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Extremal Polygonal Cacti for Wiener Index and Kirchhoff Index

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ABSTRACT

For a connected graph G, the Wiener index $W(G)$ of G is the sum of the distances of all pairs of vertices, the Kirchhoff index $Kf(G)$ of G is the sum of the resistance distances of all pairs of vertices. A k-polygonal cactus is a connected graph in which the length of every cycle is k and any two cycles have at most one common vertex. In this paper, we give the maximum and minimum values of the Wiener index and the Kirchhoff index for all k-polygonal cacti with n cycles and determine the corresponding extremal graphs, generalize results of spiro hexagonal chains with n hexagons.

1. INTRODUCTION

In this paper, we only consider the simple undirected and connected graphs. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $N_G(u)$ and $d_G(u)$ denote the neighbor set and the degree of vertex u in G, respectively, where $d_G(u) = |N_G(u)|$. For convenience, we usually simplify as N_u and d_u. The distance between any two vertices of u and v is the length of a shortest path from u to v in the graph G, denoted by $d_G(u, v)$ or $d(u, v)$. If $u \in V(G)$ and $G - u$ is not connected, then u is said to be a cut-vertex of G.

A cactus graph is a connected graph in which no edge lies in more than one cycle, for short, a cactus graph is also called a cactus. In fact, a graph G is a cactus if and only if

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each block of G is either an edge or a cycle. A cycle of length k is usuall called a k-polygon. If each block of a cactus G is a k-polygon, then G is called a k-polygonal cactus. For convenience, a k-polygon is usually referred to as a polygon.

Let $G_{n,k}$ denote the set of all k-polygon cacti with $n \geq 3$ blocks. Let $G \in G_{n,k}$ and C a k-polygon of G. If C contains exactly one cut-vertex, then C is called a terminal polygon; Otherwise, C is called a non-terminal polygon, i.e., a non-terminal polygon is a polygon contains at least two cut vertices.

A cactus chain is a special k-polygonal cactus such that each polygon has at most two cut-vertices, and each cut-vertex is shared by exactly two polygons. In fact, A k-polygonal cactus is a cactus chain if and only if the smallest connected subgraph which contains all cut-vertices is a path. If G is a cactus chain, then the number of polygons is called the length of G. Furthermore, if G is a cactus chain and the distance between two cut-vertices of each non-terminal polygon is $\left\lfloor \frac{k}{2} \right\rfloor$, then G is called a linear cactus chain. By the definition, the linear cactus chain with n polygons is unique and denoted by $L_{n,k}$.

A star-like cactus is the special k-polygonal cactus with n polygons such that all polygons have a common vertex, i.e., all polygons are terminal polygons. By the definition, it is unique and denoted by $W_{n,k}$, and $W_{n,k}$ contains exactly one cut-vertex with degree $2n$, and the degree of all the other vertices is 2.

In [17], Wang et al. gave the first three smallest Kirchhoff indices among all cacti possessing n vertices and t cycles. In [21], Ye et al. determined the minimum value and maximum values of general sum-connectivity index, general Platt index and second Zagreb index, respectively, among the class of k-polygonal cacti with n polygons. In this paper, we will give the maximum and minimum values of the Wiener index and the Kirchhoff index among all k-polygon cacti with $n \geq 3$ blocks and characterize the corresponding extremal graphs as well.

The Wiener index $W(G)$ of a graph G is based on the distances between vertex pairs, first proposed by H. Wiener [18] in 1947, and defined as the sum of the distances of all vertex pairs, i.e, $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)$. The Wiener index is used to describe the molecular structure, which was originally applied in the field of chemistry, and now is also widely used in social relationship measurement and social network, see [5, 6, 8, 14, 15, 16].

In 1993, Klein and Randić [11] introduced another distance function, the resistance distance, on the basis of electrical network theory. Inserting a unit resistance between each edge in G, the resistance distance between vertices u and v of G is the effective resistance between vertices u and v, denoted by $r_G(u,v)$ or r_{uv} . Based on the resistance distance, the Kirchhoff index $Kf(G)$ of a graph G is defined as the sum of the resistance distances of all vertex pairs, i.e., $Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r_G(u,v)$. For a vertex $u \in V(G)$, let $Kf_u(G) =$

$\sum_{u \subseteq V(G)} r_G(u, v)$, then $Kf(G) = \frac{1}{2}\sum_{u \in V(G)} Kf_u(G)$. As a useful structure-descriptor, the Kirchhoff index was well studied in [11, 13]. Much work has been done to compute the Kirchhoff index of some classes of graphs, such as complete graphs, cycles, distance transitive graphs, circulant graphs, linear hexagonal chains, unicyclic graphs and so on, see [1, 2, 3, 4, 7, 9, 10, 12, 17, 19, 20, 22, 23].

