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Some characteristics on hyper-wiener index of graphs

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ABSTRACT

Some chemical indices have been invented in theoretical chemistry, such as Hyper-Wiener index. In this paper, we present several characteristics on Hyper-Wiener index of certain special structure of graphs.

Keywords: Chemical graph theory; organic molecules; Hyper-Wiener index

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INTRODUCTION

The Hyper-Wiener index, as an extension of Wiener index, is an important topological index in Chemistry. It is used for the structure of molecule. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The Hyper-Wiener index is such a topological index and it has been widely used in Chemistry fields. Some conclusions for Hyper-Wiener index can refer to [1].

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a graph G, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v),$$

where $d(u,v)$ is the distance between u and v in G.

Several papers contributed to determine the Wiener index of special graphs. Gao and Shi [2] determined the Wiener index of gear fan graph, gear wheel graph and their r-corona graphs. Chen [3] gained the exact expression for general pepoid graph. Xing and Cai [4] characterized the tree with third-minimum wiener index and introduce the method of obtaining the order of the Wiener indices among all the trees with given order and diameter, respectively. A tricyclic graph is a connected graph with n vertices and n+2 edges. Wan and Ren [5] studied the Wiener index of tricyclic graph τ_n^3 which have at most a common vertex between any two circuits, and the smallest, the second-smallest Wiener indices of the tricyclic graphs τ_n^3 are given. The Hyper-Wiener index WW is one of the recently distance-based graph invariants. That WW clearly encodes the compactness of a structure and the WW of G is define as:

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

Pan [6] deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. Tang [7] studied the Wiener indices of unicycles graphs. Firstly, it determined a formulation for calculating the Wiener index of an unicycles graphs according its structure. And then, in terms of this formulation, it characterized the graphs with the largest, the smallest, the second largest, the second smallest, the third largest and the third smallest Wiener indies among all the unicycles graphs. Xing et al., [8] determined the n-vertex unicyclic graphs of cycle length r with the smallest and the largest Hyper-Wiener indices for $3 \le r \le n$, and the n-vertex unicyclic graphs with the smallest, the second smallest, the largest and the second largest Hyper-Wiener indices for $n \ge 5$. Yuan [9] learned the special class of unicyclic graph. Feng et al., [10] presented the extremal bicyclic graphs with maximal and minimal hyper-Wiener index. More results on Wiener index and Hyper-Wiener index can refer to [11-14].

In this paper, we discuss some characteristics about Hyper-Wiener index of special kind of graphs.

1. Main Results and Proof

Theorem 1. Let *H*, *X*, *Y* be three connected graphs disjoint in pair. Suppose that *u*, *v* are two vertices of *H*, *v'* is a vertex of *X*, *u'* is a vertex of *Y*. Let *G* be the graph obtained from *H*, *X*, *Y* by identifying *v* with *v'* and *u* with *u'*, respectively. Let G_1^* be the graph obtained from *H*, *X*, *Y* by identifying vertices *v*, *v'*, *u'*, and let G_2^* be the graph obtained from *H*, *X*, *Y* by identifying vertices *u*, *v'*, *u'* (see Fig. 1 for more detail). Then $WW(G_1^*) < WW(G)$ or $WW(G_2^*) < WW(G)$.

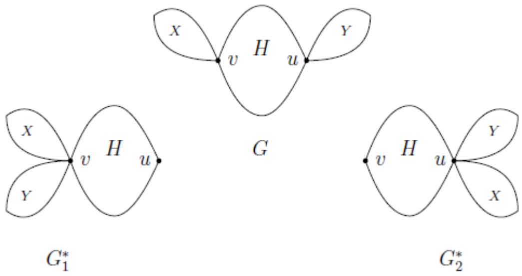

Fig. 1. Graphs described in Theorem 1.

Proof. By the definition of Hyper-Wiener index, we have

$$WW(G) = \frac{1}{2}\{\{\sum_{x,y\in V(X)} d_G(x,y) + \sum_{x,y\in V(Y)} d_G(x,y) + \sum_{x\in V(X-v),y\in V(Y-u)} d_G(x,y) + \sum_{x,y\in V(H)} d_G(x,y)$$
$$+ \sum_{x\in V(H),y\in V(Y-u)} d_G(x,y) + \sum_{x\in V(H),y\in V(X-v)} d_G(x,y)\} + \{\sum_{x,y\in V(X)} d_G(x,y)^2 + \sum_{x,y\in V(Y)} d_G(x,y)^2 +$$
$$\sum_{x\in V(X-v),y\in V(Y-u)} d_G(x,y)^2 + \sum_{x,y\in V(H)} d_G(x,y)^2 + \sum_{x\in V(H),y\in V(Y-u)} d_G(x,y)^2 + \sum_{x\in V(H),y\in V(X-v)} d_G(x,y)^2\}\}$$
$$= \frac{1}{2}\{\{\sum_{x,y\in V(X)} d_X(x,y) + \sum_{x,y\in V(Y-u)} d_Y(x,y) + \sum_{x\in V(X-v),y\in V(Y-u)} d_G(x,y) + \sum_{x,y\in V(H)} d_H(x,y)$$
$$+ \sum_{x\in V(H),y\in V(Y-u)} d_G(x,y) + \sum_{x\in V(H),y\in V(X-v)} d_G(x,y)\} + \{\sum_{x,y\in V(X)} d_X(x,y)^2 + \sum_{x,y\in V(Y-u)} d_Y(x,y)^2 +$$
$$\sum_{x\in V(X-v),y\in V(Y-u)} d_G(x,y)^2 + \sum_{x,y\in V(H)} d_H(x,y)^2 + \sum_{x\in V(H),y\in V(Y-u)} d_G(x,y)^2 + \sum_{x\in V(H),y\in V(X-v)} d_G(x,y)^2\}\}.$$

