Hyper-Wiener index of k-membered ring spiro systems

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Abstract: In this paper, the congruence relations and the lower and upper bounds of hyper-Wiener index for k-membered ring spiro systems given length n are determined respectively. As these results' applications, the congruence relations and the extremal five- and six-membered ring spiro systems with maximal and minimal hyper-Wiener index are given respectively.

Keywords: Hyper-Wiener index; k-membered ring spiro systems; para-position transformation; step transformation; grafting transformation

1 Introduction

In 1947, American physico-chemist Wiener [19] firstly introduced Wiener index, as the sum of distances between all pairs

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of vertices of the graph. He found numerous applications in the modelling of physico-chemical, pharmacological and biological properties of organic molecules. In 1993, Randić [18] extended the Wiener index for all the paths in a tree, thus resulting the so-called hyper-Wiener index. Later, Klein et al. [14] generalized Randić's definition for all connected graphs. For more information about the hyper-Wiener index in mathematics and in chemistry see [2, 3, 10, 12, 13, 22]. Eliasi et al. [7, 11, 17] computed the hyper-Wiener indices of some graph operations and F-sums of graphs. Mansour and Schork [16] computed the exact formulae of hyper-Wiener indices of bridge and chain graphs. Feng et al. [8] obtained the sharp bounds for the hyper-Wiener indices of graphs with a given matching number and completely determined the extremal graphs. Xing et al. [9, 20] also obtained the maximal and minimal hyper-Wiener indices of unicyclic and bicyclic graphs and their extremal graphs.

A *k-membered ring spiro system* is a graph in which each block is a k-membered ring. Two k-membered rings of a k-membered ring spiro system are at most linked by a spiro union (two k-membered rings have at most one common vertex, this linkage is called *spiro union*, the common vertex is designated as *spiro vertex*). A *k-membered ring spiro chain* is a k-membered ring spiro system in which each block contains at most two spiro vertices (cut-vertices) and each spiro vertex lies in exactly two blocks.

Specially, in some literatures, six-membered ring spiro chains [4, 21] were always called spiro hexagonal chains [5] or chain hexagonal cacti [6]. Chen et al. [4, 6, 21] studied the six-membered ring spiro chains having extremal values of Merrifield-Simmons index, Hosoya index and extremal energies. Recently, Deng [5] determined the extremal Wiener index of the six-membered ring spiro chains. The present authors [15] computed the hyper-Wiener index of arbitrary k-membered ring spiro chain and determined the extremal k-membered ring spiro chains for hyper-Wiener index.

In this paper, we determine congruence relations of hyper-Wiener indices for two arbitrary k-membered ring spiro systems of length n. For any k-membered ring spiro systems, we define the para-position, step and grafting transformations, and then, by virtue of them, we further determine their extremal graphs of hyper-Wiener indices. Furthermore, the lower and upper bounds of the systems are determined completely. Using these results, we give the congruence relations and the extremal graphs of five- and six-membered ring spiro systems for hyper-Wiener index respectively.

2 Main results

Suppose that $G = (V(G), E(G))$ is a connected graph and that $d(u, v)$ is the distance between u and v in the graph G. Then the *hyper-Wiener index* is defined as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d(u, v) + d^2(u, v)),$$

where $d^2(u, v) = (d(u, v))^2$. Let $d(u|G) = \sum_{v \in V(G)} d(u, v)$ and $d^2(u|G) = \sum_{v \in V(G)} d^2(u, v)$, then we further have $WW(G) = \frac{1}{4} \sum_{u \in V(G)} (d(u|G) + d^2(u|G))$. If u and v are vertices of subgraphs G_1 and G_2 of G respectively, then we set $WW_G(G_1, G_2) = \frac{1}{2} \sum_{u \in V(G_1), v \in V(G_2)} (d_G(u, v) + d_G^2(u, v))$. As the same as the work [1], we begin with a lemma which can obtain $WW(G)$ of a graph $G = G_1 \cup G_2$ with a common cut-vertex.

Lemma 2.1 [15] *Let G be a connected graph with a cut-vertex u_0 such that G_1 and G_2 are two connected subgraphs of G having u_0 as the only common vertex and $G_1 \cup G_2 = G$. Then*

$$\begin{aligned} WW(G) &= WW(G_1) + WW(G_2) + WW(G_1 \backslash u_0, G_2 \backslash u_0) \\ &= WW(G_1) + WW(G_2) + \frac{1}{2}(|V(G_2)| - 1)(d(u_0|G_1) \end{aligned}$$

$$+ d^2(u_0|G_1)) + \frac{1}{2}(|V(G_1)| - 1)(d(u_0|G_2) + d^2(u_0|G_2))$$
$$+ d(u_0|G_1)d(u_0|G_2).$$

The number of k-membered rings in a k-membered ring spiro system is called its *length*. Denote by $\mathcal{G}_{n,k}$ the set of all k-membered ring spiro systems of length n. Suppose that $\mathcal{M}$ is a number set. If there is no congruence relation between m_1 and m_2 for $m_1, m_2 \in \mathcal{M}$, then we denote it by $m_1 \equiv m_2(mod\ nonentity)$.