2. THE EXTREMAL GRAPH WITH THE MAXIMUM INDEX

In this section, we will determine the k-polygonal cactus with the maximum Wiener index and the maximum Kirchhoff index among all k-polygon cacti with n blocks for $k \geq 3$ and $n \geq 3$.

Firstly, we introduce some lemmas.

Lemma 1. [11] Let x be a cut vertex of a connected graph G and a, b be vertices occurring in different components of $G - x$. Then $r_G(a, b) = r_G(a, x) + r_G(x, b)$.

Lemma 2. [7, 17] Let G_1 and G_2 be connected graphs. $x_1 \in V(G_1)$ and $x_2 \in V(G_2)$. If G is obtained by identifying x_1 with x_2, then $Kf(G) = Kf(G_1) + Kf(G_2) + n_1 Kf_{x_2}(G_2) + n_2 Kf_{x_1}(G_1)$, where $Kf_{x_i}(G_i) = \sum_{y \epsilon V(G_i)} r_{G_i}(x_i, y)$, and $n_i = |V(G_i)| - 1$ for $i = 1,2$.

Lemma 3. If $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index, where $k \geq 3$, $n \geq 3$, and C is a k-polygon in G with exactly two cut-vertices, then the distance between two cut-vertices of C is $\left\lfloor \frac{k}{2} \right\rfloor$.

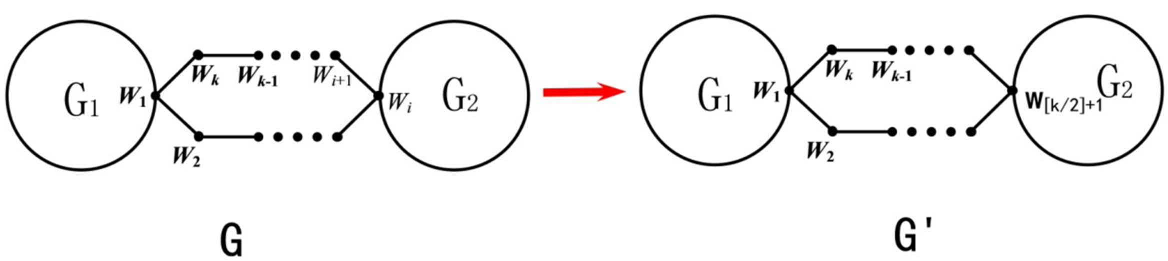

Figure 1: The graphs G and G'.

Proof. Let $C = w_1 w_2 \dots w_i \dots w_k w_1$ be a non-terminal polygon of $G \in G_{n,k}$, w_1 and w_i its two cut-vertices. G_1 and G_2 are the components of $G - E(C)$ containing w_1 and w_i, respectively. If $2 \leq i \leq \left\lfloor \frac{k}{2} \right\rfloor$, then we only need to show that $W(G') > W(G)$ and $Kf(G') > Kf(G)$, where $G' = G - w_i u - w_i v + w_{\lfloor \frac{k}{2} \rfloor + 1} u + w_{\lfloor \frac{k}{2} \rfloor + 1} v$, see Figure 1.

Let $V_1 = V(G_1)$, $V_2 = V(G_2) \cup V(C)$, $V_1' = V_1 - \{w_1\}$, $V_2' = V_2 - \{w_1\}$. We have

$$\begin{aligned}
W(G') - W(G) &= \textstyle\sum_{x,y \in V(G)} [d_{G'}(x,y) - d_G(x,y)] \\
&= \textstyle\sum_{x,y \in V_1} [d_{G'}(x,y) - d_G(x,y)] + \sum_{x,y \in V_2} [d_{G'}(x,y) - d_G(x,y)] \\
&+ \textstyle\sum_{y \in V_1', x \in V_2'} [d_{G'}(x,y) - d_G(x,y)] \\
&= \textstyle\sum_{y \in V_1', x \in V_2'} [d_{G'}(x,y) - d_G(x,y)] \\
&= \textstyle\sum_{y \in V_1', x \in V(G_2)} [d_{G'}(x,y) - d_G(x,y)] \\
&= \textstyle\sum_{y \in V_1', x \in V(G_2)} [(d_{G'}\left(x, w_{\lfloor \frac{k}{2} \rfloor + 1}\right) + d_{G'}\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_1\right) + d_{G'}(w_1, y)) \\
&- (d_G(x, w_i) + d_G(w_i, w_1) + d_G(w_1, y))] \\
&= \textstyle\sum_{y \in V_1', x \in V(G_2)} [d_{G'}\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_1\right) - d_G(w_i, w_1)] \\
&= \textstyle\sum_{y \in V_1', x \in V(G_2)} d_G\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_i\right) > 0,
\end{aligned}$$

i.e., $W(G') > W(G)$.

