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The Hyper-Wiener Index of Unicyclic Graph with Given Diameter

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Abstract The hyper-Wiener index is a kind of extension of the Wiener index, used for predicting physicochemical properties of organic compounds. The hyper-Wiener index $WW(G)$ is defined as $WW(G)=\frac{1}{2}\sum_{u,v\in V(G)}(d_G(u,v)+d_G^2(u,v))$ with the summation going over all pairs of vertices in G, $d_G(u,v)$ denotes the distance of the two vertices u and v in the graph G. In this paper, we study the minimum hyper-Wiener indices among all the unicyclic graph with n vertices and diameter d, and characterize the corresponding extremal graphs.

Keywords hyper-Wiener index; unicyclic graph; diameter

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1. Introduction

All graphs considered in this paper are finite and simple. Let G be a simple graph of order n with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. The distance between two vertices u,v of G, denoted by $d_G(u,v)$ or $d(u,v)$, is defined as the minimum length of the paths between u and v in G. The diameter of a graph G is the maximum distance between any two vertices of G. For a vertex $v\in V(G)$, the degree and the neighborhood of v, are denoted by $d_G(v)$ and $N_G(v)$ (or written as $d(v)$ and $N(v)$ for short). A vertex v of degree 1 is called pendant vertex. An edge $e=uv$ incident with the pendant vertex v is called a pendant edge. Let $PV(G)=\{v: d_G(v)=1\}$. For a subset U of $V(G)$, let $G-U$ be the subgraph of G obtained from G by deleting the vertices of U and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G-E'$ the subgraph of G obtained from G by deleting the edges of E'. If $U=\{v\}$ and $E'=\{uv\}$, the subgraphs $G-U$ and $G-E'$ will be written as $G-v$ and $G-uv$ for short, respectively. For any two nonadjacent vertices u and v in graph G, we use $G+uv$ to denote the graph obtained from G by adding a new edge uv. Denote by S_n, P_n and C_n the star, the path and cycle on n vertices, respectively.

The Wiener index of a graph G, denoted by $W(G)$, is one of the oldest topological index, which was first introduced by Wiener [1] in 1947. It is defined as $W(G)=\sum_{u,v\in V(G)}d_G(u,v)$

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where the summation goes over all pairs of vertices of G. The hyper-Wiener index of acyclic graphs was introduced by Milan Randić in 1993 (see [2]). Then Klein et al. [3], extended the definition for all connected graphs, as a generalization of the Wiener index. Similar to the symbol $W(G)$ for the Wiener index, the hyper-Wiener index is traditionally denoted by $WW(G)$. The hyper-Wiener index of a graph G is defined as

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

Let $S(G) = \sum_{u,v\in V(G)} d_G^2(u,v)$. Then

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}S(G).$$

We denote $D_G(u) = \sum_{v\in V(G)} d_G(u,v)$, $DD_G(u) = \sum_{v\in V(G)} d_G^2(u,v)$, then

$$W(G) = \frac{1}{2}\sum_{u\in V(G)} D_G(u), \quad S(G) = \frac{1}{2}\sum_{u\in V(G)} DD_G(u).$$

Recently, the properties and uses of the hyper-Wiener index have received a lot of attention. Feng et al. [4] studied hyper-Wiener indices of graphs with given matching number. Feng et al. [5] researched the hyper-Wiener index of unicyclic graphs. Feng et al. [6] discussed the hyper-Wiener index of bicyclic graphs. Feng et al. [7] studied the hyper-Wiener index of graphs with given bipartition. Xu et al. [8] discussed Hyper-Wiener index of graphs with cut edges. Liu et al. [9] determined trees with the seven smallest and fifteen greatest hyper-Wiener indices. Yu et al. [10] studied the hyper-Wiener index of trees with given parameters. Gutman [11] obtained the relation between hyper-Wiener and Wiener index. Cai et al. [12] studied the hyper-Wiener index of trees of order n with diameter d.

A unicyclic graph is a connected graph with n vertices and n edges. Let $\mathscr{U}_{n,d}$ be the set of all unicyclic graphs order n with diameter d. Obviously, $d \le n-2$. And if $d=1$, $G \cong C_3$. Therefore, in the following, we assume that $2 \le d \le n-2$. For the graphs in $\mathscr{U}_{n,d}$, some parameters, such as the spectral radius, spectral moments, energy, least eigenvalue of adjacency matrix, spectral radius of signless Laplacian et al., have been extensively studied [13–16]. Especially, in recent years Xu [17] characterized the smallest Hosoya index of unicyclic graphs with given diameter; Tan [18] investigated the minimum Wiener index of unicyclic graphs with a fixed diameter. Motivated by these articles, we will study the the minimum hyper-Wiener indices of unicyclic in the set $\mathscr{U}_{n,d}$ in this paper. Moreover, if $d \equiv 0 \pmod 2$ and $4 \le d \le n-3$, then the second minimum hyper-Wiener indices of special unicyclic graphs with girth 3 in the set $\mathscr{U}_{n,d}$ are characterized.