Theorem 2.1 *If $G, H \in \mathcal{G}_{n,k}$, then*

$$WW(G) \equiv \begin{cases} WW(H)(mod\frac{(k-1)^2}{2}), & \text{if } k \text{ is odd;} \\ WW(H)(mod\ nonentity), & \text{if } k \text{ is even.} \end{cases}$$

Proof. We first prove by induction on n that following claim is true.
Claim. For arbitrary $z \in V(G)$ and $z^* \in V(H)$, we have $d(z|G) \equiv d(z^*|H)(mod(k-1))$ for all k and

$$d^2(z|G) \equiv \begin{cases} d^2(z^*|H)(mod(k-1)), & \text{if } k \text{ is odd;} \\ d^2(z^*|H)(mod\ nonentity), & \text{if } k \text{ is even.} \end{cases}$$

The basic case $n = 1$ is clear. So suppose $n \geqslant 2$. Note that any two G and H of $\mathcal{G}_{n,k}$ can be obtained from two appropriately chosen graphs X and X^* of $\mathcal{G}_{n-1,k}$ by attaching to them two new k-membered ring B and B^*, respectively, as shown in Fig. 1.

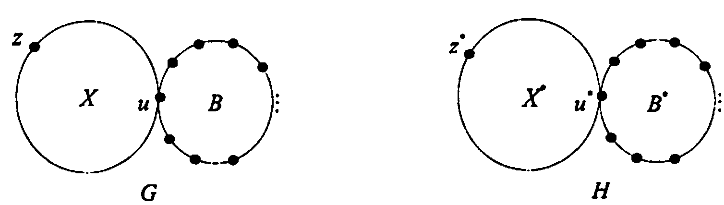

Fig. 1

For arbitrary $z \in V(X), z^* \in V(X^*)$, we have

$$\begin{aligned} d(z|G) &= d(z|X) + \sum_{v \in V(B)\backslash u} (d(z,u) + d(u,v)) \\ &= d(z|X) + (k-1)d(z,u) + d(u|B), \\ d^2(z|G) &= d^2(z|X) + \sum_{v \in V(B)\backslash u} (d(z,u) + d(u,v))^2 \\ &= d^2(z|X) + (k-1)d^2(z,u) + 2d(z,u)d(u|B) + d^2(u|B). \end{aligned}$$

Analogously, we have $d(z^*|H) = d(z^*|X^*) + (k-1)d(z^*,u^*) + d(u^*|B^*)$ and $d^2(z^*|H) = d^2(z^*|X^*)+(k-1)d^2(z^*,u^*)+2d(z^*,u^*)\cdot$

$d(u^*|B^*) + d^2(u^*|B^*)$. Note that $d(u|B) = d(u^*|B^*) = \frac{(k+1)(k-1)}{4}$ and $d^2(u|B) = d^2(u^*|B^*)$. Then

$$\begin{aligned} d(z|G) - d(z^*|H) &= (d(z|X) - d(z^*|X^*)) \\ &\quad + (k-1)(d(z,u) - d(z^*,u^*)), \\ d^2(z|G) - d^2(z^*|H) &= (d^2(z|X) - d^2(z^*|X^*)) + (k-1)(d^2(z,u) \\ &\quad - d^2(z^*,u^*)) + \frac{(k+1)(k-1)}{2}(d(z,u) - d(z^*,u^*)). \end{aligned}$$

By the inductive hypothesis, we know that the claim is fulfilled for $z \in V(X), z^* \in V(X^*)$.