Hence, we get

$$WW(G) - WW(G_1^*) = \frac{1}{2}\{\{\sum_{x\in V(X-v),y\in V(Y-u)} [d_G(x,y) - d_{G_1^*}(x,y)] +$$
$$\sum_{x\in V(H),y\in V(Y-u)} [d_G(x,y) - d_{G_1^*}(x,y)]\} + \{\sum_{x\in V(X-v),y\in V(Y-u)} [d_G(x,y)^2 - d_{G_1^*}(x,y)^2] +$$
$$\sum_{x\in V(H),y\in V(Y-u)} [d_G(x,y)^2 - d_{G_1^*}(x,y)^2]\}\}$$
$$> \frac{1}{2}\{\sum_{x\in V(H),y\in V(Y)} [d_G(x,y) - d_{G_1^*}(x,y)] + \sum_{x\in V(H),y\in V(Y)} [d_G(x,y)^2 - d_{G_1^*}(x,y)^2]\}$$
$$= \frac{1}{2}\{\sum_{x\in V(H-u-v)} [d_H(x,u) - d_H(x,v)] + \sum_{x\in V(H-u-v)} [d_H(x,u)^2 - d_H(x,v)^2]\} \quad (1)$$

$$WW(G)\text{ - }WW(G_2^*)=\frac{1}{2}\{\{\sum_{x\in V(X),y\in V(Y)}[d_G(x,y)-d_{G_2^*}(x,y)]+\sum_{x\in V(X-v),y\in V(H)}[d_G(x,y)-d_{G_2^*}(x,y)]\}+\{\sum_{x\in V(X),y\in V(Y)}[d_G(x,y)^2-d_{G_2^*}(x,y)^2]+\sum_{x\in V(X-v),y\in V(H)}[d_G(x,y)^2-d_{G_2^*}(x,y)^2]\}\}$$

$$>\frac{1}{2}\{\sum_{x\in V(H-u-v)}[d_H(x,v)-d_H(x,u)]+\sum_{x\in V(H-u-v)}[d_H(x,v)^2-d_H(x,u)^2]\}$$

(2)

If $WW(G)$ - $WW(G_1^*)$ $\le$ 0, then according to (1), $\sum_{x\in V(H-u-v)}[d_H(x,u)-d_H(x,v)]$ + $\sum_{x\in V(H-u-v)}[d_H(x,u)^2-d_H(x,v)^2]$<0. Hence, by (2), $WW(G)\text{ - }WW(G_2^*)$>0. □

Theorem 2. Suppose that G be a graph of order $n\ge 7$ obtained from a connected graph $H\ne P_1$ and a cycle $C_q=u_0u_1\cdots u_{q-1}u_0$ ($q\ge 4$) by identifying u_0 with a vertex u of the graph H (see Fig. 2 for more detail). Let $G'= G - u_{q-1}u_{q-2} + uu_{q-2}$. Then $WW(G')<WW(G)$.

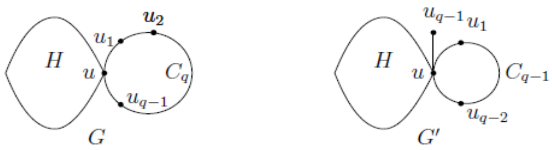

Fig. 2. Graphs described in Theorem 2.

Proof. By the definition of Hyper-Wiener index, we have

$$WW(C_q)=\begin{cases}\frac{q}{2}\sum_{i=1}^{\frac{q}{2}-1}i^2+\frac{q^3}{8} & \text{if } q \text{ is even}\\ \frac{q}{2}\sum_{i=1}^{\frac{q-1}{2}}i^2+\frac{q^3-q}{16} & \text{if } q \text{ is odd}\end{cases}$$