2. Lemmas

In this section, we list some lemmas which will be used to prove our main results.

Lemma 2.1 ([8]) *Let H, X and Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v_1 is a vertex of X, u_1 is a vertex of Y. Let G be the graph obtained from*

H, X and Y by identifying v with v_1 and u with u_1, respectively. Let G_1 be the graph obtained from H, X and Y by identifying three vertices v, v_1 and u_1, and let G_2 be the graph obtained from H, X and Y by identifying three vertices u, v_1 and u_1. Then we have

$$WW(G_1) < WW(G) \;\text{ or }\; WW(G_2) < WW(G).$$

Let G_1, G_2 be two connected graphs with $V(G_1) \cap V(G_2) = \{v\}$. Denote G_1vG_2 to be a graph with $V(G_1) \cup V(G_2)$ as its vertex set and $E(G_1) \cup E(G_2)$ as its edge set. We have the following result.

Lemma 2.2 ([8]) *Let H be a connected graph, T_m be a tree of order m, and $V(H) \cap V(T_m) = \{v\}$. Then*

$$WW(HvT_m) \geq WW(HvS_m),$$

and equality holds if and only if $HvT_m \cong HvS_m$, where v is the center of star S_m.

Lemma 2.3 ([6]) *Let G be a connected graph of order n, v be a pendant vertex of G, and $vw \in E(G)$. Then*

(1) $W(G) = W(G - v) + D_{G-v}(w) + n - 1$;

(2) $S(G) = S(G - v) + DD_{G-v}(w) + 2D_{G-v}(w) + n - 1$.

By Lemma 2.3 and the definition of hyper-Wiener index, we have the following result.

Corollary 2.4 *Let G be a connected graph of order n, v be a pendant vertex of G and $vw \in E(G)$. Then*

$$WW(G) = WW(G - v) + \frac{1}{2}DD_{G-v}(w) + \frac{3}{2}D_{G-v}(w) + n - 1.$$

Lemma 2.5 ([7]) *Let G and H be two connected graphs with $u, v \in V(G)$ and $w \in V(H)$. Let GuH (GvH, respectively) be the graph obtained from G and H by identifying u (v, respectively) with w. If $D_G(u) < D_G(v)$ and $DD_G(u) < DD_G(v)$, then $WW(GuH) < WW(GvH)$.*

Lemma 2.6 *Let G be a connected graph on $n \geq 2$ vertices and $uv \in E(G)$. Let $G^*_{k,l}$ be the graph obtained from G by attaching two new paths $P : uu_1u_2\cdots u_k$ and $Q : vv_1v_2\cdots, v_l$ of length k and l at u, v, respectively, where $u_1, \ldots, u_k$ and $v_1, \ldots, v_l$ are distinct new vertices. Let $G^*_{k+1,l-1} = G^*_{k,l} - v_{l-1}v_l + u_kv_l$. If $k \geq l \geq 1$, then*

$$WW(G^*_{k,l}) \leq WW(G^*_{k+1,l-1}).$$

Proof Let $V_0 = V(G)\backslash\{u, v\}$, $V_1 = \{w_i | w_i \in V_0, d(w_i, u) = d(w_i, v) - 1\}$, $V_2 = \{w_i | w_i \in V_0, d(w_i, u) = d(w_i, v) + 1\}$, $V_3 = \{w_i | w_i \in V_0, d(w_i, u) = d(w_i, v)\}$, then $V_0 = V_1 \cup V_2 \cup V_3$. By Corollary 2.4,

$$\begin{aligned} WW(G^*_{k+1,l-1}) =& WW(G^*_{k,l-1}) + \frac{1}{2}DD_{G^*_{k,l-1}}(u_k) + \frac{3}{2}D_{G^*_{k,l-1}}(u_k) + n + k + l - 1 \\ =& WW(G^*_{k,l-1}) + \frac{1}{2}\Big(\sum_{w_i \in V_0} d^2(w_i, u_k) + \sum_{w_i \in V(G^*_{k,l-1})\backslash V_0} d^2(w_i, u_k)\Big) + \end{aligned}$$

$$
\begin{aligned}
&\frac{3}{2}\Big(\sum_{w_i\in V_0} d(w_i,u_k)+\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,u_k)\Big)+n+k+l-1\\
=&WW(G^*_{k,l-1})+\frac{1}{2}\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d^2(w_i,u_k)+\frac{3}{2}\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,u_k)+\\
&\frac{1}{2}\Big(\sum_{w_i\in V_1} d^2(w_i,u_k)+\sum_{w_i\in V_2} d^2(w_i,u_k)+\sum_{w_i\in V_3} d^2(w_i,u_k)\Big)+\\
&\frac{3}{2}\Big(\sum_{w_i\in V_1} d(w_i,u_k)+\sum_{w_i\in V_2} d(w_i,u_k)+\sum_{w_i\in V_3} d(w_i,u_k)\Big)+n+k+l-1.
\end{aligned}
$$