Similarly, we can show that the claim is fulfilled for $z \in V(X), z^* \in V(B)$, or $z \in V(B), z^* \in V(X^*)$, or $z \in V(B), z^* \in V(B^*)$. This proves the claim. $\diamond$

Now we can proof the assertion by induction on n. The basic case $n = 1$ is fulfilled for the assertion. So suppose $n \geqslant 2$. Bearing in mind that $WW(B) = WW(B^*)$, $|V(B)| = |V(B^*)| = k$ and $|V(X)| = |V(X^*)|$. By Lemma 2.1, we have

$$\begin{aligned} WW(G) - WW(H) &= (WW(X) - WW(X^*)) \\ &\quad + \frac{1}{2}(k-1)(d(u|X) - d(u^*|X^*) + d^2(u|X) - d^2(u^*|X^*)) \\ &\quad + \frac{(k+1)(k-1)}{4}(d(u|X) - d(u^*|X^*)). \end{aligned}$$

Thus the assertion follows from the Claim and inductive hypothesis. □

A k-membered ring spiro star is such a k-membered ring spiro system that has only one spiro vertex. A k-membered ring B in a k-membered ring spiro chain is *internal* if it contains two spiro vertices, and the others *terminal*. Two vertices u and v on k-membered ring B are *para-position* if $d(u,v) = \lfloor \frac{k}{2} \rfloor$. An internal k-membered ring B is *para-position* if the two spiro vertices on B are para-position. A *para-position-k-membered ring spiro chain* is called if all internal k-membered rings are para-position. Denote the k-membered ring spiro star and the para-position-k-membered ring spiro chain of length n by S_n and L_n, respectively. Now we give an explicit relationships of k-membered ring spiro systems as follows.

Theorem 2.2 *If $S_n, L_n, G \in \mathcal{G}_{n,k}$ and $n \geq 3$, then*

$$WW(S_n) \leq WW(G) \leq WW(L_n),$$

with the left equality if and only if $G \cong S_n$, and the right equality if and only if $G \cong L_n$.

In what follows we give some lemmas before offering the proof of Theorem 2.2.

Suppose that T_i (T_i may be an empty) is the subgraph of $H_1 \in \mathcal{G}_{n,k}$ which is attaching on the k-membered ring B with a common vertex u_i ($1 \leq i \leq k$). If k is even (odd), then we call the process of transforming T_{k+2-j} from u_{k+2-j} to u_j for $2 \leq j \leq \frac{k}{2}$ ($2 \leq j \leq \frac{k+1}{2}$) the *para-position transformation* of H_1, and denote the resulting graph by H_2, as shown in Fig. 2.
Lemma 2.2 *Let $H_i \in \mathcal{G}_{n,k}$ ($i = 1, 2$) be defined as above. Then $WW(H_1) \geq WW(H_2)$.*

Proof. If k is even, by inspection of Fig. 2 and Lemma 2.1, then we have

$$
\begin{aligned}
&WW(H_1) - WW(H_2) \\
&\quad = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} (WW_{H_1}(T_i\backslash u_i, T_j\backslash u_j) - WW_{H_2}(T_i\backslash u_i, T_j\backslash u_j)) \\
&\quad + \sum_{i=1}^{k}(WW_{H_1}(T_i\backslash u_i, B\backslash u_i) - WW_{H_2}(T_i\backslash u_i, B\backslash u_i)).
\end{aligned}
$$

By simple combinatorial arguments, we obtain $WW_{H_1}(T_i\backslash u_i, T_j\backslash u_j) \geq WW_{H_2}(T_i\backslash u_i, T_j\backslash u_j)$ for $2 \leq i \leq \frac{k}{2}, \frac{k}{2} + 2 \leq j \leq k - 1$, otherwise $WW_{H_1}(T_i\backslash u_i, T_j\backslash u_j) = WW_{H_2}(T_i\backslash u_i, T_j\backslash u_j)$. Note that $WW_{H_1}(T_i\backslash u_i, B\backslash u_i) = WW_{H_2}(T_i\backslash u_i, B\backslash u_i)$, $1 \leq i \leq k$. Thus we have $WW(H_1) - WW(H_2) \geq 0$ namely $WW(H_1) \geq WW(H_2)$. Analogously, if k is odd, we can also obtain the assertion. □

