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Trees with the seven smallest and fifteen greatest hyper-Wiener indices *

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Abstract: Gutman had determined the trees on n vertices with the smallest and the greatest hyper-Wiener index (i.e., the star and path). In this paper, we identify the second up to seventh smallest hyper-Wiener indices of trees on $n \geq 17$ vertices and the second up to fifteenth greatest hyper-Wiener indices of trees on $n \geq 20$ vertices.

1 Introduction

Throughout this paper, we only concern with connected, undirected simple graphs. If $G = (V, E)$ with $|V| = n$ and $|E| = m$, then we refer to G as an (n, m) graph. Let $N(u)$ be the first neighbor vertex set of u, then $d(u) = |N(u)|$ is called the degree of u. Specially, $\Delta = \Delta(G)$ is called the *maximum degree* of vertices of G. As usual, P_n and $K_{1,n-1}$ denotes the path and star of order n, respectively.

The *distance* $d(u, v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v. Sometimes we write $d_G(u, v)$ in place of $d(u, v)$ in order to indicate the dependence on G. Let $\gamma(G, k)$ denote the number of vertex pairs of G, the distance of which is equal to k. There are

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two important graph-based structure-descriptors, called Wiener index and hyper-Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ is denoted by [1]

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \sum_{k\geq 1} k\gamma(G,k),$$

and the *hyper-Wiener index* $WW(G)$ is defined as [2]

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^2 = \frac{1}{2}\sum_{k\geq 1} k(k+1)\gamma(G,k).$$

It is well-known that the Wiener index is introduced long time ago [1], whereas the hyper-Wiener index is conceived somewhat later [2]. But it rapidly gained popularity and numerous results on it were raised [3-7]. The mathematical properties of hyper-Wiener index and its applications in chemistry can be referred to [5-10] and the references cited therein.

Gutman et al. firstly gave a partial order to Wiener index among the starlike trees in [11]. After then, the first up to fifteenth smallest and the first up to seventeenth greatest Wiener indices among trees of order n are identified in [12] and [13], respectively. Also, Gutman considered the similar order of hyper-Wiener index among trees of order n, and he had determined the trees on n vertices with the smallest and greatest hyper-Wiener index (i.e., the star and path) in [14]. Recently, among all connected graphs of order n ($n > 2k$), the first up to $(k+1)$-th smallest Wiener indices and the first up to $(k+1)$-th smallest hyper-Wiener indices are determined in [15], respectively. In this paper, we identify the second up to seventh smallest hyper-Wiener indices of trees on $n \geq 17$ vertices and the second up to fifteenth greatest hyper-Wiener indices of trees on $n \geq 20$ vertices.

2 Some preliminaries

Given a simple and undirected graph $G = (V, E)$. Let $G - u$ (resp. $G - uv$) denote the graph obtained from G by deleting the vertex $u \in V(G)$ (resp. the edge $uv \in E(G)$). Similarly, $G + uv$ is a graph obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.

Suppose v is a vertex of graph G. As shown in Fig. 1, let $G_{k,l}$ ($l \geq k \geq 1$) be the graph obtained from G by attaching two new paths P: $v(= v_0)v_1v_2\cdots v_k$ and Q:

$v(=u_0)u_1u_2\cdots u_l$ of length k and l, respectively, at v, where v_1, v_2, ..., v_k and u_1, u_2, ..., u_l are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$.

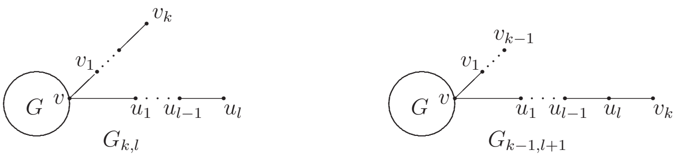

Fig. 1.

