Tricyclic graphs with minimal Kirchhoff Index*

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Abstract

The resistance distance between two vertices of a connected graph G is defined as the effective resistance between them in the corresponding electrical network constructed from G by replacing each edge of G with a unit resistor. The Kirchhoff index of $Kf(G)$ is the sum of resistance distances between all pairs of vertices of the graph G. In this paper, we'll determine the tricyclic graphs with the smallest and the second smallest Kirchhoff indices.

1 Introduction

All graphs considered here are both connected and simple if not stated in particular. For any $v \in V(G)$, we use $N_G(v)$ to denote the set of the neighbors of v, and let $N_G[v] = v \cup N_G(v)$, let $d(v)$ be the number of edges incident with v. For a graph G with $v \in V(G)$, $G - v$ denotes the graph resulting from G by deleting v (and its incident edges). For an edge uv of the graph G (the complement of G, respectively), $G - uv$ ($G + uv$, respectively) denotes the graph resulting from G by deleting (adding, respectively) uv. The distance between vertices v_i and v_j, denoted by $d_G(v_i, v_j)$ or $d(v_i, v_j)$ for short, is the length of a shortest path between them. In 1947, American Chemist H. Wiener in [1] defined the famous Wiener index as

$$W(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d(v_i, v_j) \tag{1}$$

and in 1993 Klein and Randić [2] introduced a new distance function named *resistance distance* on the basis of electrical network theory. They viewed a graph G as an electrical network N such that each edge of G is assumed to be a unit resistor. Then, the resistance distance between the vertices v_i and v_j, are denoted by $r(v_i, v_j)$, is defined to be the effective resistance between nodes v_i, $v_j \in N$. Analogous to the definition of the Wiener index,

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the Kirchhoff index $Kf(G)$ of a graph G is defined as[2, 3]

$$Kf(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} r(v_i, v_j) \tag{2}$$

If G is a tree, then $r(u, v) = d(u, v)$ for any two vertices u and v. Consequently, the Kirchhoff and Wiener indices of trees coincide.

The Kirchhoff index is an important molecular structure descriptor[4], it has been well studied in both mathematical and chemical literatures. To compute the Kirchhoff index is a hard problem, the existed results were mainly concentrate on the specific classes of graphs. For a general graph G, I. Lukovits et al. [5] showed that $Kf(G) \geq n - 1$ with equality if and only if G is complete graph K_n, and P_n has maximal Kirchhoff index. Palacios [6] showed that $Kf(G) \leq \frac{1}{6}(n^3 - n)$ with equality if and only if G is a path. In [7], Yang et al., studied the Kirchhoff index of unicyclic graphs with given girth and determined the extremal graphs. In [8], Deng et al., obtained the second maximal and minimal Kirchhoff index of unicyclic graphs. Q. Guo at al. [9] studied the Kirchhoff index of full loaded unicyclic graphs, and in [10], Deng investigated Kirchhoff index graphs with given number of cut edges. Zhou [11] obtained the extremal graphs with given matching number, connectivity and minimal Kirchhoff index. Wang et al. [12] obtained the first three minimal Kirchhoff indices among cacti. In [13], the authors studied the Kirchhoff index of bicyclic graphs with exactly two cycles. In [14], the authors studied the Kirchhoff index of linear hexagonal chains. H. Zhang et at.[15] investigated the Kirchhoff index of composite graphs. A. Nikseresht et al.[16] computed the Kirchhoff index of the T-repetition of G in terms of parameters of T and G. M. Bianchi et al.[17] studied bounds for the Kirchhoff index via majorization techniques. In [18] the authors gave the graphs with the nine largest and nine smallest Kirchhoff indices among all possible graphs. In [19] the author gave the three largest and three smallest Kirchhoff indices among graphs with diameter 2. Also, in [19] it is found that the Kirchhoff index of the so-called propeller graph $S_n(k)$ is $Kf(S_n(k)) = (n-1)^2 - \frac{2kn}{3}$.