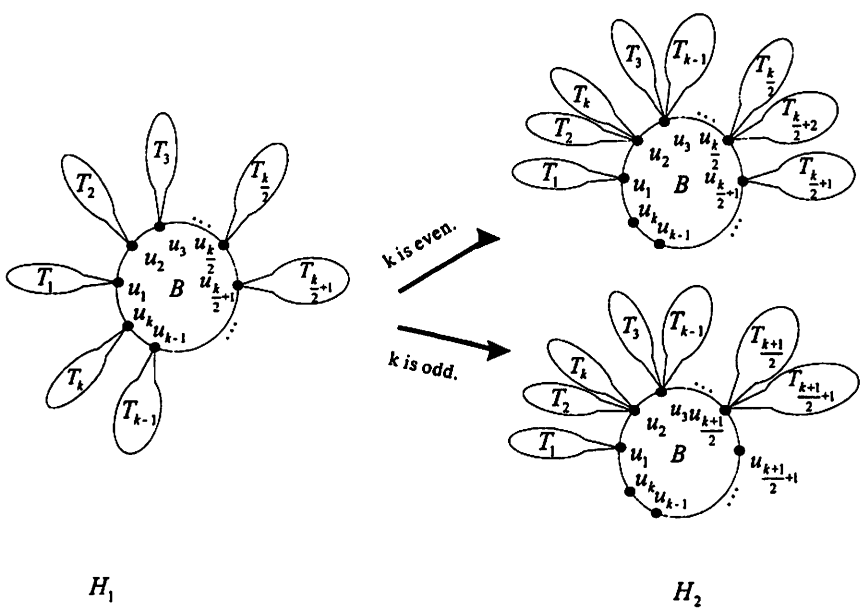

Fig. 2 Para-position transformation.

Suppose that T_i' (T_i' may be an empty) is a subgraph of $H_2' \in \mathcal{G}_{n,k}$ that has common vertex u_i with a k-membered ring B of H_2', for $i = 1, 2, \cdots, t$ (if k is even, then $t = \frac{k}{2} + 1$; if k is odd, then $t = \frac{k+1}{2}$). Take $t-1$ times transformations as follows, as shown in Fig. 3. Firstly, we transform T'_t from u_t to u_{t-1}. Secondly, we transform $T'_t \cup T'_{t-1}$ from u_{t-1} to u_{t-2}. Continuing this processes, lastly, we transform $T'_t \cup T'_{t-1} \cup \cdots \cup T'_2$ from u_2 to u_1. Then we denote successively the resulting graphs by $H_2'^{(1)}$, $H_2'^{(2)}$, $\cdots$, $H_2'^{(t-1)}$ and call the processes $u_t \to u_{t-1} \to \cdots \to u_2 \to u_1$ the *step transformation* of H'_2.

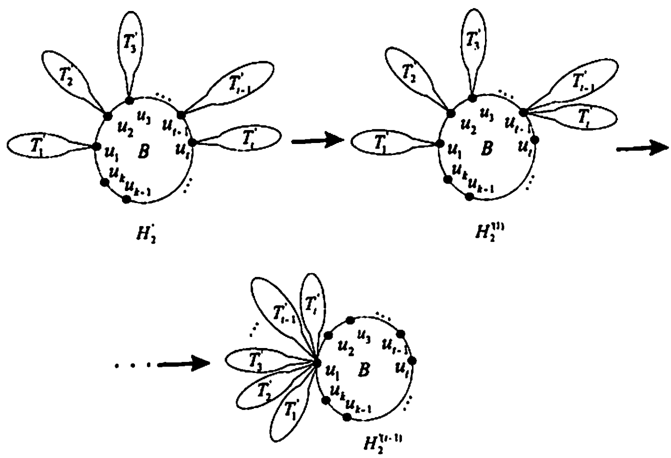

Fig. 3. Step transformation

Lemma 2.3 *Let H'_2 and $H_2'^{(i)}$ $(i = 1, 2, \cdots, t-1)$ be defined as above. Then $WW(H'_2) \geq WW(H_2'^{(t-1)})$.*

Proof. By inspection of Fig. 3 and Lemma 2.1, we have

$$\begin{aligned} & WW(H'_2) - WW(H_2'^{(1)}) \\ &= \sum_{i=1}^{t-1} \sum_{j=i+1}^{t} (WW_{H'_2}(T'_i \backslash u_i, T'_j \backslash u_j) - WW_{H_2'^{(1)}}(T'_i \backslash u_i, T'_j \backslash u_j)) \\ &+ \sum_{i=1}^{t} (WW_{H'_2}(T'_i \backslash u_i, B \backslash u_i) - WW_{H_2'^{(1)}}(T'_i \backslash u_i, B \backslash u_i)). \end{aligned}$$

By simple combinatorial argument, we obtain

$WW_{H_2'}(T_t'\backslash u_t, T_j'\backslash u_j) \geq WW_{H_2'^{(1)}}(T_t'\backslash u_t, T_j'\backslash u_j)$ $(j = 1, 2, \cdots, t-1)$, otherwise $WW_{H_2'}(T_i'\backslash u_i, T_j'\backslash u_j) = WW_{H_2'^{(1)}}(T_i'\backslash u_i, T_j'\backslash u_j)$. Note that $WW_{H_2'}(T_i'\backslash u_i, B\backslash u_i) = WW_{H_2'^{(1)}}(T_i'\backslash u_i, B\backslash u_i)$ $(i = 1, 2, \cdots, t)$. Then we have $WW(H_2') \geq WW(H_2'^{(1)})$. Analogously, we can obtain $WW(H_2'^{(1)}) \geq WW(H_2'^{(2)}), \cdots,$ $WW(H_2'^{(t-2)}) \geq WW(H_2'^{(t-1)})$. This proves the assertion. □