Next, we consider the Kirchhoff index. Let H_2 and H_2' be the induced subgraphs by $V(C) \cup V(G_2)$ in G and G', respectively, $n_1 = |V_1| - 1$ and $n_2 = |V_2| - 1$. By Lemma 2 and Lemma 1, we have

$$\begin{aligned}
Kf(G') - Kf(G) &= [Kf(G_1) + Kf(H_2') + n_1 Kf_{w_1}(H_2') + n_2 Kf_{w_1}(G_1)] \\
&- [Kf(G_1) + Kf(H_2) + n_1 Kf_{w_1}(H_2) + n_2 Kf_{w_1}(G_1)] \\
&= n_1 [Kf_{w_1}(H_2') - Kf_{w_1}(H_2)] \\
&= n_1 \textstyle\sum_{x \in V(G_2)} [(r_{G'}\left(x, w_{\lfloor \frac{k}{2} \rfloor + 1}\right) + r_{G'}\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_1\right)) \\
&- (r_G(x, w_i) + (w_i, w_1))] \\
&= n_1 \textstyle\sum_{x \in V(G_2)} [r_{G'}\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_1\right) - r_G(w_i, w_1)] \\
&= n_1 \textstyle\sum_{x \in V(G_2)} r_{G'}\left(w_{\lfloor \frac{k}{2} \rfloor + 1}, w_i\right) > 0,
\end{aligned}$$

i.e., $Kf(G') > Kf(G)$.

$\square$

Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$, and let $C_1, C_2, \dots, C_s$ be $s (s \geq 1)$ cycles of length k in G, $V_1 = V(C_1) \cup V(C_2) \cup \dots \cup V(C_s)$, $u \in C_1$ is a cut vertex of G but not a cut vertex of $G[V_1]$. If $G[V_1]$ is a cactus chain and each k-polygon of $\{C_1, C_2, \dots, C_s\}$ has at most two cut-vertices in G, C_s is a terminal polygon of G, the degree of each vertex of $\mathbf{V_1} - \{\mathrm{u}\}$ is at most four in G, then $G[V_1]$ is called a pendent cactus chain of length s of G, and C_{s-1} is called a neighbor polygon of the pendent cactus chain [21].

From the definition, if $G[V_1]$ is a pendent cactus chain of length $s \geq 2$, then for $1 \leq i \leq s-1$ and $2 \leq j \leq s-1$, each C_i contains exactly two cut-vertices in G, and the degree of every cut-vertex of C_j is equal to four in G.

Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$ and let $C_1, C_2, \cdots, C_{s+t}$ *be* $s+t(s \geq 1, t \geq 1)$ cycles in G such that the induced subgraphs $G[V(C_1) \cup V(C_2) \cup \cdots \cup V(C_s)]$ and $G[V(C_{s+1}) \cup V(C_{s+2}) \cup \cdots \cup V(C_{s+t})]$ are two pendent linear cactus chains of length s and t respectively, i.e., the distance between two cut-vertices in the each cycle C_i is $\left\lfloor \frac{k}{2} \right\rfloor$.

(i) If $u_0 \in V(C_1) \cap V(C_{s+1})$ and $d_G(u_0) \geq 6$, then u_0 is called a special vertex of G;

(ii) If C_0 is a k-polygon of G with at least three cut-vertices in G such that $V(C_1) \cap V(C_0) = v_0$ and $V(C_{s+1}) \cap V(C_0) = w_0$ with $d_G(w_0) = d_G(v_0) = 4$, then C_0 is called a special polygon of G.

The following result shows that the k-polygon cactus with the maximum Wiener index or the maximum Kirchhoff index has no special vertices.

Lemma 4. If $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index, then G has no special vertices.

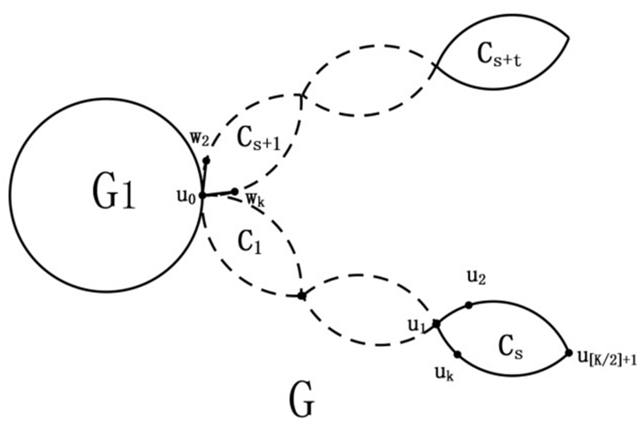

Figure 2: The graph G in Lemma 4.