$$
\begin{aligned}
WW(G^*_{k,l})=&WW(G^*_{k,l-1})+\frac{1}{2}DD_{G^*_{k,l-1}}(v_{l-1})+\frac{3}{2}D_{G^*_{k,l-1}}(v_{l-1})+n+k+l-1\\
=&WW(G^*_{k,l-1})+\frac{1}{2}\Big(\sum_{w_i\in V_0} d^2(w_i,v_{l-1})+\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d^2(w_i,v_{l-1})\Big)+\\
&\frac{3}{2}\Big(\sum_{w_i\in V_0} d(w_i,v_{l-1})+\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,v_{l-1})\Big)+n+k+l-1\\
=&WW(G^*_{k,l-1})+\frac{1}{2}\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d^2(w_i,v_{l-1})+\frac{3}{2}\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,v_{l-1})+\\
&\frac{1}{2}\Big(\sum_{w_i\in V_1} d^2(w_i,v_{l-1})+\sum_{w_i\in V_2} d^2(w_i,v_{l-1})+\sum_{w_i\in V_3} d^2(w_i,v_{l-1})\Big)+\\
&\frac{3}{2}\Big(\sum_{w_i\in V_1} d(w_i,v_{l-1})+\sum_{w_i\in V_2} d(w_i,v_{l-1})+\sum_{w_i\in V_3} d(w_i,v_{l-1})\Big)+n+k+l-1.
\end{aligned}
$$

Obviously,

$$\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,u_k)=\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d(w_i,v_{l-1}),$$

$$\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d^2(w_i,u_k)=\sum_{w_i\in V(G^*_{k,l-1})\backslash V_0} d^2(w_i,v_{l-1}),$$

$$\sum_{w_i\in V_1} d(w_i,u_k)\ge\sum_{w_i\in V_1} d(w_i,v_{l-1}),\ \sum_{w_i\in V_1} d^2(w_i,u_k)\ge\sum_{w_i\in V_1} d^2(w_i,v_{l-1}),$$

$$\sum_{w_i\in V_2} d(w_i,u_k)\ge\sum_{w_i\in V_2} d(w_i,v_{l-1}),\ \sum_{w_i\in V_2} d^2(w_i,u_k)\ge\sum_{w_i\in V_2} d^2(w_i,v_{l-1}),$$

$$\sum_{w_i\in V_3} d(w_i,u_k)\ge\sum_{w_i\in V_3} d(w_i,v_{l-1}),\ \sum_{w_i\in V_3} d^2(w_i,u_k)\ge\sum_{w_i\in V_3} d^2(w_i,v_{l-1}).$$

So, $WW(G^*_{k,l})\le WW(G^*_{k+1,l-1})$. $\square$

Lemma 2.7 ([12]) *Let $P=v_0v_1\cdots v_d$ be a path of order $d+1$. Then*

$$D_P(v_j)=\frac{2j^2-2dj+d^2+d}{2},$$

and

$$DD_P(v_j)=\frac{6j^2+6dj^2-6d^2j-6dj+2d^3+3d^2+d}{6},$$

for $1 \le j \le d-1$. Moreover, if $1 \le i < j \le \frac{d}{2}$, $D_P(v_i) > D_P(v_j)$, and $DD_P(v_i) > DD_P(v_j)$; if $\frac{d}{2} \le i < j \le (d-1)$, $D_P(v_i) < D_P(v_j)$, and $DD_P(v_i) < DD_P(v_j)$.

3. Conclusions

In this section, we will give the minimum hyper-Wiener index in the set $\mathscr{U}_{n,d}$ $(2 \le d \le n-2)$. For any graph $G \in \mathscr{U}_{n,d}$, a path with length d of G is called the diametrical path of G, the only cycle of G is called a unique cycle of G. Note that the number of diametrical paths in $\mathscr{U}_{n,d}$ is possibly more than one. The following propositions present some properties of graphs from $\mathscr{U}_{n,d}$ with the smallest hyper-Wiener index.

Proposition 3.1 *Let $G \in \mathscr{U}_{n,d}$ such that $WW(G)$ is as small as possible. Let C_g be a unique cycle of G, then there exists a diametrical path P_{d+1} of G such that $V(C_g) \cap V(P_{d+1}) \neq \varnothing$.*

Proof If $V(C_g) \cap V(P_{d+1}) = \varnothing$, since G is connected, there exists an only path

$$P = v_i v_k v_{k+1} \cdots v_{l-1} v_l$$

connecting C_g and P_{d+1}, where $v_i \in V(C_g), v_l \in V(P_{d+1})$ and $v_k, \dots, v_{l-1} \in V(G) \backslash (V(C_g) \cup V(P_{d+1}))$. Let $u_1, \dots, u_p \in N_G(v_l) \backslash \{v_{l-1}\}, p = d(v_l)-1, w_1, \dots, w_q \in N_G(v_i) \backslash \{v_k\}$, $q = d(v_i)-1$ and $G_1 = G - v_l u_1 - \cdots - v_l u_p + v_i u_1 + \cdots + v_i u_p$, $G_2 = G - v_i w_1 - \cdots v_i w_q + v_l w_1 + \cdots + v_l w_q$. Thus by Lemma 2.1, $WW(G_1) < WW(G)$ or $WW(G_2) < WW(G)$, a contradiction. $\Box$