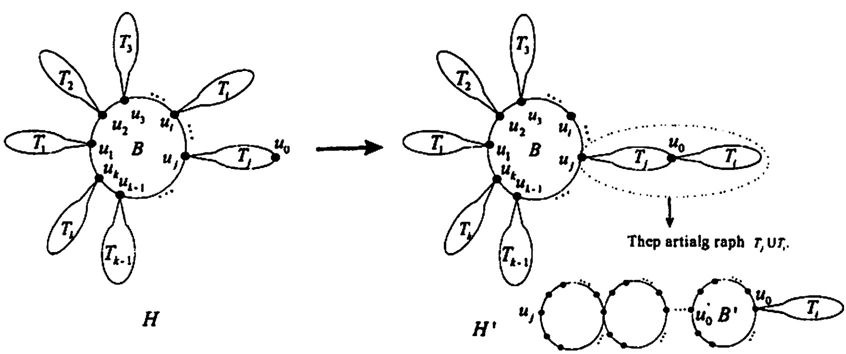

Fig. 4. Grafting transformation

Given a graph $H \in \mathcal{G}_{n,k}$, we can appropriately choose a k-membered ring B, the subgraphs T_i of H (T_i may be an empty) has common vertices v_i with the k-membered ring B $(i = 1, 2, \cdots, k)$. There exists some T_j such that $B \cup T_j$ is a para-position-k-membered ring spiro chain. If u_0 is the farthest vertex to vertex u_j in T_j, then we call the process of transforming arbitrary T_i from u_i to u_0 $(i \neq j)$ the *grafting transformation* of H, and denote the resulting graph by H', as shown in Fig. 4.

Lemma 2.4 *Let H and H' be defined as above. Then* $WW(H) \leq WW(H')$.

Proof. By inspection of Fig. 4 and Lemma 2.1, we have

$$WW(H) = \sum_{l=1, l\neq i,j}^{k} WW(T_l) + WW(T_i \cup B \cup T_j)$$

$$+\sum_{l=1,l\neq i,j}^{k-1}\sum_{m=l+1,m\neq i,j}^{k} WW_H(T_l\backslash u_l, T_m\backslash u_m)$$

$$+\sum_{l=1,l\neq i,j}^{k} WW_H(T_i\backslash u_i, T_l\backslash u_l)+\sum_{l=1,l\neq i,j}^{k} WW_H(T_j\backslash u_j, T_l\backslash u_l)$$

$$+\sum_{l=1,l\neq i,j}^{k} WW_H(T_l\backslash u_l, B\backslash u_i),$$

$$WW(H') = \sum_{l=1,l\neq i,j}^{k} WW(T_l) + WW(B\cup T_j\cup T_i)$$

$$+\sum_{l=1,l\neq i,j}^{k-1}\sum_{m=l+1,m\neq i,j}^{k} WW_{H'}(T_l\backslash u_l, T_m\backslash u_m)$$

$$+\sum_{l=1,l\neq i,j}^{k} WW_{H'}(T_i\backslash u_i, T_l\backslash u_l)+\sum_{l=1,l\neq i,j}^{k} WW_{H'}(T_j\backslash u_j, T_l\backslash u_l)$$

$$+\sum_{l=1,l\neq i,j}^{k} WW_{H'}(T_l\backslash u_l, B\backslash u_i).$$

Then we can observe that

$$WW(H)-WW(H') = (WW(T_i\cup B\cup T_j) - WW(B\cup T_j\cup T_i))$$

$$+(\sum_{l=1,l\neq i,j}^{k} WW_H(T_i\backslash u_i, T_l\backslash u_l) - \sum_{l=1,l\neq i,j}^{k} WW_{H'}(T_i\backslash u_i, T_l\backslash u_l)).$$