Proof. Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemma 3, all pendent chains in G are linear. If G has a special vertex u_0, then there are $s+t(s \geq 1, t \geq 1)$ cycles $C_1, C_2, \cdots, C_{s+t}$ in G such that the induced subgraphs $G[V(C_1) \cup V(C_2) \cup \cdots \cup V(C_s)]$ and $G[V(C_{s+1}) \cup V(C_{s+2}) \cup \cdots \cup V(C_{s+t})]$ are two pendent linear cactus chains of length s and t, respectively, and $u_0 \in V(C_1) \cap V(C_{s+1})$ and $d_G(u_0) \geq 6$, see Figure 2, i.e., G is obtained from G_1 and G_2 by identifying $u_0 \in V(G_1)$ with $w_1 \in V(C_{s+1})$, where $G_2 = G[V(C_{s+1}) \cup V(C_{s+2}) \cup \cdots \cup V(C_{s+t})]$ is the linear chain $L_{n,s+t}$.

Let $' = G - u_0w_2 - u_0w_k + u_{\lfloor \frac{k}{2} \rfloor+1}w_1 + u_{\lfloor \frac{k}{2} \rfloor+1}w_k$, then $G' \in G_{n,k}$. Note that $W(G) = W(G_1) + W(G_2) + \sum_{x\in V_1, y\in V_2} d_G(x,y)$, $W(G') = W(G_1) + W(G_2) + \sum_{x\in V_1, y\in V_2} d_{G'}(x,y)$, where $V_1 = V(G_1) - \{u_0\}$ and $V_1 = V(G) - V(G_1)$, we have $W(G') - W(G) = \sum_{x\in V_1, y\in V_2}[d_{G'}(x,y) - d_G(x,y)] > 0$.Similarly,

$$Kf(G') - Kf(G) = \sum_{x\in V_1, y\in V_2}[r_{G'}(x,y) - r_G(x,y)] > 0.$$

So, $W(G') > W(G)$ and $Kf(G') > Kf(\mathrm{G})$, a contradiction to G with the maximum Wiener index or the maximum Kirchhoff index. □

Now, we will show that the k-polygon cactus with the maximum Wiener index or the maximum Kirchhoff index also has no special polygons.

Lemma 5. If $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index, then G has no special polygon.

Proof. Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemmas 3 and 4, all pendent chains in G are linear and G has no special vertices.

If G has a special polygon C_0 , then there are $s + t (s \geq 1, t \geq 1)$ cycles $\mathrm{C}_1, \mathrm{C}_2, \dots,$ C_{s+t} in G such that the induced subgraphs $L_{n,s} = G[V(C_1) \cup V(C_2) \cup \dots \cup V(C_s)]$ *and* $L_{n,t} = G[V(C_{s+1}) \cup V(C_{s+2}) \cup \dots \cup V(C_{s+t})]$ are two pendent linear cactus chains of length s and t, respectively, $v_0 \in V(C_1) \cap V(C_0)$, $w_0 \in V(C_{s+1}) \cap V(C_0)$ and $d_G(w_0) = d_G(v_0) = 4$, i.e., G is obtained from $C_0 \cup G_1 \cdots \cup G_r$, $L_{n,s}$ and $L_{n,t}$ by identifying $v_0 \in V(C_0)$ with $v_1 \in V(C_1)$ and identifying $w_0 \in V(C_0)$ with $w_1 \in V(C_{s+1})$, where $C_1 = v_1v_2 \dots v_kv_1$ with two cut-vertices v_1 and $v_{\lfloor \frac{k}{2} \rfloor+1}$, $C_{s+1} = w_1w_2 \dots w_kw_1$ with two cut-vertices w_1 and $w_{\lfloor \frac{k}{2} \rfloor+1}$ and $C_0 \cup G_1 \cdots \cup G_r$ is obtained by attaching k-polygons G_i $(1 \leq \mathrm{i} \leq \mathrm{r})$ to cut-vertices v_i of C_0 , see Figure 3. Let $G' = G - w_0w_2 - w_0w_k + u_{\lfloor \frac{k}{2} \rfloor+1}w_2 + u_{\lfloor \frac{k}{2} \rfloor+1}w_k$ where u_1 and $u_{\lfloor \frac{k}{2} \rfloor+1}$ are two cut-vertices of $C_s = u_1u_2 \cdots u_ku_1$ in G_0. Then $G_0 \in G_{n,k}$, and $W(G) = \sum_{i=1}^{r} W(G_i)$, $+ W(H) + \sum_{x\in V_1, y\in V_2} d_G(x,y)$ $W(G') = \sum_{i=1}^{r} W(G_i) + W(L_{n,s+t+1}) + \sum_{x\in V_1, y\in V_2} d_{G'}(x,y)$, where H is the induced subgraph of G by $V(C_1) \cup V(C_2) \cup \dots \cup V(C_{s+t})$, $L_{n,s+t+1}$ is the linear chain consisted of $C_0 \cup C_1 \cdots \cup C_{s+t}$ in G_0 , $V_1 = V(H) - R$ and $V_2 = V(G) - V(H)$ and $R = \{w_0, v_0, v_1, \cdots, v_t\}$ is the set of cut-vertices of C_0 in G. Note that $W(H) \leq W(L_{n,s+t+1})$ since $d_G(v_0, w_0) \leq \frac{k}{2}$, and $\sum_{x\in V_1, y\in V_2} d_G(x,y) - \sum_{x\in V_1, y\in V_2} d_{G'}(x,y) = \sum_{x\in V_1, y\in V_2'}[d_G(x,y) - d_{G'}(x,y)]$, where $V_2' = V\ (C_{s+1} \cup \dots \cup C_{s+t}) - \{w_1\}$. Therefore,

