

Uniform cacti with extremal Wiener indices*

Zhengxin Qin^{1,2}, Xianyong Li², Guoping Wang^{2†}

¹The College of Mathematics and Systems Sciences,

Xinjiang University, Urumqi, Xinjiang 830046, P.R.China

² School of Mathematical Sciences, Xinjiang Normal University,
Urumqi 830054, Xinjiang, P. R. China

Abstract. The Wiener index of a graph is the sum of the distances between all pairs of vertices. In this paper we determine h -cacti and h -cactus chains with the extremal Wiener indices, respectively.

Key words: Wiener index, h -cactus, h -cactus chain

MR classification: O 157.5

1 Introduction

The Wiener index was introduced by H. Wiener [8] in 1947. A lot more is done on the Wiener index than what could be mentioned here. The significant applications of the Wiener index in chemistry can be found in [7]. I. Gutman et al. [6] detailed the correlation of Wiener index with certain physicochemical properties of nonpolar organic substances. A. A. Dobrynin et al. [3, 4] have extensively researched the Wiener index in mathematics.

A *cactus* G is a connected graph in which each edge lies on at most one cycle. Therefore, each block in G is either an edge or a cycle. An *h -cactus* is a cactus in which each block is an h -cycle. An *h -cactus chain* is an h -cactus in which each block contains at most two cut-vertices and each cut-vertex lies in exactly two blocks. Certain invariants of a closely related class of block-cactus graphs have been studied in [2, 9]. T. Došlić and F.

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†Corresponding author. Email: xj.wgp@163.com.

Måløy [5] considered a type of cactus chain and studied their matching and independence related properties.

In this paper we determine the h -cacti and h -cactus chains with the extremal Wiener indices, respectively.

2 Main results

Suppose that $d_G(u, v)$ is the distance between vertices u and v in a graph G , and let $d(v|G) = \sum_{u \in V(G)} d_G(u, v)$. Then $W(G) = \frac{1}{2} \sum_{v \in V(G)} d(v|G)$ is Wiener index of G . The following lemma is important and will be repeatedly used to obtain our main results.

Lemma 2.1. [1] *Let G be a connected graph with a cut-vertex u such that G_1 and G_2 are two connected subgraphs of G having u as the only common vertex and $G_1 \cup G_2 = G$. Then*

$$W(G_1 \cup G_2) = W(G_1) + W(G_2) + (|V(G_1)| - 1)d(u|G_2) + (|V(G_2)| - 1)d(u|G_1).$$

The number of h -cycles in an h -cactus is its length. Denote by $\mathcal{C}(k)$ the set of all h -cacti of length k .

Theorem 2.1. *If $Y, Y^* \in \mathcal{C}(k)$, then $W(Y) \equiv W(Y^*) \pmod{h-1}$.*

Proof. We proceed by induction on k . The case $k = 2$ is obviously true. So suppose $k \geq 3$.

Note that any two Y and Y^* of $\mathcal{C}(k)$ can be obtained from two appropriately chosen graphs X and X^* of $\mathcal{C}(k-1)$ by attaching to them two new h -cycles C_h and C_h^* , respectively, as in Fig. 1.

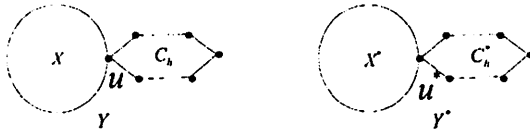


Fig. 1

By Lemma 2.1, we know that

$$W(Y) = W(X) + W(C_h) + (|V(X)| - 1)d(u|C_h) + (|V(C_h)| - 1)d(u|X),$$

$$W(Y^*) = W(X^*) + W(C_h^*) + (|V(X^*)| - 1)d(u^*|C_h^*) + (|V(C_h^*)| - 1)d(u^*|X^*).$$

Since $W(C_h) = W(C_h^*)$, $|V(X)| = |V(X^*)|$ and $d(u|C_h) = d(u^*|C_h^*)$, we obtain

$$W(Y) - W(Y^*) = (W(X) - W(X^*)) + (h - 1)(d(u|X) - d(u^*|X^*)).$$

The result follows from inductive hypothesis that $W(X) \equiv W(X^*) \pmod{h-1}$. \square