Proposition 3.2 *Let $G \in \mathscr{U}_{n,d}$ such that $WW(G)$ is as small as possible. Let C_g be a unique cycle of G and P_{d+1} be a diametrical path of G. Then for $v \in V(G) \backslash (V(C_g) \cup V(P_{d+1}))$, $d(v) = 1$ and they are adjacent to the same vertex in $V(C_g) \cup V(P_{d+1})$.*

Proof By Lemmas 2.1 and 2.2, we have for $v \in V(G) \setminus (V(C_g) \cup V(P_{d+1}))$, $d(v) = 1$ and they are adjacent to the same vertex in $V(P_{d+1})$. $\Box$

By Proposition 3.1, denote

$$C_g = v_k v_{k+1} \cdots v_{l-1} v_l v_{d+2} v_{d+3} \cdots v_s v_k, \quad s \ge d+2,$$

where

$$\{v_k, v_{k+1}, \dots, v_{l-1}, v_l\} = V(C_g) \cap V(P_{d+1}) \text{ and } \{v_{d+2}, v_{d+3}, \dots, v_s\} = V(C_g) \setminus V(P_{d+1}).$$

Proposition 3.3 *Let $G \in \mathscr{U}_{n,d}$ such that $WW(G)$ is as small as possible. Let $P = v_1 v_2 \cdots v_k v_{k+1} \cdots v_d v_{d+1}$ $(d(v_1) = 1)$ be the diametrical path and C_g the unique cycle of G. Then*

(i) $k \neq l$.

(ii) If $l = k+1$, then $s - d = 2$; and if $l \ge k+2$, then $s - d = l - k$.

Proof (i) If $k = l$, then $s \ge d+3$ and $k \neq 1, d+1$. Denote $u_1, \dots, u_p \in N_G(v_{d+2}) \backslash \{v_k\}, p = d(v_{d+2}) - 1$. Let $G^* = G - v_{d+2} u_1 - \cdots - v_{d+2} u_p + v_{k+1} u_1 + \cdots + v_{k+1} u_p$, $G^* \in \mathscr{U}_{n,d}$. Denote $V_1 = \{v_i : v_i \in C_g \backslash \{v_k\}, d(v_i, v_{d+2}) < d(v_i, v_k) + 1\}$, $V_2 = \{v_j : v_j \in (\bigcup_{v_i \in V_1} N_G(v_i)) \backslash V(C_g)\}$.

Then for any $v \in V_1 \bigcup V_2$,

$$d_{G^*}(v, v_{d+2}) - d_G(v, v_{d+2}) = 2,$$
$$d^2_{G^*}(v, v_{d+2}) - d^2_G(v, v_{d+2}) = 4d_G(v, v_{d+2}) + 4 \leq 4d_G(v, v_k) + 4 = 4d_G(v, v_{k+2}) - 4,$$
$$d_{G^*}(v, v_{k+1}) - d_G(v, v_{k+1}) = -2,\ d^2_{G^*}(v, v_{k+1}) - d^2_G(v, v_{k+1}) = -4d_G(v, v_{k+1}) + 4 < 0,$$
$$d_{G^*}(v, v_{k+2}) - d_G(v, v_{k+2}) = -2.\ d^2_{G^*}(v, v_{k+2}) - d^2_G(v, v_{k+2}) = -4d_G(v, v_{k+2}) + 4.$$

The distance between all other vertices is unchanged or reduced. So, $WW(G^*) < WW(G)$, a contradiction.

(ii) Otherwise, since $s - d > l - k$, we have $s - d \geq 3$. Thus v_{s-1} exists. Denote $u_1, \ldots, u_p \in N_G(v_{d+2})\backslash\{v_l\}, p = d(v_{d+2}) - 1$,

Let $G^* = G - v_{d+2}u_1 - \cdots - v_{d+2}u_p + v_lu_1 + \cdots + v_lu_p$, $G^* \in \mathscr{U}_{n,d}$. Denote $V_1 = \{v_i : v_i \in C_g\backslash\{v_k, \ldots, v_l\}, d(v_i, v_{d+2}) < d(v_i, v_l) + 1\}$, $V_2 = \{v_j : v_j \in (\bigcup\limits_{v_i \in V_1} N_G(v_i))\backslash V(C_g)\}$. Then for any $v \in V_1 \bigcup V_2$,

$$d_{G^*}(v, v_{d+2}) - d_G(v, v_{d+2}) = 1,$$
$$d^2_{G^*}(v, v_{d+2}) - d^2_G(v, v_{d+2}) = 2d_G(v, v_{d+2}) + 1 \leq 2d_G(v, v_l) + 1,$$
$$d_{G^*}(v, v_l) - d_G(v, v_l) = -1,$$
$$d^2_{G^*}(v, v_l) - d^2_G(v, v_l) = -2d_G(v, v_l) + 1,$$
$$d_{G^*}(v_{d+3}, v_{l-1}) - d_G(v_{d+3}, v_{l-1}) = -1,$$
$$d^2_{G^*}(v_{d+3}, v_{l-1}) - d^2_G(v_{d+3}, v_{l-1}) = -2d_G(v_{d+3}, v_{l-1}) + 1 = -5.$$