$$\sum_{x\in V_1, y\in V_2'}[d_G(x,y) - d_{G'}(x,y)]$$
$$= \sum_{x\in V_1, y\in V_2'}[(d_G(x,w_0)+d_G(w_0,y)) - (d_{G'}\left(x,u_{\lfloor \frac{k}{2}\rfloor+1}\right) + d_{G'}\left(u_{\lfloor \frac{k}{2}\rfloor+1},y\right))]$$
$$= \sum_{x\in V_1, y\in V_2'}[d_G(x,w_0) - d_{G'}\left(x,u_{\lfloor \frac{k}{2}\rfloor+1}\right)] > 0.$$

So, $W(G) < W(G')$. Similarly, by Lemmas 1 and 2, we can get $Kf(G) < Kf(G')$, a contradiction to G with the maximum Wiener index or the maximum Kirchhoff index. □

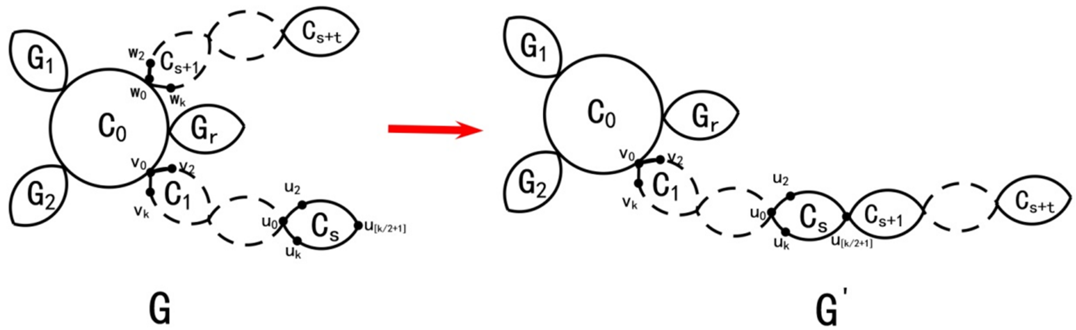

Figure 3: The graph G and G_0 in Lemma 5.

Theorem 6. Let $\in G_{n,k}$, $k \geq 3$ and $n \geq 3$. Then

$$W(G) \leq \binom{n}{3}(k-1)^2\left\lfloor\frac{k}{2}\right\rfloor + \left(\frac{1}{2}nk + (k-1)(n^2-n)\right)\left\lfloor\frac{k^2}{4}\right\rfloor,$$
$$Kf(G) \leq \binom{n}{3}\frac{(k-1)^2}{k}\left\lfloor\frac{k}{2}\right\rfloor\left\lceil\frac{k}{2}\right\rceil + \frac{1}{12}\left(nk + 2(k-1)(n^2-n)\right)(k^2-1),$$

with equality if and only if $G = L_{n,k}$ is a linear chain with n k-polygons.

Proof. Let $G \in G_{n,k}$ with the maximum Wiener index or the maximum Kirchhoff index. By Lemmas 3, 4 and 5, we know that G is the linear chain $L_{n,k}$. So, we only need to compute $W(L_{n,k})$ and $Kf(L_{n,k})$. Let $D_u(G) = \sum_{u\in V(G)} d_G(x,u)$, If C is a k-polygon and $u \in V(C)$, then $a = D_u(G) = \left\lfloor\frac{k^2}{4}\right\rfloor$ and $W(C) = \frac{1}{2}ka$.