An h -cactus star is an h -cactus that has only one cut-vertex. Denote by F_k the h -cactus star of length k . Suppose that F_{k_i} is a subgraph of $G_1 \in \mathcal{C}(k)$ whose cut-vertex u_i is on a cycle C ($i = 1, 2$). Two vertices u and v on cycle C are in t -position if $d_C(u, v) = t$. If u_1 and u_2 are in t -position on C and $1 \leq t \leq \lfloor \frac{h}{2} \rfloor$, then we call the process of moving F_{k_2} from u_2 to u_1 the *flower transformation* of G_1 , and denote the resulting graph by G_2 , as in Fig. 2.

Lemma 2.2. *Let G_i and u_i ($i = 1, 2$) be defined as above, and $T_0 = G_1 \setminus \{F_{k_1}, F_{k_2}\}$. If $d_{G_2}(u_1|T_0) \leq d_{G_1}(u_2|T_0)$, then $W(G_1) > W(G_2)$.*

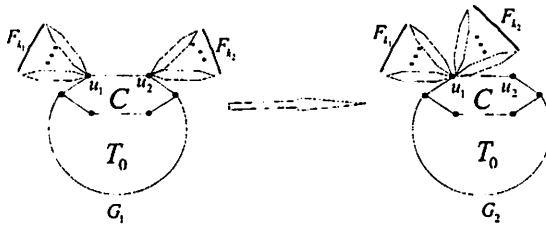


Fig. 2. Flower transformation

Proof. By Lemma 2.1, we have

$$W(G_1) = W(T_0 \cup F_{k_1}) + W(F_{k_2}) + (|V(T_0 \cup F_{k_1})| - 1)d_{G_1}(u_2|F_{k_2})$$

$$+ (|V(F_{k_2})| - 1)d_{G_1}(u_2|T_0 \cup F_{k_1}),$$

$$W(G_2) = W(T_0 \cup F_{k_1}) + W(F_{k_2}) + (|V(T_0 \cup F_{k_1})| - 1)d_{G_2}(u_1|F_{k_2})$$

$$+ (|V(F_{k_2})| - 1)d_{G_2}(u_1|T_0 \cup F_{k_1}).$$

Since $d_{G_1}(u_2|F_{k_2}) = d_{G_2}(u_1|F_{k_2})$, we have

$$W(G_1) - W(G_2) = (|V(F_{k_2})| - 1)(d_{G_1}(u_2|T_0 \cup F_{k_1}) - d_{G_2}(u_1|T_0 \cup F_{k_1})).$$

Note that

$$d_{G_1}(u_2|T_0 \cup F_{k_1}) = d_{G_1}(u_2|T_0) + (|V(F_{k_1})| - 1)d_{G_1}(u_2, u_1) + d_{G_1}(u_1|F_{k_1}),$$

$$d_{G_2}(u_1|T_0 \cup F_{k_1}) = d_{G_2}(u_1|T_0) + d_{G_2}(u_1|F_{k_1}).$$

Since $d_{G_1}(u_2|T_0) \geq d_{G_2}(u_1|T_0)$, we have $W(G_1) - W(G_2) = (|V(F_{k_2})| - 1)(d_{G_1}(u_2|T_0) - d_{G_2}(u_1|T_0) + (|V(F_{k_1})| - 1)d_{G_1}(u_2, u_1)) > 0$. \square

Suppose that $T_i \in \mathcal{E}(k_i)$ is a subgraph of $G_3 \in \mathcal{E}(k)$ that has common vertex u_i with a cycle C of G_3 ($i = 3, 4$). If u_3 and u_4 are in t -position on C and $1 \leq t \leq \lfloor \frac{h}{2} \rfloor$, then we call the process of moving T_4 from u_4 to u_3 the *inner transformation* of G_3 , and denote the resulting graph by G_4 , as in Fig. 3.