The distance between all other vertices is unchanged or reduced. So, $WW(G^*) < WW(G)$, a contradiction. $\Box$

Let U_0 be the unicyclic graph of order $d+2$ shown in Figure 1. Let $U_0(n_2, \ldots, n_d, n_{d+2})$ be a graph of order n obtained from U_0 by attaching n_i pendant vertices to each $v_i \in V(U_0)\backslash\{v_1, v_{d+1}\}$, respectively, where $n_{d+2} = 0$ when $k = 1$ or $k = d$. Denote $\tilde{\mathscr{U}}_{n,d} = \{U_0(n_2, \ldots, n_d, n_{d+2}) : \sum_{i=2}^{d} n_i + n_{d+2} = n - d - 2\}$ and $\bar{\mathscr{U}}_{n,d} = \{U_0(0, \ldots, 0, n_i, 0, \ldots, 0) : n_i \geq 0\}$.

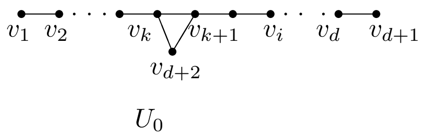

Figure 1 Graph U_0

By Lemma 2.1, we have the following result.

Proposition 3.4 *Let $G \in \tilde{\mathscr{U}}_{n,d}\backslash\bar{\mathscr{U}}_{n,d}$. Then there is a graph $G^* \in \bar{\mathscr{U}}_{n,d}$ such that $WW(G^*) < WW(G)$.*

Let $\triangle(n, d)$ be a graph of order n obtained from a triangle C_3 by attaching $n - d - 2$ pendant edges and a path of length $\lceil \frac{d}{2} \rceil$ at one vertex of the triangle C_3, and a path of length $\lceil \frac{d}{2} \rceil - 1$ to another vertex of the triangle C_3, respectively. Let $\nabla(n, d)$ be a graph of order n obtained from a triangle C_3 by attaching $n-d-2$ pendant edges and a path of length $\lceil \frac{d}{2} \rceil - 1$ at one vertex of the triangle C_3, and a path of length $\lceil \frac{d}{2} \rceil$ to another vertex of the triangle C_3, respectively. Note that if $d = n-2$ or $d \equiv 1 \pmod 2$, then $\triangle(n,d) \cong \nabla(n,d)$.

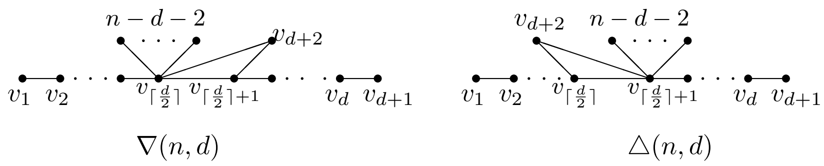

Figure 2 Graphs $\nabla(n,d)$ and $\triangle(n,d)$

Proposition 3.5 *Let $\nabla(n,d)$ and $\triangle(n,d)$ be the above two graphs shown in Figure 2. Suppose that $4 \le d \le n-3$ and $d \equiv 0 \pmod 2$. Then $WW(\triangle(n,d)) < WW(\nabla(n,d))$.*

Proof By Corollary 2.4,

$$WW(\triangle(n,d)) = WW(\triangle(n,d) - v_{d+1}) + \frac{1}{2} DD_{\triangle(n,d)-v_{d+1}}(v_d) + \frac{3}{2} D_{\triangle(n,d)-v_{d+1}}(v_d) + n - 1,$$

$$WW(\nabla(n,d)) = WW(\nabla(n,d) - v_{d+1}) + \frac{1}{2} DD_{\nabla(n,d)-v_{d+1}}(v_d) + \frac{3}{2} D_{\nabla(n,d)-v_{d+1}}(v_d) + n - 1.$$

Since $\triangle(n,d) - v_{d+1} \cong \nabla(n,d) - v_{d+1}$, so

$$\begin{aligned} WW(\triangle(n,d)) - WW(\nabla(n,d)) =& \frac{1}{2}(DD_{\triangle(n,d)-v_{d+1}}(v_d)) - DD_{\nabla(n,d)-v_{d+1}}(v_d) + \\ & \frac{3}{2}(D_{\triangle(n,d)-v_{d+1}}(v_d) - D_{\nabla(n,d)-v_{d+1}}(v_d)) \\ =& -\frac{1}{2}(d+1)(n-d-2) - \frac{3}{2}(n-d-2) \\ =& -(\lceil \frac{d}{2} \rceil + 2)(n-d-2) < 0. \quad \square \end{aligned}$$