Let $L_{n,k} = C_1 \cup C_2 \cdots \cup C_n$ consist of n k-polygons $C_1, C_2, \cdots, C_n$, u_i is the common cut-vertex of C_i and C_{i+1}, the distance $b = d(u_i, u_{i+1}) = \left\lfloor\frac{k}{2}\right\rfloor$, $1 \leq i < n$.

$$W(L_{n+1,k}) = W(L_{n,k}) + W(C_{n+1}) + (k-1)D_{u_n}(L_{n,k}) + (k-1)nD_{u_n}(C_{n+1})$$
$$= W(L_{n,k}) + \frac{1}{2}ka + (k-1)D_{u_n}(L_{n,k}) + (k-1)na$$
$$= W(L_{n,k}) + (k-1)D_{u_n}(L_{n,k}) + \left[\frac{1}{2}k + (k-1)n\right]a.$$

Now, $D_{u_1}(L_{1,k}) = a$, $D_{u_2}(L_{2,k}) = a + a + (k-1)b = 2a + (k-1)b$, $D_{u_3}(L_{3,k}) = 2a + (k-1)b + a + 2(k-1)b = 3a + 3(k-1)b$, and we have by induction that $D_{u_n}(L_{n,k}) = na + \binom{n}{2}(k-1)b$. So,

$$\begin{aligned}W(L_{n+1,k}) &= W(L_{n,k}) + \binom{n}{2}(k-1)^2\boldsymbol{b} + \left[\frac{1}{2}k + 2(k-1)n\right]a\\ &= W(L_{n-1,k}) + \left[\binom{n-1}{2} + \binom{n}{2}\right](k-1)^2 b\\ &+ \left[\frac{1}{2}k + 2(k-1)(n-1) + \frac{1}{2}k + 2(k-1)n\right]\\ &= W(L_{1,k}) + \sum_{i=1}^{n}\binom{i}{2}(k-1)^2 b + \sum_{i=1}^{n}[\frac{1}{2}k + 2(k-1)i]a\\ &= \frac{1}{2}ka + \binom{n+1}{3}(k-1)^2 b + \sum_{i=1}^{n}[\frac{1}{2}k + 2(k-1)i]a\\ &= \binom{n+1}{3}(k-1)^2\left\lfloor\frac{k}{2}\right\rfloor + \left(\frac{1}{2}k(n+1) + (k-1)n(n+1)\right)\left\lfloor\frac{k^2}{4}\right\rfloor\end{aligned}$$

Similarly, let $Kf_u(G) = \sum_{x\in V(G)} r_G(x,u)$. If C is a k-polygon and $u \in V(C)$, then $a' = Kf_u(C) = \frac{k^2-1}{6}$ and $Kf(C) = \frac{1}{2}ka' = \frac{k^3-k}{12}$. Let $b' = r_{C_{i+1}}(u_{\boldsymbol{i}}, u_{i+1}) = \frac{1}{k}\left\lfloor\frac{k}{2}\right\rfloor\left\lceil\frac{k}{2}\right\rceil, 1 \le i < n$. Then, $Kf(L_{n+1,k}) = Kf(L_{n,k}) + Kf(C_{n+1}) + (k-1)\,Kf_{u_n}(L_{n,k}) + (k-1)\,n\,Kf_{u_n}(C_{n+1}) = Kf(L_{n,k}) + (k-1)Kf_{u_n}(L_{n,k}) + \left[\frac{1}{2}k + 2(k-1)n\right]a'$, $Kf_{u_n}(L_{n,k}) = na' + \binom{n}{2}(k-1)b'$ and $Kf(G) = \binom{n+1}{3}(k-1)^2 b' + \left(\frac{1}{2}k(n+1) + (k-1)n(n+1)\right)a = \binom{n+1}{3}\frac{(k-1)^2}{k}\left\lfloor\frac{k}{2}\right\rfloor\left\lceil\frac{k}{2}\right\rceil + \frac{1}{12}\big(k(n+1) + 2(k-1)n(n+1)\big)(k^2-1)$,

Hence the result. □

Theorem 6 gives the maximum values of Wiener index and Kirchhoff index for all k-polygonal cacti with n cycles and characterizes the extremal graphs. For $k = 6$, we can get the maximum values of Wiener index and Kirchhoff index for all spiro hexagonal chains with n hexagons.

Corollary 7. [3, 4, 9] Among all spiro hexagonal chains with n hexagons, we have

(i) the unique spiro hexagonal chain with the maximum Wiener index is the spiro para-chain P_n, and $W(P_n) = \frac{25}{2}n^3 + \frac{15}{2}n^2 + 7n$;

(ii) the unique spiro hexagonal chain with the maximum Kirchhoff index is the spiro para-chain P_n, and $Kf(P_n) = \frac{25}{2}n^3 + \frac{125}{12}n^2 + \frac{5}{6}n$.

3. THE EXTREMAL GRAPH WITH THE MINIMUM INDEX

In this section, we determine the minimum values of Wiener index and Kirchhoff index for all k-polygonal cacti with n cycles and characterizes the extremal graphs and the corresponding extremal graphs.