The cyclomatic number of a connected graph G is defined as $c(G) = m-n+1$. A graph G with $c(G) = k$ is called a $k-$cyclic graph, for $c(G) = 3$, we named G as a tricyclic graph. Let $\mathscr{T}_n$ be the set of all tricyclic graphs with n vertices. By [20-26], a tricyclic graph G contains at least 3 cycles and at most 7 cycles, furthermore, there do not exist 5 cycles in G. Let $\mathscr{T}_n = \mathscr{T}_n^3 \bigcup \mathscr{T}_n^4 \bigcup \mathscr{T}_n^6 \bigcup \mathscr{T}_n^7$, where $\mathscr{T}_n^i$ denotes the set of tricyclic graph on n vertices with exact i cycles for $i = 3, 4, 6, 7$. Note that the induced subgraph of vertices on the cycles of $G \in \mathscr{T}_n^i (i = 3, 4, 6, 7)$ are depicted in Figure 1.

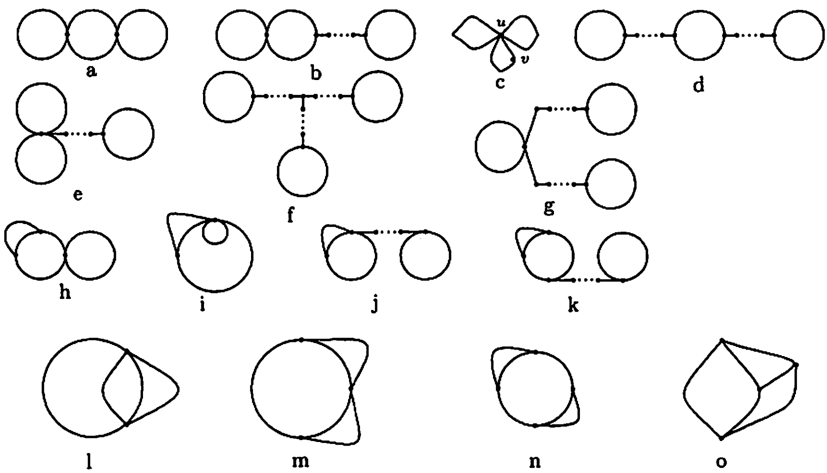

Figure 1. The arrangement of cycles of a tricyclic graph in $\mathscr{T}_n^i (i = 3, 4, 6, 7)$

For any graph $G \in \mathscr{T}_n$, G can be obtained from some graphs showed in Figure 1 by attaching trees to some vertices.

To our best knowledge, the Kirchhoff index for tricyclic graphs has not been considered so far, and the most similar result about it gave in [19]. In this paper, we'll investigate the Kirchhoff indices of tricyclic graphs, and determine the tricyclic graphs with the smallest and the second smallest Kirchhoff indices.

2 Preliminary Results

Let G_1, G_2 be two disjoint connected graphs, and let $v_1 \in V(G_1)$, $v_2 \in V(G_2)$. We obtain a graph G from $(G_1 - v_1) \bigcup (G_2 - v_2)$ by adding a new vertex u and together with edges joining u to the vertices of $N_{G_1}(v_1) \bigcup N_{G_2}(v_2)$. The graph G is called a coalescence of G_1 and G_2 at vertices v_1, v_2, denoted by $G_1 u G_2$.

For a vertex $u \in V(G)$, let $Kf_u(G) = \sum\limits_{v \in V(G)} r(v, u)$. C_n be the cycle on $n \geq 3$ vertices, for any two vertices $v_i, v_j \in V(C_n)$ with $i < j$, by Ohm's law, we have $r_{C_n}(v_i, v_j) = \dfrac{(j-i)(n+i-j)}{n}$, and for a vertex $u \in V(C_n)$, one has $Kf_u(C_n) = \dfrac{n^2-1}{6}$.