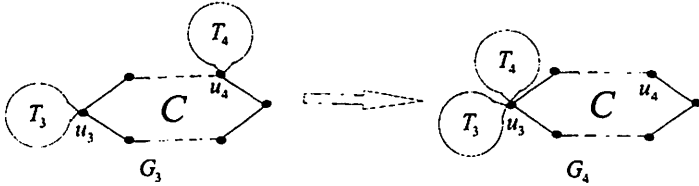


Fig. 3. Inner transformation

Lemma 2.3. *Let G_i and u_i ($i = 3, 4$) be defined as above. Then we have $W(G_3) > W(G_4)$.*

Proof. By Lemma 2.1, we have

$$W(G_3) = W(T_3 \cup C) + W(T_4) + (|V(T_3 \cup C)| - 1)d_{G_3}(u_4|T_4) + (|V(T_4)| - 1)d_{G_3}(u_4|T_3 \cup C),$$

$$W(G_4) = W(T_3 \cup C) + W(T_4) + (|V(T_3 \cup C)| - 1)d_{G_4}(u_3|T_4) + (|V(T_4)| - 1)d_{G_4}(u_3|T_3 \cup C).$$

Since $d_{G_3}(u_4|T_4) = d_{G_4}(u_3|T_4)$, we have

$$W(G_3) - W(G_4) = (|V(T_4)| - 1)(d_{G_3}(u_4|T_3 \cup C) - d_{G_4}(u_3|T_3 \cup C)).$$

Note that

$$d_{G_3}(u_4|T_3 \cup C) = (|V(T_3)| - 1)d_{G_3}(u_4, u_3) + d_{G_3}(u_3|T_3) + d_{G_3}(u_4|C),$$

$$d_{G_4}(u_3|T_3 \cup C) = d_{G_4}(u_3|T_3) + d_{G_4}(u_3|C) \text{ and } d_{G_3}(u_4|C) = d_{G_4}(u_3|C).$$

Therefore, we have

$$W(G_3) - W(G_4) = (|V(T_4)| - 1)(|V(T_3)| - 1)d_{G_3}(u_4, u_3) > 0. \quad \square$$

We easily observe that a graph $G \in \mathcal{C}(k)$ can be transformed into some F_k through a finite number of steps of flower or inner transformation. Thus, by Lemmas 2.2 and 2.3, we have the following

Theorem 2.2. *If $G \in \mathcal{C}(k)$ and $k \geq 3$, then $W(G) \geq W(F_k)$, with equality if and only if $G \cong F_k$.*

A cycle C in an h -cactus chain is *internal* if it contains two cut-vertices. An internal cycle C is *para* if the two cut-vertices on C are in $\lfloor \frac{h}{2} \rfloor$ -position. Denote by L_k the *para*- h -cactus chain of length k whose internal cycles are all *para*.

Suppose that L_{k_i} is a subgraph of $G_5 \in \mathcal{C}(k)$ that has a common vertex u_i with cycle C of G_5 ($i = 5, 6$) and that $u_7 \in V(L_{k_5})$ is the farthest vertex from u_5 . If u_5 and u_6 are in t -position ($0 \leq t \leq \lfloor \frac{h}{2} \rfloor$), then we call the process of moving L_{k_6} from u_6 to u_7 the *lengthening transformation* of G_5 , and denote the resulting graph by G_6 , as in Fig. 4.

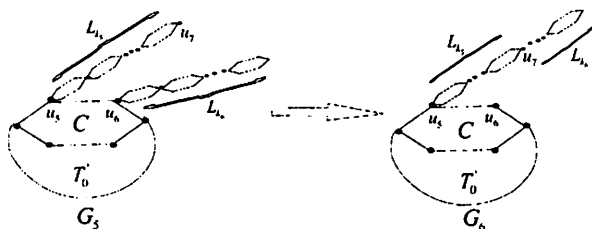


Fig. 4. Lengthening transformation.