Theorem 8. Let $G \in G_{n,k}$, $k \geq 3$ and $n \geq 3$. Then

$$W(G) \geq \frac{1}{2} n\big(k + 2(n-1)(k-1)\big)\left\lfloor \frac{k^2}{4} \right\rfloor,$$
$$Kf(G) \geq \frac{1}{12} n\big(k + 2(n-1)(k-1)\big)(k^2-1),$$

with equality if and only if $G = W_{n,k}$ is a star-like cactus with n k-polygons.

Proof. Let $G \in G_{n,k}$ be a cactus with the minimum Wiener index or the minimum Kirchhoff index. We first show that G is a star-like cactus, i.e., each polygon in G has only one cut-vertex. If there is a k-polygon C_0 in G such that C_0 has at least two cut-vertices, then we only need to show that there is $C_0 \in G_{n,k}$ such that $W(G_0) < W(G)$ and $Kf(G_0) < Kf(G)$. Let $v_1, v_2, \ldots, v_t$ be all cut-vertices in C_0, $t \geq 2$, and G_i the components of $G - E(C_0)$ containing v_i, $i = 1,2, \ldots, t$, i.e, G is obtained by attaching G_i to the cut-vertex v_i of G_0. Now, we take G_0 to be the cactus obtained by attaching all $G_i (i = 1,2, \ldots, t)$ to the same vertex v_1 of C_0, see Figure 4, then $W(G) = \sum_{i=1}^{t} W(G_i) + W(C_0) + \sum_{1 \leq i<j \leq t} \sum_{x \in V_i, y \in V_j} d_G(x,y) + \sum_{i=1}^{t} \sum_{x \in V_i, y \in V_0} d_G(x,y)$, where $V_0 = V(C_0) - \{v_1, \ldots, v_t\}$, $V_i = V(G_i) - \{v_i\}$, $1 \leq i \leq t$, and $W(G') = \sum_{i=1}^{t} W(G_i) + W(C_0) + \sum_{1 \leq i<j \leq t} \sum_{x \in V_i, y \in V_j} d_{G'}(x,y) + \sum_{i=1}^{t} \sum_{x \in V_i, y \in V_0} d_{G'}(x,y)$. Note that $\sum_{i=1}^{t} \sum_{x \in V_i, y \in V_0} d_{G'}(x,y) = \sum_{i=1}^{t} \sum_{x \in V_i, y \in V_0} d_G(x,y)$ and

$$\sum_{1 \leq i<j \leq t} \sum_{x \in V_i, y \in V_j} d_{G'}(x,y) < \sum_{1 \leq i<j \leq t} \sum_{x \in V_i, y \in V_j} d_G(x,y).$$

So, we have $W(G') < W(G)$. Similarly, by Lemmas 1 and 2, we can get $Kf(G') < Kf(G)$.

Next, we compute $W(W_{n,k})$ and $Kf(W_{n,k})$. Let $W_{n,k} = C_1 \cup C_2 \cdots \cup C_n$ consist of n k-polygons $C_1, C_2, \cdots, C_n$, v_0 is the common cut-vertex of all $C_1 (1 \leq i \leq t)$. Then

$$\begin{aligned}
W(W_{n+1,k}) &= W(W_{n,k}) + W(C_{n+1}) + (k-1)D_{v_0}(W_{n,k}) + (k-1)nD_{v_0}(C_{n+1}) \\
&= W\big(W_{n,k}\big) + \frac{1}{2}ka + (k-1)D_{v_0}(W_{n,k}) + (k-1)na \\
&= W\big(W_{n,k}\big) + \frac{1}{2}ka + (k-1)na + (k-1)na \\
&= W\big(W_{1,k}\big) + \sum_{i=1}^{n} [\tfrac{1}{2}k + 2(k-1)i]a \\
&= \frac{1}{2}ka + \sum_{i=1}^{n} [\tfrac{1}{2}k + 2(k-1)i]a \\
&= \frac{1}{2}(n+1)(k + 2nk - 2n)\left\lfloor \frac{k^2}{4} \right\rfloor,
\end{aligned}$$

and

$$\begin{aligned}
Kf(W_{n+1,k}) &= Kf(W_{n,k}) + Kf(C_{n+1}) + (k-1)Kf_{v_0}(W_{n,k}) + (k-1)nKf_{v_0}(C_{n+1}) \\
&= Kf\big(W_{n,k}\big) + \frac{1}{2}ka' + (k-1)na' + (k-1)na' \\
&= Kf\big(W_{1,k}\big) + \sum_{i=1}^{n} \left[\frac{1}{2}k + 2(k-1)i\right] a' \\
&= \frac{1}{2}ka' + \sum_{i=1}^{n} [\tfrac{1}{2}k + 2(k-1)i]a'
\end{aligned}$$

$$= \frac{1}{12}(n+1)(k+2nk-2n)(k^2-1).$$

□

Theorem 8 gives the minimum values of Wiener index and Kirchhoff index for all k-polygonal cacti with n cycles and characterizes the extremal graphs.

