0$, namely, $Kf(S_n^{p,q}) > Kf(S_n^{p-1,q})$. On the other hand, $g(4) < 0$, $Kf(S_n^{4,q}) < Kf(S_n^{3,q})$. So when the length of the cycle is 4, the Kirchhoff index is minimal. Hence $S_n^{4,4}$ has the minimal Kirchhoff index.

Subcase 2.3. $n = 12$. Then $p_1 = 4$, namely, $g(4) = 0$. So $Kf(S_{12}^{4,q}) = Kf(S_{12}^{3,q})$. On the other hand, for $p \ge 5$, $g(p) > 0$. That is, $Kf(S_{12}^{p,q}) > Kf(S_{12}^{p-1,q})$. So when the length of cycle is 4 or 3, the Kirchhoff index is minimal. Hence $S_{12}^{4,4}$, $S_{12}^{3,4}$ and $S_{12}^{3,3}$ have the minimal Kirchhoff index.

Subcase 2.4. $n > 12$. Then $p_1 < 4$. For $p \ge 4$, $g(p) > 0$, namely, $Kf(S_n^{p,q}) > Kf(S_n^{p-1,q})$. So when the length of cycle is 3, the Kirchhoff index is minimal. Hence $S_n^{3,3}$ has the minimal Kirchhoff index . □

From Theorems 3.1 and 3.2, we arrive at our main result.

Theorem 3.3. *Among n-vertex bicyclic graphs with exactly two cycles*

(a) $P_n^{3,3}$ has the maximal Kirchhoff index.

(b) The following graphs have the minimal Kirchhoff indices: $S_5^{3,3}$*;* $S_6^{3,4}$*;* $S_7^{4,4}$*;* $S_8^{4,4}$ *and* $S_8^{4,5}$*;* $S_n^{4,4}$ *(*$9 \le n \le 11$*);* $S_{12}^{4,4}$*,* $S_{12}^{3,4}$ *and* $S_{12}^{3,3}$*;* $S_n^{3,3}$ *(*$n > 12$*).*

By formulae (1) and (2), we can obtain the following formulae.

(i) $Kf(S_n^{3,3}) = n^2 - \frac{10n}{3} + 1$;

(ii) $Kf(S_n^{3,4}) = n^2 - \frac{19n}{6} - 1$;

(iii) $Kf(S_n^{4,4}) = n^2 - 3n - 3$;

(iv) $Kf(S_n^{4,5}) = n^2 - \frac{5n}{2} - 7$;

(v) $Kf(P_n^{3,3}) = \frac{n^3-21n+36}{6}$.

Combining these formulae with Theorem 3.3, sharp bounds for Kirchhoff indices of bicyclic graphs are obtained.

Theorem 3.4. *For n-vertex bicyclic graph G with exactly two cycles,*

(i) *if* $n = 6$, $n^2 - \frac{19n}{6} - 1 \le Kf(G) \le \frac{n^3-21n+36}{6}$;

(ii) *if* $7 \le n \le 12$, $n^2 - 3n - 3 \le Kf(G) \le \frac{n^3-21n+36}{6}$;

(iii) *if* $n = 5$ *or* $n > 12$, $n^2 - \frac{10n}{3} + 1 \le Kf(G) \le \frac{n^3-21n+36}{6}$.

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References

[1] D.J. Klein and M. Randić, Resistance distance, J. Math. Chem. 12 (1993) 81–95.

[2] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.

[3] W. Xiao and I. Gutman, Relations between resistance and Laplacian matrices and their applications, MATCH Commun. Math. Comput. Chem. 51 (2004) 119-127.

[4] R. B. Bapat, I. Gutman and W. Xiao, A simple method for computing resistance distance, Z. Naturforsch. 58a (2003) 494-498.

[5] W. Xiao and I. Gutman, Resistance distance and Laplacian spectrum, Theoret. Chem. Acc. 110 (2003) 284-289.

[6] W. Xiao and I. Gutman, On resistance matrices, MATCH Commun. Math. Comput. Chem. 49 (2003) 67-81.

[7] W.J. Xiao and I. Gutman, Resistance distance and Laplacian spectrum, Theor. Chem. Acc. 110 (2003) 284-289.

[8] I. Lukovits, S. Nikolić and N. Trinajstić, Resistance distance in regular graphs, Int. J. Quantum Chem. 71 (1999) 217–225.

[9] D.J. Klein, I. Lukovits and I. Gutman, On the definition of the hyper-wiener index for cycle-containing structures, J. Chem. Inf. Comput. Sci. **35** (1995) 50–52.

[10] I. Lukovits, S. Nikolić and N. Trinajstić, Note on the resistance distances in the dodecahedron, Croat. Chem. Acta 73 (2000) 957–967.

[11] A.T. Balaban, X. Liu, D.J. Klein, D. Babic, T.G. Schmalz, W.A. Seitz and M. Randić, Graph invariants for fullerenes, J. Chem. Inf. Comput. Sci. 35 (1995) 396–404.

[12] P.W. Fowler, Resistance distances in fullerene graphs, Croat. Chem. Acta 75 (2002) 401–408.

[13] D. Babić, D.J. Klein, I. Lukovits, S. Nikolić and N. Trinajstić, Resistance-distance matrix: A computational algorithm and its application, Int. J. Quantum Chem. 90 (2002) 166–176.

[14] J.L. Palacios, Closed-form formulas for Kirchhoff index, Int. J. Quantum Chem. 81 (2001) 135–140.

[15] H.P. Zhang and Y.J. Yang, Resistance distance and Kirchhoff index in circulant graphs, Int. J. Quantum Chem. 107 (2007) 330–339.

[16] Y.J. Yang and H.P. Zhang, Kirchhoff index of linear hexagonal chains, Int. J. Quantum Chem. 108 (2008) 503–512.

[17] J.L. Palacios, Resistance distance in graphs and random walks, Int. J. Quantum Chem. 81 (2001) 29–33.

[18] D.J. Klein, Resistance-distance sum rules, Croat. Chem. Acta 75 (2002) 633–649.

[19] Y.J. Yang and X.Y. Jiang, Unicyclic graphs with extremal Kirchhoff index, MATCH Commun. Math Comput. Chem. 60 (2008) 107-120.

[20] R.C. Entringer, D.E. Jackson and D.A. Snyder, Distance in graphs, Czechoslovak Math. J. 26 (1976) 283–296.