Lemma 2.1([2]). 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

$$r_G(a,b) = r_G(a,x) + r_G(x,b). \tag{3}$$

Lemma 2.2([7]). Let G_1 and G_2 be two connected graphs with exactly one common vertex x, and $G = G_1 x G_2$. Then

$$Kf(G) = Kf(G_1)+Kf(G_2)+(|V(G_1)|-1)Kf_x(G_2)+(|V(G_2)|-1)Kf_x(G_1). \tag{4}$$

Lemma 2.3. Let $G_1, G_2, \cdots, G_t$ be connected graphs with exactly one common vertex x, and $|V(G_i)| = n_i (i = 1, 2, \cdots, t)$. Then

$$Kf(G) = \sum_{1\le i\le t} Kf(G_i) + \sum_{1\le i\le t}\sum_{1\le j\le t, j\ne i} (n_i - 1)Kf_x(G_j). \tag{5}$$

Proof. Let $H_t = G_1 x G_2 x \cdots x G_t$, by Lemma 2.2, one has

$$\begin{aligned} & Kf(H_t) \\ &= Kf(H_{t-1}) + Kf(G_t) + (|V(H_{t-1})| - 1)Kf_x(G_t) + (n_t - 1)Kf_x(H_{t-1}) \\ &= \cdots \\ &= \sum_{1\le i\le t} Kf(G_i) + \sum_{1\le i\le t}\sum_{1\le j\le t, j\ne i} (n_i - 1)Kf_x(G_j). \end{aligned}$$

For convenience, we provide some grafting transformations, which will decrease the Kirchhoff index of graphs as follows.

Let v be a vertex of degree $p+1$ in a graph G, such that $vv_1, vv_2, \cdots, vv_p$ are pendant edges incident with v, and u is the neighbor of v distinct from $v_1, v_2, \cdots, v_p$, and $G' = \alpha(G, v)$ by removing the edges $vv_1, vv_2, \cdots, vv_p$ and adding new edges $uv_1, uv_2, \cdots, uv_p$, see Figure 2.

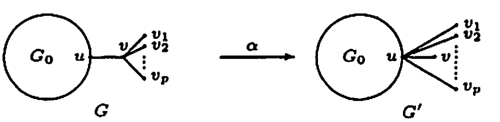

Figure 2. Transformation α.

Lemma 2.4. Let $G' = \alpha(G, v)$ be a graph transformed from the graph G, described above. Then $Kf(G) \ge Kf(G')$, with equality holds if and only if G is a star with v as its center.

Proof. Let $|V(G_0)| = n_0$, by the definition of Kirchhoff index and Lemma 2.2, one has

$$\begin{aligned} Kf(G) &= Kf(G_0) + Kf(S_{p+2}) + (n_0 - 1)Kf_u(S_{p+2}) + (p+1)Kf_u(G_0) \\ &= Kf(G_0) + (p+1)^2 + (n_0 - 1)(2p+1) + (p+1)Kf_u(G_0) \\ Kf(G') &= Kf(G_0) + (p+1)^2 + (n_0 - 1)(p+1) + (p+1)Kf_u(G_0) \end{aligned}$$

Thus, $Kf(G) - Kf(G') = p(n_0 - 1) \geq 0$.

This proves the result.

Remark 1. Repeating Transformation α, any tree can be changed into a star, any cyclic graph can be changed into a cyclic graph such that all the edges not on the cycles are pendant edges.

Transformations β. Let u, v be two vertices in G. $u_1, u_2, \cdots, u_s$ are the leaves adjacent to u, $v_1, v_2, \cdots, v_t$ are the leaves adjacent to v. $G' = G - \{vv_1, vv2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, $G'' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, depicted in Figure 3.

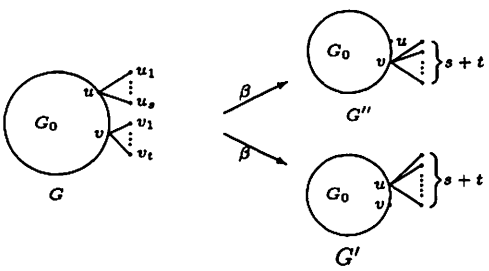

Figure 3. Transformation β.

Lemma 2.5. Let G' and G'' be the graphs depicted in transformation β, then either $Kf(G) > Kf(G')$ or $Kf(G) > Kf(G'')$.