Note that $d_H(u,u_l) + d_H(u_l,v) \leq d_{H'}(u,u_0) + d_{H'}(u_0,u_j) + d_{H'}(u_j,u_l) + d_{H'}(u_l,v)$. Then we can easily obtain $WW_H(T_i\backslash u_i, T_l\backslash u_l) - WW_{H'}(T_i\backslash u_i, T_l\backslash u_l) \leq 0$. Thus we further have

$$WW(H)-WW(H') \leq WW(T_i\cup B\cup T_j)-WW(B\cup T_j\cup T_i). \quad (*)$$

Let B', u_0' be an hexagon and a vertex labeled in the partial graph $T_j \cup T_i$ as shown in Fig. 4. Then we have

$$\begin{aligned}
&WW(T_i \cup B \cup T_j) \\
&\quad = WW(T_i) + WW(B) + WW(T_j) + WW_H(B\backslash u_j, T_j\backslash u_j) \\
&\quad + WW_H(T_i\backslash u_i, B\backslash u_i) + WW_H(T_i\backslash u_i, T_j\backslash u_j), \\
&WW(B \cup T_j \cup T_i) = WW(B \cup (T_j\backslash B')) + WW(B') + WW(T_i) \\
&\quad + WW_{H'}(B'\backslash u_0, T_i\backslash u_0) + WW_{H'}((B \cup (T_j\backslash B'))\backslash u_0', B'\backslash u_0') \\
&\quad + WW_{H'}((B \cup (T_j\backslash B'))\backslash u_0', T_i\backslash u_0).
\end{aligned}$$

By some combinatorial argument, we further have

$$WW(T_i \cup B \cup T_j) - WW(B \cup T_j \cup T_i) = WW_H(T_i\backslash u_i, T_j\backslash u_j)$$

$$-WW_{H'}((B \cup (T_j\backslash B'))\backslash u_0', T_i\backslash u_0).$$

Since $d_{H'}(u_0, u_0') \geq d_{H'}(u_j, u_i)$, we can easily observe that $WW_H(T_i\backslash u_i, T_j\backslash u_j) \leq WW_{H'}((B \cup (T_j\backslash B'))\backslash u_0', T_i\backslash u_0)$. Thus we have $WW(T_i \cup B \cup T_j) - WW(B \cup T_j \cup T_i) \leq 0$, and by the inequality $(*)$ we prove the assertion. □

Proof of Theorem 2.2. By Lemma 2.2 and Lemma 2.3, we easily observe that a graph $G \in \mathcal{G}_{n,k}$ can be transformed into S_n through some steps of the para-position or step transformations. Thus we have $WW(G) \geq WW(S_n)$.

By Lemma 2.4, we easily observe that a graph $G \in \mathcal{G}_{n,k}$ can be transformed into L_n through some steps of the grafting transformations. Thus we have $WW(G) \leq WW(L_n)$.□

Now we give the formulae for computing the hyper-Wiener indices of S_n and L_n, respectively.

Theorem 2.3 For $S_n \in \mathcal{G}_{n,k}$,

$$WW(S_n) = \begin{cases} \frac{k^2(k+1)(k+2)n}{48} + \frac{(7k^3+36k^2-4k-48)kn(n-1)}{96}, & 2 \mid k; \\ \frac{k(k^2-1)(k+3)n}{48} + \frac{(7k+15)(k+1)(k-1)^2n(n-1)}{96}, & 2 \nmid k. \end{cases}$$

Proof. By [11], $WW(B) = \begin{cases} \frac{k^2(k+1)(k+2)}{48}, & 2 \mid k \\ \frac{k(k^2-1)(k+3)}{48}, & 2 \nmid k \end{cases}$. By Lemma 2.1 and some calculations with Maple 9.5, we easily obtain the assertion. □

Theorem 2.4 For $L_n \in \mathcal{G}_{n,k}$,

$$WW(L_n) = \begin{cases} \frac{1}{96}kn(k(k^2-2k+1)n^3 + 4(2k^2 \\ -3k+1)n^2 - (2k^2-25k+20)n \\ +k^3+2k^2-10k+16), & 2 \mid k; \\ \frac{1}{96}(k-1)((k^3-3k^2+3k-1)n^3 \\ +12(k^2-2k+1)n^2 + 44(k-1)n \\ +k^3-k^2-17k+33), & 2 \nmid k. \end{cases}$$

Proof. Let the k-membered rings of L_n be $B_1, B_2, \cdots, B_n$ with spiro vertices $s_1, s_2, \cdots, s_{n-1}$ in sequence and denote $L_n = B_1B_2\cdots B_n$. By Lemma 2.1, we have

$$WW(L_n) = WW(L_{n-1}) + WW_{L_n}(L_{n-1}, B_n \setminus s_{n-1})$$

$$+ \sum_{\{u,v\} \subseteq V(B_n \setminus s_{n-1})} (d_{L_n}(u,v) + d^2_{L_n}(u,v)).$$