Theorem 3.6 *Let $G \in \mathscr{U}_{n,2}$. Then $WW(G) \ge WW(\triangle(n,2)$, and equality holds if and only if (i) $n=4$, $G \cong C_4$ or $G \cong \triangle(4,2)$; (ii) $n=5$, $G \cong C_5$ or $G \cong \triangle(5,2)$; (iii) $n \ge 6$, $G \cong \triangle(n,2)$.*

Proof If $d=2$, then $G \cong C_4$, $G \cong C_5$ or $G \cong \triangle(n,2)$. $WW(C_4) = WW(\triangle(4,2)) = 20$. $WW(C_5) = WW(\triangle(5,2)) = 40$. The results hold for $d=2$. $\square$

Theorem 3.7 *For any graph $G \in \tilde{\mathscr{U}}_{n,d}$, $3 \le d \le n-2$, we have $WW(G) \ge WW(\triangle(n,d))$, and equality holds if and only if $G \cong \triangle(n,d)$.*

Proof Let $G \in \tilde{\mathscr{U}}_{n,d}$ such that the $WW(G)$ is as small as possible. Then by Lemma 2.1, $G \in \bar{\mathscr{U}}_{n,d}$. Let $N(v_i) \cap PV(G) = \{w_1, w_2, \ldots, w_{n_i}\}$ if $n_i > 0$, $P = v_1 v_2 \cdots v_k v_{k+1} \cdots v_d v_{d+1}$ be a path length d of G and $C = v_k v_{k+1} v_{d+2} v_k$ the only cycle of G. Since $\min\{d(v_1), d(v_{d+1})\} = 1$, we assume $d(v_1) = 1, k \ne 1$.

Claim 1. If $n_i > 0$, then $i \ne d+2$.

If $i = d+2$, let $G_1 = G - v_{d+2}w_1 - v_{d+2}w_2 - \cdots - v_{d+2}w_{n_i} + v_k w_1 + v_k w_2 + \cdots + v_k w_{n_i}$, $G_2 = G - v_{k-1}v_k + v_{d+2}v_{k-1}$. Then $G_1, G_2 \in \bar{\mathscr{U}}_{n,d}$. By Lemma 2.1, we have $WW(G_1) < WW(G)$ or $WW(G_2) < WW(G)$, a contradiction.

Claim 2. If $n_i > 0$, then $i \in \{k, k+1\}$.

Assume to the contrary. According to symmetry, we consider the case $v_i \in V(P)\backslash V(C)$ and $i > k+1$.

Case 1. If $i-1 > d+1-i$.

Let $G^* = G - v_i w_1 - v_i w_2 - \cdots - v_i w_{n_i} + v_{i-1} w_1 + v_{i-1} w_2 + \cdots + v_{i-1} w_{n_i}$, $G^* \in \bar{\mathscr{U}}_{n,d}$.

$$\begin{aligned}
&2(WW(G^*) - WW(G))\\
&\quad = (d-i+3-i+(i-k)-(i-k+1)+(d-i+3)^2-i^2+(i-k)^2-(i-k+1)^2)n_i\\
&\quad < (d-i+3-i+(i-k)-(i-k+1)+(d-i+3)^2-i^2)n_i\\
&\quad = (d+1-i-(i-1))+(d+1-i-(i-2))(d+3)n_i < 0,
\end{aligned}$$

a contradiction.

Case 2. If $i-1 \le d+1-i$.

Since $i-1 \le d+1-i$, then $k < i-1 \le d+1-i < d+1-k-1 = d-k$.

Let $G^* = G - v_k v_{d+2} + v_{k+2} v_{d+2}$, $G^* \in \bar{\mathscr{U}}_{n,d}$.

$$\begin{aligned}
&2(WW(G) - WW(G^*))\\
&\quad = -(k+1)+d-k+1+n_i-(k+1)^2+(d-k+1)^2+n_i((i-k)^2-(i-k-1)^2\\
&\quad = d-k-k+n_i+(d+2)(d-k-k)+n_i((i-k)^2-(i-k-1)^2\\
&\quad > d-k-k+(d+2)(d-k-k) > 0,
\end{aligned}$$

a contradiction.

Combining Cases 1 and 2, if $G \in \bar{\mathscr{U}}_{n,d}$ and $WW(G)$ is as small as possible, then $i \in \{k, k+1\}$.

Claim 3. $k \ne d$.

If $k = d$, let $G^* = G - v_{d+1} v_{d+2} + v_{d-1} v_{d+2}$, $G^* \in \bar{\mathscr{U}}_{n,d}$.

$2(WW(G^*) - WW(G)) = -d + 2 - d^2 + 4 < 0$, a contradiction.

Claim 4. $k = \lceil \frac{d}{2} \rceil$.

If $k < \lceil \frac{d}{2} \rceil$, let $G^* = G - v_d v_{d+1} + v_1 v_{d+1}$. If $k > \lceil \frac{d}{2} \rceil$, let $G^* = G - v_1 v_2 + v_{d+1} v_1$. In all cases, $G^* \in \bar{\mathscr{U}}_{n,d}$. By Lemma 2.6, $WW(G^*) \le WW(G)$, a contradiction.