Proof. Let $|V(G_0)| = n_0$, by the definition of Kirchhoff index and Lemma 2.2, one has,

$$Kf(G) = Kf(G_0) - sKf_u(G_0) + tKf_v(G_0) + (n_0 - 1)(s + t) + (s + t)^2 + str(u, v),$$

$$Kf(G') = Kf(G_0) + (s + t)Kf_u(G_0) + (n_0 - 1)(s + t) + (s + t)^2,$$

$$Kf(G'') = Kf(G_0) + (s + t)Kf_v(G_0) + (n_0 - 1)(s + t) + (s + t)^2.$$

Thus, $\Delta_1 = Kf(G) - Kf(G') = t(Kf_v(G_0) - Kf_u(G_0) + sr(u, v))$,

$\Delta_2 = Kf(G) - Kf(G'') = s(Kf_u(G_0) - Kf_v(G_0) + tr(u, v))$.

Hence, if $Kf(G) - Kf(G') > 0$ and $Kf(G) - Kf(G'') > 0$ hold, then the result follows.

If at least one difference is negative, say $\Delta_1 < 0$, then $Kf_v(G_0) - Kf_u(G_0) + sr(u, v) < 0$, i.e., $Kf_u(G_0) - Kf_v(G_0) > sr(u, v)$, and therefore $\Delta_2 > s(s + t)r(u, v) > 0$.

This completes the proof.

Remark 2. Repeating Transformation β, any cyclic graph can be changed into a cyclic graph such that all the pendant edges are attached to the same vertex.

Suppose that G is obtained from a connected graph $G_0 \ncong P_1(|V(G_0)| \geq 9)$ and a cycle $C_p = v_0v_1\cdots v_{p-1}v_0(p \geq 4$ for p is even; otherwise $p \geq 5)$ by identifying v_0 with a vertex v of the graph G_0 (see Figure 4), i.e.,$G = G_0vC_p$. Let $G' = G - v_{p-1}v_{p-2} + vv_{p-2}$, i.e., $G' = G_0vC_{p-1}vK_1$. We name above operation as grafting transformation γ.

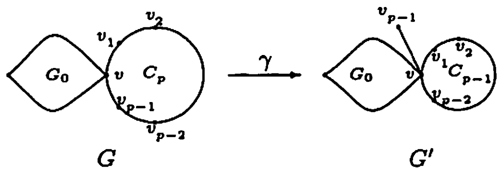

Figure 4. Transformation γ

Lemma 2.6. Let G and G' be the graphs depicted in Figure 4, then $Kf(G') < Kf(G)$.

Proof. Let $|V(G_0)| = n_0$. By the definition of Kirchhoff index and Lemma 2.2, one has,

$$Kf(G) = Kf(G_0) + (p-1)Kf_v(G_0) + (n_0 - 1)\frac{p^2-1}{6} + \frac{p^3-p}{12},$$

$$Kf(G') = Kf(G_0) + (p-1)Kf_v(G_0) + (n_0 - 1)\frac{p^2-2p+6}{6} + \frac{p^3-p^2+10p-12}{12}.$$

Thus, $Kf(G) - Kf(G') = (n_0 - 1)\frac{2p-7}{6} + \frac{p^2-11p+12}{12} \geq 0$.
The proof is completed.

3 The smallest Kirchhoff indices of $\mathscr{T}_n^i$

In this section we shall determine the graphs that achieve the smallest Kirchhoff indices in $\mathscr{T}_n^i(i = 3, 4, 6, 7)$, respectively.

3.1 The smallest Kirchhoff index of $\mathscr{T}_n^3$

Let H be a graph formed by attaching three cycles C_a, C_b, C_c to a common vertex u; see Figure 1.(c), and let $G_{a,b,c}^k$ be the graph on n vertices obtained from H by attaching k pendant edges to the vertex u, where $a+b+c+k = n+2(n \geq 13)$. We also set $\mathcal{G} = \{G \in \mathscr{T}_n : G$ is a graph obtained from H by attaching k pendant vertices to the vertex v of H except $u\}$, $\widetilde{G}_{a,b,c}^k$ is one of the resulted graph, see Figure 5.