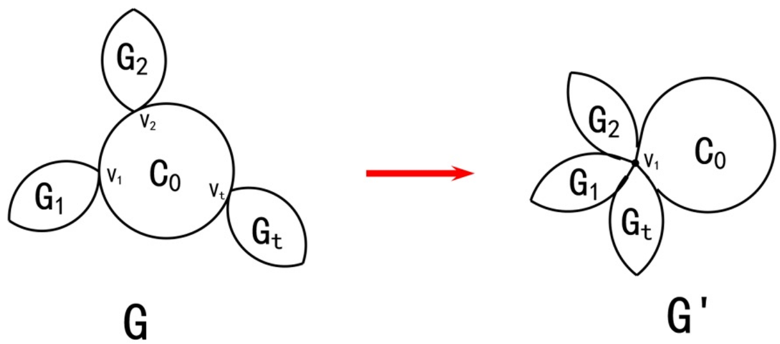

Figure 4: The graphs G and G' in Theorem 8.

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REFERENCES

1. D. Babić, D. J. Klein, I. Lukovits, S. Nikolić, N. Trinajstić, Resistance-distance matrix: A computational algorithm and its application, *Int. J. Quantum Chem.* **90** (2002) 166−176.
2. H. Deng, On the minimum Kirchhoff index of graphs with a given number of cut-edges, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 171−180.
3. H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Comput. Model.* **55** (2012) 634−644.
4. H. Deng, Z. Tang, Kirchhoff indices of spiro and polyphenyl hexagonal chains, *Util. Math.* **95** (2014) 113−128.
5. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211−249.
6. A. Dobrynin, I. Gutman, S. Klavˇ zar, P. Zigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247−294.

7. Q. Guo, H. Deng, D. Chen, The extremal Kirchhoff index of a class of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 713−722.
8. I. Gutman, S. Li, W. Wei, Cacti with n vertices and t cycles having extremal Wiener index, *Discrete Appl. Math.* **232** (2017) 189−200.
9. G. Huang, M. Kuang, H. Deng, The expected values of Kirchhoff indices in the random polyphenyl and spiro chains, *ARS Math. Contem.* **9** (2) (2015) 207−217.
10. D. J. Klein, Resistance-distance sum rules, *Croat. Chem. Acta* **75** (2002) 633−649.
11. D. J. Klein, M. Randi´ c, Resistance distance, *J. Math. Chem.* **12** (1993) 81−95.
12. J. Palacios, Resistance distance in graphs and random walks, *Int. J. Quantum Chem.* **81** (2001) 29−33.
13. J. Palacios, Closed-form formulas for Kirchhoff index, *Int. J. Quantum Chem.* **81** (2001) 135−140.
14. O. E. Polansky, D. Bonchev, The Wiener number of graphs I: general theory and changes due to graph operations, *MATCH Commun. Math. Comput. Chem.* **21** (1986) 133−186.
15. O. E. Polansky, D. Bonchev, Theory of the Wiener number of graphs II: Transfer graphs and some of their metric properties, *MATCH Commun. Math. Comput. Chem.* **25** (1990) 3−39.
16. Z. Tang, H. Deng, The (n,n)-graphs with the first three extremal Wiener indices, *J. Math. Chem.* **43** (2008) 60−74.
17. H. Wang, H. Hua, D. Wang, Catic with minimum, second-minimum, and third-minimum Kirchhoff indices, *Math. Commun.* **15** (2) (2010) 347−358.
18. H. Wiener, Structural determination of paraffin boiling point, *J. Am. Chem. Soc.* **69** (1947) 17−20.12
19. Y. Yang, X. Jiang, Unicyclic graphs with extremal Kirchhoff index, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 107−120.
20. Y. Yang, H. Zhang, Kirchhoff index of linear hexagonal chains, *Int. J. Quantum Chem.* **108** (2008) 503−512.
21. J. Ye, M. Liu, Y. Yao, K. Ch. Das, Extramal polygonal cacti for bond incident degree indices, *Discrete Applied Math.* **257** (2019) 289−298.
22. W. Zhang, H. Deng, The second maximal and minimal Kirchhoff indices of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **69** (2009) 683−695.
23. H. Zhang, Y. Yang, Resistance distance and Kirchhoff index in circulant graphs, *Int. J. Quantum Chem.* **107** (2007) 330−339.