Lemma 2.1 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $l \geq k \geq 1$, then $W(G_{k,l}) \leq W(G_{k-1,l+1})$, the equality holds if and only if G is an isolated vertex.*

Proof. It is easy to see that

$$W(G_{k-1,l+1}) - W(G_{k,l}) = \sum_{w \in V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(w, v_k) - \sum_{w \in V(G_{k,l})} d_{G_{k,l}}(w, v_k). \quad (1)$$

Let $V_1 = V(G) \setminus \{v\}$, then $V(G_{k,l}) \setminus V_1 = V(G_{k-1,l+1}) \setminus V_1$. Let $V_2 = V(G_{k,l}) \setminus V_1$. Clearly,

$$\sum_{w \in V(G_{k,l})} d_{G_{k,l}}(w, v_k) = \sum_{w \in V_1} d_{G_{k,l}}(w, v_k) + \sum_{w \in V_2} d_{G_{k,l}}(w, v_k). \quad (2)$$

$$\sum_{w \in V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(w, v_k) = \sum_{w \in V_1} d_{G_{k-1,l+1}}(w, v_k) + \sum_{w \in V_2} d_{G_{k-1,l+1}}(w, v_k). \quad (3)$$

Note that the subgraph of $G_{k,l}$ induced by V_2 is a path of length $k+l$, which is isomorphic to the subgraph of $G_{k-1,l+1}$ induced by V_2, thus

$$\sum_{w \in V_2} d_{G_{k,l}}(w, v_k) = \sum_{w \in V_2} d_{G_{k-1,l+1}}(w, v_k). \quad (4)$$

Therefore, by combining equalities (1)-(4), we have

$$W(G_{k-1,l+1}) - W(G_{k,l}) = \sum_{w \in V_1} d_{G_{k-1,l+1}}(w, v_k) - \sum_{w \in V_1} d_{G_{k,l}}(w, v_k)$$

$$= \sum_{w \in V_1} (d_{G_{k-1,l+1}}(w, v_k) - d_{G_{k,l}}(w, v_k)). \quad (5)$$

If G is an isolated vertex, then $V_1 = \emptyset$. By equality (5), it follows that $W(G_{k-1,l+1}) = W(G_{k,l})$. If G is not an isolated vertex, since $l \geq k$, then $d_{G_{k-1,l+1}}(w, v_k) > d_{G_{k,l}}(w, v_k)$ holds for every $w \in V_1$. Thus, the result follows from equality (5). ∎

Proposition 2.1 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $l \geq k \geq 1$, then $WW(G_{k,l}) \leq WW(G_{k-1,l+1})$, the equality holds if and only if G is an isolated vertex.*

Proof. As in the proof of Lemma 2.1, let $V_1 = V(G) \setminus \{v\}$, $V_2 = V(G_{k,l}) \setminus V_1$. It can be proved analogously with Lemma 2.1 that

$$\sum_{\{u,w\}\subseteq V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(u,w)^2 - \sum_{\{u,w\}\subseteq V(G_{k,l})} d_{G_{k,l}}(u,w)^2$$

$$= \sum_{w\in V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(w,v_k)^2 - \sum_{w\in V(G_{k,l})} d_{G_{k,l}}(w,v_k)^2$$

$$= \sum_{w\in V_1} d_{G_{k-1,l+1}}(w,v_k)^2 - \sum_{w\in V_1} d_{G_{k,l}}(w,v_k)^2 + \sum_{w\in V_2} d_{G_{k-1,l+1}}(w,v_k)^2 - \sum_{w\in V_2} d_{G_{k,l}}(w,v_k)^2$$

$$= \sum_{w\in V_1} (d_{G_{k-1,l+1}}(w,v_k)^2 - d_{G_{k,l}}(w,v_k)^2). \tag{6}$$

If G is not an isolated vertex, since $l \geq k$, then $d_{G_{k-1,l+1}}(w,v_k)^2 > d_{G_{k,l}}(w,v_k)^2$ holds for every $w \in V_1$. Recall that $WW(G_{k,l}) = \frac{1}{2}W(G_{k,l}) + \frac{1}{2}\sum_{\{u,w\}\subseteq V(G_{k,l})} d_{G_{k,l}}(u,w)^2$, and $WW(G_{k-1,l+1}) = \frac{1}{2}W(G_{k-1,l+1}) + \frac{1}{2}\sum_{\{u,w\}\subseteq V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(u,w)^2$, then the result follows from Lemma 2.1 and equality (6). ■

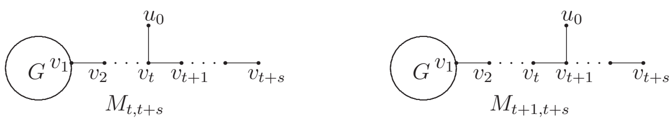

Fig. 2.