Lemma 2.4. *Let G_i ($i = 5, 6$) and u_j ($j = 5, 6, 7$) be defined as above, and $T'_0 = G_5 \setminus \{L_{k_5}, L_{k_6}\}$. If $d_{G_6}(u_5|T'_0) \geq d_{G_5}(u_6|T'_0)$, then $W(G_5) < W(G_6)$.*

Proof. By Lemma 2.1, we have

$$\begin{aligned} W(G_5) &= W(T'_0 \cup L_{k_5}) + W(L_{k_6}) + (|V(T'_0 \cup L_{k_5})| - 1)d_{G_5}(u_6|L_{k_6}) \\ &\quad + (|V(L_{k_6})| - 1)d_{G_5}(u_6|T'_0 \cup L_{k_5}), \end{aligned}$$

$$\begin{aligned} W(G_6) &= W(T'_0 \cup L_{k_5}) + W(L_{k_6}) + (|V(T'_0 \cup L_{k_5})| - 1)d_{G_6}(u_7|L_{k_6}) \\ &\quad + (|V(L_{k_6})| - 1)d_{G_6}(u_7|T'_0 \cup L_{k_5}). \end{aligned}$$

Since $d_{G_5}(u_6|L_{k_6}) = d_{G_6}(u_7|L_{k_6})$, we have

$$W(G_6) - W(G_5) = (|V(L_{k_6})| - 1)(d_{G_6}(u_7|T'_0 \cup L_{k_5}) - d_{G_5}(u_6|T'_0 \cup L_{k_5})).$$

Note that

$$\begin{aligned} d_{G_5}(u_6|T'_0 \cup L_{k_5}) &= d_{G_5}(u_6|T'_0) + d_{G_5}(u_5|L_{k_5}) + (|V(L_{k_5})| - 1)t, \\ d_{G_6}(u_7|T'_0 \cup L_{k_5}) &= d_{G_6}(u_5|T'_0) + \lfloor \frac{h}{2} \rfloor k_8 (|V(T'_0)| - 1) + d_{G_6}(u_7|L_{k_5}). \end{aligned}$$

Since $d_{G_6}(u_5|T'_0) \geq d_{G_5}(u_6|T'_0)$, we have

$$\begin{aligned} W(G_6) - W(G_5) &= (|V(L_{k_6})| - 1)(d_{G_6}(u_5|T'_0) - d_{G_5}(u_6|T'_0)) \\ &\quad + (\lfloor \frac{h}{2} \rfloor (k - k_5 - k_6) - t)(h - 1)k_5 > 0. \quad \square \end{aligned}$$

We easily observe that a graph $G \in \mathcal{C}(k)$ can be transformed into some L_k through a finite number of steps of the lengthening transformation. Thus, by Lemma 2.4, we have the following

Theorem 2.3. *If $G \in \mathcal{C}(k)$ and $k \geq 3$, then $W(G) \leq W(L_k)$, with equality if and only if $G \cong L_k$.*

An internal cycle C in an h -cactus chain is *ortho* if the two cut-vertices on C are in 1-position. Denote by H_k the *ortho*- h -cactus chain of length k whose internal cycles are all ortho. Now we give explicit expression of Wiener indices of F_k , L_k and H_k .

Remark 2.1. *The Wiener index of the h -cactus star F_k is given by*

$$W(F_k) = \begin{cases} \frac{h^2(h-1)k^2}{4} - \frac{h^2(h-2)k}{8}, & \text{if } h \text{ is even;} \\ \frac{(h-1)^2(h+1)k^2}{4} - \frac{(h-2)(h-1)(h+1)k}{8}, & \text{if } h \text{ is odd.} \end{cases}$$

Proof. Let C be an h -cycle in F_k . Then $F_k = F_{k-1} \cup C$. Let x be the cut-vertex of F_k . By Lemma 2.1, we have

$$W(F_k) = W(C) + W(F_{k-1}) + (h-1)d(x|F_{k-1}) + (h-1)(k-1)d(x|C).$$

If h is even, then $W(C) = \frac{h^3}{8}$, $d(x|C) = \frac{h^2}{4}$ and $d(x|F_{k-1}) = \frac{h^2(k-1)}{4}$, and so

$$W(F_k) = W(F_{k-1}) + \frac{h^3}{8} + \frac{h^2(h-1)(k-1)}{2}.$$

Using iteration method, we obtain $W(F_k) = \frac{h^2(h-1)k^2}{4} - \frac{h^2(h-2)k}{8}$.