By Claims 1–4, $G \in \{\triangle(n,d)), \nabla(n,d)\}$. By Proposition 3.4, our result holds. $\Box$

By Proposition 3.5, we have the following result.

Theorem 3.8 *For $G \in \bar{\mathscr{U}}_{n,d} \backslash \triangle(n,d)$ with $d \equiv 0 \pmod 2$ and $4 \le d \le n-3$, we have $WW(G) \ge WW(\nabla(n,d))$ and equality holds if and only if $G \cong \nabla(n,d)$.*

Let n, m and d be integers with $3 \le d \le n-2$. For $a \ge b \ge 0$ and $a \ge 1$, let $U^x_{n,2m,d}(a,b)$ be the unicyclic graph obtained from the cycle $C_{2m} = a_0 a_1 \cdots a_{2m-1} a_0$ by attaching a path P_{a+1} to a_0 and a path P_{b+1} to a_m, respectively, where $a+b = d-m$, and attaching $l = n-d-m$ pendent vertices $w_1, w_2, \ldots, w_l$ to the vertex x, where $x \in \{v_{a-1}, \ldots, v_1, a_0, a_1, \ldots, a_m, u_1, u_2, \ldots, u_{b-1}\}$. Denote $U^i_{n,2m,d}(a,b) = U^x_{n,2m,d}(a,b), x \in \{a_0, a_1, \ldots, a_{\lfloor \frac{m}{2} \rfloor}\}$.

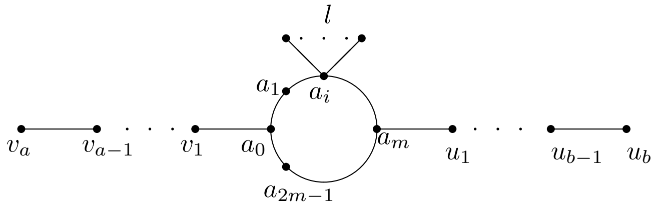

Figure 3 Graphs $U^i_{n,2m,d}(a,b)$

Proposition 3.9 *Let $G \in U^x_{n,2m,d}(a,b)$ such that $WW(G)$ is as small as possible. Then $x \notin \{u_1, u_2, \dots, u_{b-1}\}$.*

Proof Otherwise, if $x = u_j$ $(1 \le j \le b-1)$, let $G_1 = G - xw_1 - xw_2 - \cdots - xw_l$, $G^* = G - xw_1 - xw_2 - \cdots - xw_l + a_m w_1 + a_m w_2 + \cdots + a_m w_l$. By Lemma 2.7, let $k_1 = a + m + j$, $k_2 = a + m$, $d = a + m + b$. So

$$\begin{aligned} D_{G_1}(u_j) - D_{G_1}(a_m) =& k_1^2 - dk_1 - k_2^2 + dk_2 + (m-1)j \\ =& j(m + j + a - b) + (m-1)j > 0, \\ DD_{G_1}(v_j) - DD_{G_1}(a_m) =& (d+1)(k_1 - d)k_1 + (j+1)^2 + (j+2)^2 + \cdots + \\ & (j + m - 1)^2 - ((d+1)(k_2 - d)k_2 + 1^2 + 2^2 + \cdots + (m-1)^2) \\ =& (a + m + b + 1)j(m + j + a - b) + (m-1)j^2 + m(m-1)j > 0. \end{aligned}$$

By Lemma 2.5, $WW(G^*) < WW(G)$ a contradiction. □

Proposition 3.10 *Let $G \in U^x_{n,2m,d}(a,b)$ such that $WW(G)$ is as small as possible. Then $x \notin \{v_1, v_2, \dots, v_{a-1}\}$.*

Proof Otherwise, let $x = v_i$ $(1 \le i \le a-1)$. If $m + b > a$, let $G_1 = G - xw_1 - xw_2 - \cdots - xw_l$, $G^* = G - xw_1 - xw_2 - \cdots - xw_l + a_0 w_1 + a_0 w_2 + \cdots + a_0 w_l$. By Lemma 2.7, let $k_1 = a - i$, $k_2 = a$, $d = a + m + b$. So

$$\begin{aligned} D_{G_1}(v_i) - D_{G_1}(a_0) =& k_1^2 - dk_1 - k_2^2 + dk_2 + (m-1)i = -i(2a - i - d) + (m-1)i \\ =& (m - 1 + m - a + b + i)i > 0, \\ DD_{G_1}(v_i) - DD_{G_1}(a_0) =& (d+1)(k_1 - d)k_1 + (i+1)^2 + (i+2)^2 + \cdots + \\ & (i + m - 1)^2 - ((d+1)(k_2 - d)k_2 + 1^2 + 2^2 + \cdots + (m-1)^2) \\ =& (-2a + d + i)i(1 + d) + (m-1)i^2 + m(m-1)i \\ =& (m - a + b + i)i(1 + d) + (m-1)i^2 + m(m-1)i > 0. \end{aligned}$$

By Lemma 2.5, $WW(G^*) < WW(G)$, a contradiction.