Case 1. If $2 \nmid k$, then

$$WW_{L_n}(L_{n-1}, B_n \setminus s_{n-1}) = \frac{1}{2} \sum_{u \in V(L_{n-1})} \sum_{v \in V(B_n \setminus s_{n-1})} ((d(u, s_{n-1})$$

$$+ d(s_{n-1}, v)) + (d(u, s_{n-1}) + d(s_{n-1}, v))^2)$$

$$= \frac{1}{2} \sum_{u \in V(L_{n-1})} 2(((d(u, s_{n-1}) + 1) + (d(u, s_{n-1}) + 1)^2) + \cdots$$

$$+ ((d(u, s_{n-1}) + \frac{k-1}{2}) + (d(u, s_{n-1}) + \frac{k-1}{2})^2))$$

$$= \sum_{u \in V(L_{n-1})} \sum_{i=1}^{\frac{k-1}{2}} ((d(u, s_{n-1}) + i) + (d(u, s_{n-1}) + i)^2)$$

$$= \frac{1}{24}(k-1)(k+1)(k+3)(n(k-1)-k+2)$$
$$+ \frac{1}{4}(k-1)(k+3) \sum_{u \in V(L_{n-1})} d(u, s_{n-1})$$
$$+ \frac{1}{2}(k-1) \sum_{u \in V(L_{n-1})} d^2(u, s_{n-1}).$$

From the graph L_n, we can see that

$$\sum_{u \in V(L_{n-1})} d(u, s_{n-1}) = (1 + 2 + \cdots + \frac{(k-1)(n-1)}{2})$$
$$+ ((1 + 2 + \cdots + \frac{k-1}{2}) + ((\frac{k-1}{2} + 1)$$
$$+ (\frac{k-1}{2} + 2) + \cdots + (\frac{k-1}{2} + \frac{k-1}{2})) + \cdots +$$
$$((\frac{(k-1)(n-2)}{2} + 1) + (\frac{(k-1)(n-2)}{2} + 2)$$
$$+ \cdots + (\frac{(k-1)(n-2)}{2} + \frac{k-1}{2})))$$
$$= \sum_{i=1}^{\frac{(k-1)(n-1)}{2}} i + \sum_{i=0}^{n-2} \sum_{j=1}^{\frac{k-1}{2}} (\frac{k-1}{2} i + j)$$
$$= \frac{(k-1)(n-1)((k-1)n-k+3)}{4},$$

Similarly, we have

$$\sum_{u \in V(L_{n-1})} d^2(u, s_{n-1})$$
$$= \frac{(k-1)(n-1)((k-1)n-k+2)((k-1)n-k+3)}{12}.$$

Thus we have

$$WW_{L_n}(L_{n-1}, B_n \setminus s_{n-1}) = \frac{1}{48}(k-1)(2(k^3 - 3k^2 + 3k - 1)n^3$$
$$- 3(k^3 - 9k^2 + 15k - 7)n^2 + 2(k^3 - 12k^2 + 43k - 32)n$$
$$- k^3 + 5k^2 - 39k + 51).$$

Note that $\sum\limits_{\{u,v\}\subseteq V(B_n\setminus s_{n-1})} (d_{L_n}(u,v) + d^2_{L_n}(u,v))$ $= \frac{(k-1)(k-2)(k+3)(k+1)}{48}$. Therefore, we have

$$WW(L_n) = WW(L_{n-1}) + \frac{1}{48}(k-1)(2(k^3-3k^2+3k-1)n^3 - 3(k^3-9k^2+15k-7)n^2 + 2(k^3-12k^2+43k-32)n + 7k^2-44k+45).$$

Note that $WW(B_1) = \frac{k(k^2-1)(k+3)}{48}$. Using the recurrence, we have

$$\begin{aligned} WW(L_n) &= WW(B_1) + \sum_{i=2}^{n} \frac{1}{48}(k-1)(2(k^3-3k^2+3k-1)i^3 \\ &\quad - 3(k^3-9k^2+15k-7)i^2 + 2(k^3-12k^2+43k-32)i \\ &\quad + 7k^2-44k+45) \\ &= \frac{1}{96}(k-1)((k^3-3k^2+3k-1)n^3 + 12(k^2-2k+1)n^2 \\ &\quad + 44(k-1)n + k^3-k^2-17k+33). \end{aligned}$$

Case 2. If $2 \mid k$, as the same as the argument of Case 1, we can easily obtain the assertion. □

Corollary 2.5 [16]

(i) For $L_n \in \mathcal{G}_{n,3}$, $WW(L_n) = \frac{n^2}{6}(n^2+6n+11)$;

(ii) For $L_n \in \mathcal{G}_{n,4}$, $WW(L_n) = \frac{n}{2}(3n^3+7n^2+4n+6)$;

(iii) For $L_n \in \mathcal{G}_{n,6}$, $WW(L_n) = \frac{n}{8}(75n^3+110n^2+29n+122)$.