Suppose v_1 is a vertex of graph G, and v_2, ..., v_{t+s}, u_0 are distinct new vertices (not in G). Let G' be the graph obtained from G by attaching a new path P: $v_1v_2\cdots v_{t+s}$. Let $M_{t,t+s} = G' + v_tu_0$ and $M_{t+i,t+s} = G' + v_{t+i}u_0$, where $1 \leq i \leq s$. For instance, $M_{t,t+s}$ and $M_{t+1,t+s}$ are depicted in Fig. 2.

Lemma 2.2 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $t \geq s \geq 1$, then $W(M_{t,t+s}) \leq W(M_{t+1,t+s})$. Moreover, the equality holds if and only if $t = s$ and G is an isolated vertex.*

Proof. For convenience, sometimes we write $M_{t,t+s}$ as M, and $M_{t+1,t+s}$ as M' in the proof of this lemma. Let $V_1 = V(G) \setminus \{v_1\}$, then $V(M_{t,t+s}) \setminus V_1 = V(M_{t+1,t+s}) \setminus V_1$. Let $V_2 = V(M_{t,t+s}) \setminus V_1$. Thus,

$$W(M_{t+1,t+s}) - W(M_{t,t+s}) = \sum_{w \in V(M')} d_{M'}(w, u_0) - \sum_{w \in V(M)} d_M(w, u_0)$$

$$= \sum_{w \in V_1} (d_{M'}(w, u_0) - d_M(w, u_0)) + \sum_{w \in V_2} d_{M'}(w, u_0) - \sum_{w \in V_2} d_M(w, u_0). \quad (7)$$

Note that $d_{M'}(w, u_0) > d_M(w, u_0)$ holds for every $w \in V_1$, and

$$\sum_{w \in V_2} d_{M'}(w, u_0) - \sum_{w \in V_2} d_M(w, u_0) = t + 1 - (s + 1) = t - s \geq 0.$$

Thus, the result follows by equality (7). ■

Lemma 2.3 *suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $t \geq s \geq 1$, then $WW(M_{t,t+s}) \leq WW(M_{t+1,t+s})$. Moreover, the equality holds if and only if $t = s$ and G is an isolated vertex.*

Proof. As in the proof of Lemma 2.2, sometimes we write $M_{t,t+s}$ as M, and $M_{t+1,t+s}$ as M' for convenience. Let $V_1 = V(G) \setminus \{v_1\}$, and $V_2 = V(M_{t,t+s}) \setminus V_1$. By Lemma 2.2 and the definition of hyper-Wiener index, we only need to show that

$$\sum_{\{u,v\} \subseteq V(M')} d_{M'}(u, v)^2 \geq \sum_{\{u,v\} \subseteq V(M)} d_M(u, v)^2. \quad (8)$$

Clearly, $\sum_{\{u,v\} \subseteq V(M')} d_{M'}(u, v)^2 - \sum_{\{u,v\} \subseteq V(M)} d_M(u, v)^2$

$$= \sum_{w \in V(M')} d_{M'}(w, u_0)^2 - \sum_{w \in V(M)} d_M(w, u_0)^2$$

$$= \sum_{w \in V_1} (d_{M'}(w, u_0)^2 - d_M(w, u_0)^2) + \sum_{w \in V_2} d_{M'}(w, u_0)^2 - \sum_{w \in V_2} d_M(w, u_0)^2. \quad (9)$$

Note that $d_{M'}(w, u_0)^2 > d_M(w, u_0)^2$ holds for every $w \in V_1$, and

$$\sum_{w \in V_2} d_{M'}(w, u_0)^2 - \sum_{w \in V_2} d_M(w, u_0)^2 = (t + 1)^2 - (s + 1)^2 \geq 0.$$

Thus, inequality (8) follows by equality (9). This completes the proof. ■

By Lemma 2.3, we obtain the next result immediately.

Proposition 2.2 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $t \geq s \geq 1$, then $WW(M_{t,t+s}) \leq WW(M_{t+i,t+s})$, where $1 \leq i \leq s$.*

Recall that a vertex u of a tree T is called a *branching point* of T if $d(u) \geq 3$. Furthermore, u is said to be an *out-branching point* if at most one of the components of $T - u$ is not a path; otherwise, u is an *in-branching point* of T.