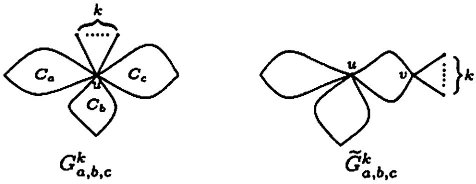

Figure 5. The graphs $G^k_{a,b,c}$ and $\widetilde{G}^k_{a,b,c}$

Theorem 3.1.1. Let $G^k_{a,b,c}$, $\widetilde{G}^k_{a,b,c}$ be the two graphs depicted above, then $Kf(G^k_{a,b,c}) < Kf(\widetilde{G}^k_{a,b,c})$.

Proof. Let $H = C_a u C_b u C_c$ in $G^k_{a,b,c}$ and $\widetilde{G}^k_{a,b,c}$, then

$$Kf(G^k_{a,b,c}) = Kf(H) + Kf(S_{k+1}) + (|V(H)| - 1)Kf_u(S_{k+1}) + kKf_u(H),$$
$$Kf(\widetilde{G}^k_{a,b,c}) = Kf(H) + Kf(S_{k+1}) + (|V(H)| - 1)Kf_v(S_{k+1}) + kKf_v(H).$$

and $Kf_u(S_{k+1}) = Kf_v(S_{k+1})$, $Kf_u(S_{k+1}) < Kf_v(S_{k+1})$.

Thus, $Kf(G^k_{a,b,c}) < Kf(\widetilde{G}^k_{a,b,c})$.

Further, one has,

Theorem 3.1.2. Let G be a n vertex tricyclic graph with exactly three cycles C_a, C_b and C_c, then $Kf(G) \geq Kf(G^k_{a,b,c})$ with the equality if and only if $G \cong G^k_{a,b,c}$.

Theorem 3.1.3. For any given positive integers a, b, c and k, one has

(i) $Kf(G^k_{a,b,c}) > Kf(G^{k+1}_{a-1,b,c})$, if $a \geq 4$, $b, c \geq 3$;

(ii) $Kf(G^k_{a,b,c}) > Kf(G^{k+1}_{a,b-1,c})$, if $a, c \geq 3$, $b, c \geq 4$;

(iii) $Kf(G^k_{a,b,c}) > Kf(G^{k+1}_{a,b,c-1})$, if $a, b \geq 3$, $b, c \geq 4$.

Proof. By the symmetry of three cycles C_a, C_b and C_c contained in G, here we only show that (i) holds. We omit the proofs for (ii) and (iii).

Let $G_0 = C_b u C_c$, $H = C_a u S_{k+1}$, by the definition of Kirchhoff index and Lemma 2.2, one has,

$$\begin{aligned}
&Kf(G^k_{a,b,c})\\
&= Kf(G_0) + Kf(H) + (b + c - 2)Kf_u(H) + (a + k - 1)Kf_u(G_0),\\
&= Kf(G_0) + (a + k - 1)Kf_u(G_0) + \frac{1}{6}(b + c - 2)(a^2 + 6k - 1)\\
&\quad + \frac{1}{12}(a^3 + 2a^2k + 12ak + 12k^2 - a - 14k);\\
&Kf(G^{k+1}_{a-1,b,c})\\
&= Kf(G_0) + (a + k - 1)Kf_u(G_0) + \frac{1}{6}(b + c - 2)(a^2 + 6k - 2a + 6)\\
&\quad + \frac{1}{12}(a^3 + 2a^2k - a^2 + 8ak + 12k^2 + 10a - 12).
\end{aligned}$$

$$
\begin{aligned}
Kf(G^k_{a,b,c}) - Kf(G^{k+1}_{a-1,b,c}) &= \frac{1}{12}(n(4a-14) - 3a^2 + 3a + 12) \\
&\geq \frac{1}{12}((a+9)(4a-14) - 3a^2 + 3a + 12) \\
&> 0, \quad \text{since } n \geq 13.
\end{aligned}
$$

This completes the proof.

Theorem 3.1.4. Let $G \in \mathscr{T}_n^3$, then $Kf(G) \geq n^2 - 4n + 1$, the equality holds if and only if $G \cong G^{n-7}_{3,3,3}$.