3 Examples

As the applications of the results in the section 2, we take five- and six-membered ring spiro systems for examples.

Example 3.1 For $G, H \in \mathcal{G}_{n,5}$, by Theorem 2.1, we have $WW(G) \equiv WW(H)(mod 8)$. By Theorem 2.2, the extremal graphs with maximal and minimal hyper-Wiener index are the five-membered ring spiro star and the para-position-five-membered ring spiro chain respectively. By Theorem 2.3 and Theorem 2.4, we further obtain $10n(5n-3) \leq WW(G) \leq \frac{2}{3}n(4n^3+12n^2+11n+3)$.

Example 3.2 For $G, H \in \mathcal{G}_{n,6}$, by Theorem 2.1, we have $WW(G) \equiv WW(H)(mod\ nonentity)$. By Theorem 2.2, the extremal graphs with maximal and minimal hyper-Wiener index are the six-membered ring spiro star and the para-position-six-membered ring spiro chain respectively. By Theorem 2.3 and Theorem 2.4, we further obtain $3n(57n-43) \leq WW(G) \leq \frac{1}{8}n(75n^3+110n^2+29n+122)$.

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References

[1] R. Balakrishnan, N. Sridharan, K. V. Tyer, Wiener index of graphs with more than one cut-vertex, *Appl. Math. Lett.* 21 (2008) 922-927.

[2] G. G. Cash, Polynomial expressions for the hyper-Wiener index of extended hydrocarbon networks, *Comput. Chem.* 25 (2001) 577-582.

[3] G. G. Cash, Relationship between the Hosoya polynomial and the hyper-Wiener index, *Appl. Math. Lett.* 15 (2002) 893-895.

[4] X. Chen, B. Zhao, P. Zhao, Six-membered ring spiro chains with extremal Merrifield-Simmons index and Hosoya index, *MATCH Commun. Math. Comput. Chem.* 62 (2009) 657-665.

[5] H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Comput. Model.* (2011), doi:10.1016/j.mcm.2011.08.037.

[6] T. Došlić, F. Måløy, Chain hexagonal cacti: matchings and independent sets, *Discrete Math.* 310 (2010) 1676-1690.

[7] M. Eliasi, A. Iranmanesh, The hyper-Wiener index of the generalized hierarchical product of graphs, *Discrete Appl. Math.* 159 (2011) 866-871.

[8] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* 23 (2010) 943-948.

[9] L. Feng, W. Liu, K. Xu, The hyper-Wiener index of bicyclic graphs, *Utilitas Math.* 84 (2011) 97-104.

[10] I. Gutman, Relation between hyper-Wiener and Wiener index, *Chem. Phys. Lett.* 364 (2002) 352-356.

[11] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, The hyper-Wiener index of graph operations, *Comput. Math. Appl.* 56 (2008) 1402-1407.

[12] S. Klavžar, I. Gutman, A theorem on Wiener-type invariants for isometric subgraphs of hypercubes, *Appl. Math. Lett.* 19 (2006) 1129-1133.

[13] S. Klavžar, P. Žigert, I. Gutman, An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons, *Comput. Chem.* 24 (2000) 229-233.

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

[15] X. Li, X. Yang, R. Hu, k-membered ring spiro chains with extremal hyper-Wiener index, *ARS Combin.* in press.

[16] T. Mansour, M. Schork, Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs, *J. Math. Chem.* 581 (2009) 59-69.

[17] M. Metsidik, W. Zhang, F. Duan, Hyper- and reverse-Wiener indices of F-sums of graphs, *Discrete Appl. Math.* 158 (2010) 1433-1440.

[18] M. Randić, Novel molecular descriptor for structure-property studies, *Chem. Phys. Lett.* 211 (1993) 478-483.

[19] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* 60 (1947) 17.

[20] R. Xing, B. Zhou, X. Qi, Hyper-Wiener index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 66 (2011) 315-328.

[21] P. Zhao, B. Zhao, X. Chen, Y. Bai, Two classes of chains with maximal and minmal total π-electron energy, *MATCH Commun. Math. Comput. Chem.* 62 (2009) 525-536.

[22] B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, *Chem. Phys. Lett.* 394 (2004) 93-95.