Similarly, we can prove that $W(F_k) = \frac{(h-1)^2(h+1)k^2}{4} - \frac{(h-2)(h-1)(h+1)k}{8}$ if h is odd. \square

We also have the following Remarks 2.2 and 2.3

Remark 2.2. The Wiener index of the para- h -cactus chain L_k is given by

$$W(L_k) = \begin{cases} \frac{h(h-1)^2 k^3}{12} + \frac{(h^2-h)k^2}{2} - \frac{(h^3-2h^2-2h)k}{24}, & \text{if } h \text{ is even;} \\ \frac{(h-1)^3 k^3}{12} + \frac{(h-1)^2 k^2}{2} - \frac{(5h^3+6h^2-21h+10)k}{24}, & \text{if } h \text{ is odd.} \end{cases}$$

Remark 2.3. The Wiener index of the ortho- h -cactus chain H_k is given by

$$W(H_k) = \begin{cases} \frac{h(h-1)k^3}{6} + \frac{h(h-1)(h-2)k^2}{4} + \frac{(5h^3+6h^2-8h)k}{24}, & \text{if } h \text{ is even;} \\ \frac{(h-1)hk^3}{6} + \frac{(h^3+h^2+h+1)k^2}{4} - \frac{(3h^3-14h^2+5h+6)k}{24}, & \text{if } h \text{ is odd.} \end{cases}$$

Theorem 2.4. Suppose that $G \in \mathcal{C}(k)$ is an h -cactus chain. Then $W(H_k) \leq W(G)$, with equality if and only if $G \cong H_k$.

Proof. Suppose that $T_i \in \mathcal{C}(k_i)$ is a subgraph of h -cactus chain G that has a common vertex v_i ($i = 1, 2$) with cycle C so that $G = T_1 \cup C \cup T_2$, as in Fig. 5.

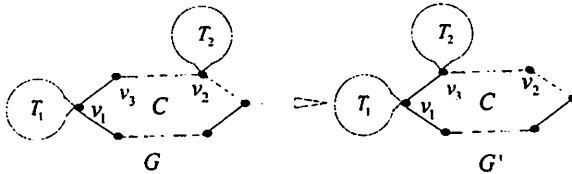


Fig. 5

Suppose that $v_3 \in C$ is adjacent to v_1 . Then we denote by G' the graph obtained from G by moving T_2 from v_2 to v_3 . If v_1 and v_2 are in t -position ($1 \leq t \leq \lfloor \frac{h}{2} \rfloor$), then, by Lemma 2.1, we have

$$\begin{aligned} W(G) &= W(T_1) + W(C \cup T_2) + (|V(T_1)| - 1)d_G(v_1|C \cup T_2) \\ &\quad + (|V(T_2)| + h - 2)d_G(v_1|T_1) \\ &= W(T_1) + W(T_2) + (h - 1)d_G(v_2|T_2) + (|V(T_2)| - 1)d_G(v_2|C) \\ &\quad + W(C) + (|V(T_1)| - 1)d_G(v_1|C \cup T_2) + (|V(T_2)| + h - 2)d_G(v_1|T_1) \\ &= W(T_1) + W(C) + W(T_2) + (|V(T_2)| - 1)d_G(v_2|C) \\ &\quad + (|V(T_1)| - 1)(d_G(v_1|C) - t) + t(|V(T_1)| - 1)|V(T_2)| \\ &\quad + (|V(T_1)| + h - 2)d_G(v_2|T_2) + (|V(T_2)| + h - 2)d_G(v_1|T_1). \end{aligned}$$

Similarly, we can obtain

$$\begin{aligned}W(G') &= W(T_1) + W(C) + W(T_2) + (|V(T_2)| - 1)d_{G'}(v_3|C) \\ &\quad + (|V(T_1)| - 1)(d_{G'}(v_1|C) - 1) + (|V(T_1)| - 1)|V(T_2)| \\ &\quad + (|V(T_1)| + h - 2)d_{G'}(v_3|T_2) + (|V(T_2)| + h - 2)d_{G'}(v_1|T_1).\end{aligned}$$

Note that $d_G(v_2|C) = d_{G'}(v_3|C)$, $d_G(v_2|T_2) = d_{G'}(v_3|T_2)$ and $d_G(v_1|T_1) = d_{G'}(v_1|T_1)$. Therefore, we have

$$W(G) - W(G') = (t - 1)(|V(T_1)| - 1)(|V(T_2)| - 1) \geq 0.$$

This shows that the assertion is true. \square

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