Proof. It's sufficient to see that for any graph $G \in \mathscr{T}_n^3$, $Kf(G) \geq Kf(G^{n-7}_{3,3,3})$.

By a simple calculation, one has, $Kf(G^{n-7}_{3,3,3}) = n^2 - 4n + 1$.

3.2 The smallest Kirchhoff index of $\mathscr{T}_n^4$

Let P_{a+1}, P_{b+1}, P_{c+1} be three vertex disjoint paths with $a, b, c \geq 1$, and at most one of them is 1. Identifying the three initial vertices and terminal vertices of them, *resp.* The resulting graph, denote as $\Theta-$graph $\Theta(a, b, c)$. Connecting the cycle C_d and $\Theta(a, b, c)$ by a path P_k, where $k \geq 1$, naming the resulting graph as $\widetilde{\Theta}-$graph. From [20-26], we know that the are exactly four types of $\widetilde{\Theta}-$graph, see Figure 1 h,i,j,k. $\mathscr{T}_n^4$ is the set of graphs each of which is a $\widetilde{\Theta}-$graph, has some trees attached, if possible. Let $\mathcal{H}_0 = \Theta(a, b, c)vC_d$, and $H^k_{a,b,c,d}$ is a n vertex graph formed from $\mathcal{H}_0$ by attaching $k(k = n + 5 - a - b - c - d)$ pendant vertices to v, see Figure 6.

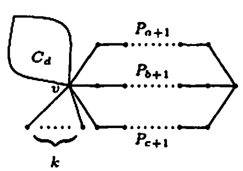

Figure 6. The graph $H^k_{a,b,c,d}$

Similar to the discussion way of section 3.1, one has,

Theorem 3.2.1. Let $G \in \mathscr{T}_n^4$ such that G contains the $\Theta(a, b, c)$ and the cycle C_d with $E(\Theta(a, b, c)) \bigcap E(C_d) = \emptyset$. Then $Kf(G) \geq Kf(H^k_{a,b,c,d})$.

Similarly, one has,

Theorem 3.2.2. For any given positive integers a, b, c, d and k, then

(i) $Kf(H^k_{a,b,c,d}) > Kf(H^{k+1}_{a-1,b,c,d})$ for either $a \geq 4$, $b, c \geq 2$ and $bc \geq 6$, $d \geq 3$ or $a = 3$, $b, c, d \geq 3$;

(ii) $Kf(H^k_{a,b,c,d}) > Kf(H^{k+1}_{a,b-1,c,d})$ for either $b \geq 4$, $a, c \geq 2$ and $ac \geq 6$, $d \geq 3$ or $b = 3$, $a, c, d \geq 3$;

(iii) $Kf(H^k_{a,b,c,d}) > Kf(H^{k+1}_{a,b,c-1,d})$ for either $c \geq 4$, $a, b \geq 2$ and $ab \geq 6$, $d \geq 3$ or $c = 3$, $a, b, d \geq 3$;

(iv) $Kf(H^k_{a,b,c,d}) > Kf(H^{k+1}_{a,b,c,d-1})$ for either $d \geq 4$, $abc \geq 18$.

And

Theorem 3.2.3. Let $G \in \mathscr{T}_n^4$, then $Kf(G) \geq n^2 - \frac{47n}{12} + 1$, the equality holds if and only if $G \cong H^{n-6}_{2,3,3,3}$ (or $H^{n-6}_{3,2,3,3}$, $H^{n-6}_{3,3,2,3}$).

Proof. It is noted that $H^{n-6}_{2,3,3,3} \cong H^{n-6}_{3,2,3,3} \cong H^{n-6}_{3,3,2,3}$.

By Theorem 3.2.2, for any graph $G \in \mathscr{T}_n^4$, $Kf(G) \geq Kf(H^{n-6}_{2,3,3,3})$, and

$$Kf(H^{n-6}_{2,3,3,3}) = n^2 - \frac{47n}{12} + 1.$$

3.3 The smallest Kirchhoff index of $\mathscr{T}_n^6$

Let $I^k_{a,b,c,d}$ be a tricyclic graph with exact 6 cycles on n vertices obtained from Figure 1(l) by attaching k pendant vertices to v showed in Figure 7(i).