If $m+b \le a$, let $G^* = G - v_i w_1 - v_i w_2 - \cdots - v_i w_l + v_{i-1} w_1 + v_{i-1} w_2 + \cdots + v_{i-1} w_l - v_a v_{a-1} + u_b v_a$. Since $d_G(w_i, a_j) - d_{G^*}(w_i, a_j) = 1$ $(i = 1, 2, \dots, r, j = m+1, m+2, \dots, 2m-1)$,

$$\begin{aligned} & \sum_{j=m+1}^{2m-1} d_G(v_a, a_j) - \sum_{j=m+1}^{2m-1} d_{G^*}(v_a, a_j) \\ & = (a + 1 + a + 2 + \cdots + a + m - 1) - ((b+1) + 1 + (b+1) + 2 + \cdots + (b+1) + m - 1)) \end{aligned}$$

$$= (a-b-1)(m-1) > 0.$$

$$\sum_{j=m+1}^{2m-1} d_G^2(v_a, a_j) - \sum_{j=m+1}^{2m-1} d_{G^*}^2(v_a, a_j)$$
$$= ((a+1)^2 + (a+2)^2 + \cdots + (a+m-1)^2) - (((b+1)+1)^2 +$$
$$((b+1)+2)^2 + \cdots + ((b+1)+m-1))^2)$$
$$= (a-b-1)(m-1)(a+b+1+m) > 0.$$

So

$$2WW(G) - 2WW(G^*) = \sum_{i,j}(d_G(w_i, a_j) - d_{G^*}(w_i, a_j)) + \sum_{j=m+1}^{2m-1} d_G(v_a, a_j) - \sum_{j=m+1}^{2m-1} d_{G^*}(v_a, a_j) + \sum_{i,j}(d_G^2(w_i, a_j) - d_{G^*}^2(w_i, a_j)) + \sum_{j=m+1}^{2m-1} d_G^2(v_a, a_j) - \sum_{j=m+1}^{2m-1} d_{G^*}^2(v_a, a_j) > 0,$$

a contradiction.

The result holds. □

Proposition 3.11 *Let $G \in U_{n,2m,d}^x(a,b)$ such that $WW(G)$ is as small as possible. If $a = b$, then $x = a_{\lfloor \frac{m}{2} \rfloor}$. If $a > b$, then $x \notin \{a_{\lfloor \frac{m}{2} \rfloor + 1}, \ldots, a_m\}$.*

Proof Let $G_1 = G - xw_1 - xw_2 - \cdots - xw_l$, $0 \le i \le m$,

$D_{G_1}(a_i) = (i+1+i+2+\cdots+i+a) + (m-i+1+m-i+2+\cdots+m-i+b) + (1+2+\cdots+m+1+2+\cdots+m-1) = (a-b)i + mb + \frac{a(a+1)}{2} + \frac{b(b+1)}{2} + m^2$.

$DD_{G_1}(a_i) = ((i+1)^2 + (i+2)^2 + \cdots + (i+a)^2) + ((m-i+1)^2 + (m-i+2)^2 + \cdots + (m-i+b)^2) + (1^2 + 2^2 + \cdots + m^2 + 1^2 + 2^2 + \cdots + (m-1)^2) = (a+b)i^2 + a(a+1)i - b(b+1)i - 2mbi + bm^2 + mb(b+1) + \frac{a(a+1)(2a+1)}{6} + \frac{b(b+1)(2b+1)}{6} + \frac{m(2m^2+1)}{3}$.

$D_{G_1}(a_i) - D_{G_1}(a_j) = (a-b)(i-j)$.

$DD_{G_1}(a_i) - DD_{G_1}(a_j) = ((a+b)(i+j) + a(a+1) - b(b+1) - 2mb)(i-j)$.

If $a = b$, $\lfloor \frac{m}{2} \rfloor \ge i > j \ge 1$, $D_{G_1}(a_i) = D_{G_1}(a_j), DD_{G_1}(a_i) - DD_{G_1}(a_j) = 2b(i+j-m)(i-j) < 0$, $m \ge i > j \ge \lfloor \frac{m}{2} \rfloor$, $D_{G_1}(a_i) = D_{G_1}(a_j), DD_{G_1}(a_i) - DD_{G_1}(a_j) = 2b(i+j-m)(i-j) > 0$. So, if $a = b$, then $x = a_{\lfloor \frac{m}{2} \rfloor}$.

If $a > b, m \ge i > j \ge \lfloor \frac{m}{2} \rfloor$, $D_{G_1}(a_i) > D_{G_1}(a_j), DD_{G_1}(a_i) > DD_{G_1}(a_j)$. By Lemma 2.5, $x \notin \{a_{\lfloor \frac{m}{2} \rfloor + 1}, \ldots, a_m\}$. □

By Theorem 3.7, Propositions 3.9–3.11, we have the following result.

Theorem 3.12 *Let G be a graph in $\mathscr{U}_{n,d}$ $(3 \le d \le n-2)$ having the minimum hyper-Wiener index. Then $G \cong \triangle(n,d)$ or $G \cong U_{n,2m,d}^i(a,b)$.*

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