Note that if $q\ge 4$ is even, then $\sum_{j=0}^{q-2}\{d_{G'}(u_{q-1},u_j)+d_{G'}(u_{q-1},u_j)^2\}=2+2\sum_{i=2}^{q/2}(i+i^2)$. Hence,

$$WW(G)\text{ - }WW(G')=\frac{1}{2}\{\sum_{x\in V(H)-u_0}\sum_{i=0}^{q-1}\{[d_G(x,u_i)-d_{G'}(x,u_i)]+[d_G(x,u_i)^2-d_{G'}(x,u_i)^2]\}+\sum_{0\le i<j\le q-1}\{[d_G(u_i,u_j)-d_{G'}(u_i,u_j)]+[d_G(u_i,u_j)^2-d_{G'}(u_i,u_j)^2]\}\}$$

$$\ge\frac{q-2}{4}\sum_{x\in V(H)-u_0}d_H(x,u_0)+(\frac{q^2}{4}+q-3)+(\frac{q}{2}\sum_{i=1}^{\frac{q}{2}-1}i^2+\frac{q^3}{8})\text{-}(\frac{q-1}{2}\sum_{i=1}^{\frac{q-2}{2}}i^2+\frac{(q-1)^3-(q-1)}{16})\text{-}\frac{1}{2}(2+2\sum_{i=2}^{q/2}(i+i^2))$$

$$\ge\frac{q-2}{4}+(\frac{q^2}{4}+q-3)+(\frac{q}{2}\sum_{i=1}^{\frac{q}{2}-1}i^2+\frac{q^3}{8})\text{-}(\frac{q-1}{2}\sum_{i=1}^{\frac{q-2}{2}}i^2+\frac{(q-1)^3-(q-1)}{16})\text{-}(1+\sum_{i=2}^{q/2}(i+i^2))>0.$$

Note that if $q\ge 4$ is odd, then $\sum_{j=0}^{q-2}\{d_{G'}(u_{q-1},u_j)+d_{G'}(u_{q-1},u_j)^2\}=2+2\sum_{i=2}^{(q-1)/2}(i+i^2)+\frac{q+1}{2}+\frac{(q+1)^2}{4}$.

Hence,

$$WW(G)-WW(G')=\frac{1}{2}\Big\{\sum_{x\in V(H)-u_0}\sum_{i=0}^{q-1}\{[d_G(x,u_i)-d_{G'}(x,u_i)]+[d_G(x,u_i)^2-d_{G'}(x,u_i)^2]\}+\sum_{0\le i<j\le q-1}\{[d_G(u_i,u_j)-d_{G'}(u_i,u_j)]+[d_G(u_i,u_j)^2-d_{G'}(u_i,u_j)^2]\}\Big\}$$

$$=\frac{q-3}{4}\sum_{x\in V(H)-u_0}d_H(x,u_0)+\Big(\frac{(q-1)^2}{4}-q-2\Big)+\Big(\frac{q}{2}\sum_{i=1}^{\frac{q-1}{2}}i^2+\frac{q^3-q}{16}\Big)-\Big(\frac{q-1}{2}\sum_{i=1}^{\frac{q-1}{2}-1}i^2+\frac{(q-1)^3}{8}\Big)-\frac{1}{2}\Big(2+2\sum_{i=2}^{(q-1)/2}(i+i^2)+\frac{q+1}{2}+\frac{(q+1)^2}{4}\Big)$$

$$\ge\frac{q-3}{4}+\Big(\frac{(q-1)^2}{4}-q-2\Big)+\Big(\frac{q}{2}\sum_{i=1}^{\frac{q-1}{2}}i^2+\frac{q^3-q}{16}\Big)-\Big(\frac{q-1}{2}\sum_{i=1}^{\frac{q-1}{2}-1}i^2+\frac{(q-1)^3}{8}\Big)-\Big(1+\sum_{i=2}^{(q-1)/2}(i+i^2)+\frac{q+1}{4}+\frac{(q+1)^2}{8}\Big)>0.$$

Thus, we get the desired result. □

Let $G^0(n,r)$ be the cactus obtained from the *n*-vertex star by adding *r* mutually independent edges (see Fig. 3 for more detail).

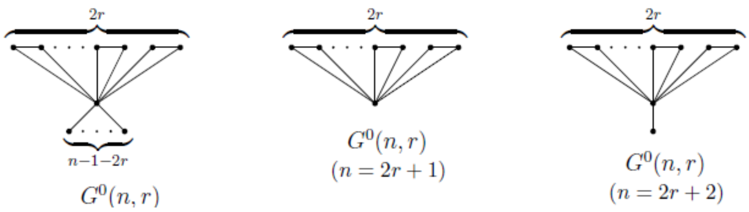

Fig. 3. The structure of $G^0(n,r)$.

Theorem 3. $WW(G^0(n,r))=\frac{1}{2}\{(3(n-1)^2-(n-1)-4r)\}$.

Proof. Since $W(K_{1,n-1})=(n-1)^2$ and $W(G^0(n,r))=(n-1)^2-r$. We get $WW(G^0(n,r))=\frac{1}{2}\{(2(n-1)^2-(n-1)-3r)+((n-1)^2-r)\}=\frac{1}{2}\{(3(n-1)^2-(n-1)-4r)\}$.

□

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