Let $J^k_{a,b,c}$ be a tricyclic graph with exact 6 cycles on n vertices obtained from Figure 1(m) by attaching k pendant vertices to v showed in Figure 7(ii).

Let $K^k_{a,b,c}$ be a tricyclic graph with exact 6 cycles on n vertices obtained from Figure 1(n) by attaching k pendant vertices to v showed in Figure 7(iii).

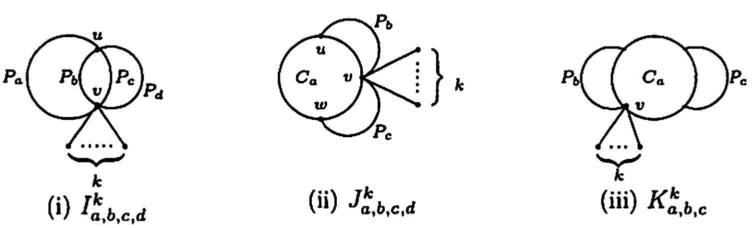

Figure 7. The graphs $I^k_{a,b,c,d}$, $J^k_{a,b,c}$, $K^k_{a,b,c}$

Theorem 3.3.1. Let $G \in \mathscr{T}_n^6$, then

(i) $Kf(G) \geq Kf(I^k_{a,b,c,d})$ if the six cycles in G are arranged the same way as the graphs depicted in Figure 1(l);

(ii) $Kf(G) \geq Kf(J^k_{a,b,c})$ if the six cycles in G are arranged the same way as the graphs depicted in Figure 1(m);

(iii) $Kf(G) \geq Kf(K^k_{a,b,c})$ if the six cycles in G are arranged the same as with the graphs depicted in Figure 1(n).

Similarly, one has,

Theorem 3.3.2. Let $G \in \mathscr{T}_n^6$,

(i) If the arrangement of the six cycles is the same as Fig 1(l), then $Kf(G) \geq Kf(I^{n-5}_{3,3,3,2})$, the equality holds if and only if $G \cong I^{n-5}_{3,3,3,2}$;

(ii) If the arrangement of the six cycles is the same as Fig 1(m), then $Kf(G) \geq Kf(J^{n-5}_{3,3,3})$, the equality holds if and only if $G \cong J^{n-5}_{3,3,3}$;

(iii) If the arrangement of the six cycles is the same as Fig 1(n), then $Kf(G) \geq Kf(K^{n-5}_{4,3,3})$, the equality holds if and only if $G \cong K^{n-6}_{4,3,3}$.

Moreover, It is ease to compute out that $Kf(I^{n-5}_{3,3,3,2}) = n^2 - \frac{19n}{5} + 1$, $Kf(J^{n-5}_{3,3,3}) = n^2 - \frac{80n}{21} + \frac{181}{1155}$, $Kf(K^{n-6}_{4,3,3}) = n^2 - \frac{221n}{70} - \frac{907}{210}$.

Combining the above results, one arrives at,

Theorem 3.3.3. Let $G \in \mathscr{T}_n^6$, then $Kf(G) \geq n^2 - \frac{19n}{5} + 1$, the equality holding if and only if $G \cong I^{n-5}_{3,3,3,2}$.

3.4 The smallest Kirchhoff index of $\mathscr{T}_n^7$

Let $R^k_{a,b,c,d,e,f}$ be a tricyclic graph with exact seven cycles on n vertices obtained from Figure 1(o) by attaching k pendant vertices to v, shown in Figure 8, where $a + b + c + d + e + f + k = n + 8$.

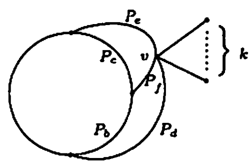

Figure 8. The graph $R^k_{a,b,c,d,e,f}$

Applying the similar methods above, we can obtain the following results, and we omit the proof here.

Theorem 3.4.1. Let $G \in \mathscr{T}_n^7$, then $Kf(G) \geq Kf(R^{n-4}_{2,2,2,2,2,2})$, the equality holds if and only if $G \cong R^{n-4}_{2,2,2,2,2,2}$.

It's noted that $Kf(R^{n-4}_{2,2,2,2,2,2}) = n^2 - \frac{7n}{2} + 1$.

4 Extremal Kirchhoff indices of $\mathscr{T}_n$

In this section, we'll determine the graphs in $\mathscr{T}_n$ with the smallest and the second smallest Kirchhoff indices.

By combining the theorems 3.1.4, 3.2.3, 3.3.3 with 3.4.1, one arrives at,

Theorem 4.1. Let $G \in \mathscr{T}_n (n \geq 12)$, then $Kf(G) \geq n^2 - 4n + 1$, the equality holds if and only if $G \cong G^{n-7}_{3,3,3}$.

The derived result coincides with the Kirchhoff index of $S_n(3)$ characterized in [19], and $G_{3,3,3}^{n-7}$ has the diameter 2.

In the following, we'll determine the graph in $\mathscr{T}_n$ with second smallest Kirchhoff index.

In the first place, we determine the graph in $\mathscr{T}_n^3$ with the second smallest Kirchhoff index.

Now suppose first that G has the second smallest Kirchhoff index among all elements of $\mathscr{T}_n^3$. Evidently, G can be changed into $G_{3,3,3}^{n-7}$ by using exactly one step of transformation α, β or γ, for otherwise, one can employ one step of transformation α, β or γ on G, and obtain a new graph G', which is still in $\mathscr{T}_n^3$ but not isomorphic to $G_{3,3,3}^{n-7}$, which gives

$$Kf(G) < Kf(G') < Kf(G_{3,3,3}^{n-7}),$$

contradicting to the choice of G.

By the above arguments, one can conclude that G must be one of the graphs H_1, H_2, and H_3, depicted in Figure 9.

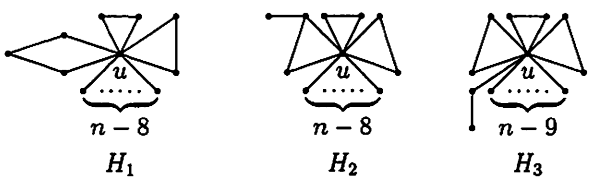

Figure 9. The graphs H_1, H_2 and H_3 in T_n^3

Theorem 4.2. Let $G \in \mathscr{T}_n^3 (n \geq 8)$, then $Kf(G) \geq n^2 - \frac{23}{6}n - 1$, the equality holds if and only if $G \cong H_1$.

Proof. By Lemma 2.3, one has,

$$\begin{aligned} & Kf(H_1) \\ &= Kf(C_4) + 2Kf(C_3) + Kf(S_{n-7}) + 3\big(2Kf_u(C_3) + Kf_u(S_{n-7})\big) + \\ &\quad 4\big(Kf_u(C_4) + Kf_u(C_3) + Kf_u(S_{n-7})\big) + (n-8)\big(Kf_u(C_4) + 2Kf_u(C_3)\big) \\ &= n^2 - \frac{23}{6}n - 1. \end{aligned}$$

Similarly, $Kf(H_2) = n^2 - \frac{10}{3}n - \frac{5}{3}$, $Kf(H_3) = n^2 - 3n - 2$.

It's easy to check that $Kf(H_3) > Kf(H_2) > Kf(H_1)$.

This completes the proof.

By combining the theorems 3.2.3, 3.3.3, 3.4.1 with 4.2, one arrives at,

Theorem 4.3. Let $G \in \mathscr{T}_n$, and $G \ncong G_{3,3,3}^{n-7}$,

(i) If $n \geq 24$, then $Kf(G) \geq n^2 - \frac{47}{12}n + 1$, the equality holds if and only if $G \cong H^{n-6}_{2,3,3,3}$.

(ii) If $9 \leq n \leq 24$, then $Kf(G) \geq n^2 - \frac{23}{6}n - 1$, the equality holds if and only if $G \cong H_1$.

Remark 3. Continuing to explore in this way, we'll determine graphs with the third smallest, the fourth smallest, etc., Kirchhoff indices, we omit the details here.

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