For convenience, we introduce a transfer operation: $T \to T_A \to T_B \to T_C$, as shown in Fig. 3, where T is a tree of order n, u is an out-branching point of T, $d(u) = m$, and all the components $T_1, T_2, ... T_m$ of $T - u$ except T_1 are paths.

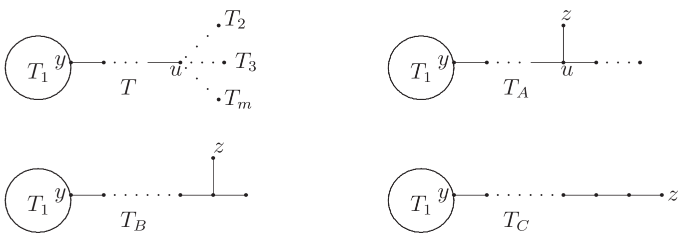

Fig. 3.

Lemma 2.4 [13] *Let u be an out-branching point of a tree T of order n, $d(u) = m$ ($m \geq 3$), and let all components T_1, T_2, ..., T_m of $T - u$ except T_1 be paths. Then,*

$$W(T) \leq W(T_A) \leq W(T_B) < W(T_C),$$

and $W(T) = W(T_A)$ (or $W(T_B)$) if and only if $T = T_A$ (or T_B).

Proposition 2.3 *Let u be an out-branching point of a tree T of order n, $d(u) = m$ ($m \geq 3$), and let all components T_1, T_2, ..., T_m of $T - u$ except T_1 be paths. Then,*

$$WW(T) \leq WW(T_A) \leq WW(T_B) < WW(T_C),$$

and $WW(T) = WW(T_A)$ (or $WW(T_B)$) if and only if $T = T_A$ (or T_B).

Proof. By Proposition 2.1, it is easy to see that $WW(T) \leq WW(T_A)$ with the equality holding if and only if $T = T_A$. Moreover, Proposition 2.1 implies that $WW(T_B) < WW(T_C)$. Next we shall prove that $WW(T_A) \leq WW(T_B)$ with the equality holding if and only if $T_A = T_B$. By Lemma 2.4 and the definition of hyper-Wiener index, we only need to prove that

$$\sum_{\{w,v\}\subseteq V(T_B)} d_{T_B}(w,v)^2 \geq \sum_{\{w,v\}\subseteq V(T_A)} d_{T_A}(w,v)^2, \tag{10}$$

where the equality holds if and only if $T_A = T_B$. Once this is proved, we are done.

Let T_u denote the component of $T_A - y$, which contains u. Set $V_1 = V(T_u) \cup \{y\}$. Then, $V(T_A) \setminus V_1 = V(T_B) \setminus V_1$. Let $V_2 = V(T_A) \setminus V_1$. It is easy to see that

$$\sum_{\{w,v\}\subseteq V(T_B)} d_{T_B}(w,v)^2 - \sum_{\{w,v\}\subseteq V(T_A)} d_{T_A}(w,v)^2$$

$$= \sum_{w\in V(T_B)} d_{T_B}(w,z)^2 - \sum_{w\in V(T_A)} d_{T_A}(w,z)^2$$

$$= \sum_{w\in V_1} d_{T_B}(w,z)^2 - \sum_{w\in V_1} d_{T_A}(w,z)^2 + \sum_{w\in V_2} (d_{T_B}(w,z)^2 - d_{T_A}(w,z)^2). \tag{11}$$

Note that $\sum_{w\in V_1} d_{T_B}(w,z)^2 \geq \sum_{w\in V_1} d_{T_A}(w,z)^2$, and $d_{T_B}(w,z)^2 \geq d_{T_A}(w,z)^2$ holds for every $w \in V_2$, then inequality (10) holds by equality (11), and the equality holds in inequality (10) if and only if $T_A = T_B$. This completes the proof. ∎

3 The ordering of the greatest hyper-Wiener indices of trees

Let $T(n; n_1, n_2, ..., n_m)$ denote the starlike tree of order n obtained by inserting $n_1 - 1$, ..., $n_m - 1$ vertices into m edges of the star $K_{1,m}$ of order $m + 1$ respectively, where $n_1 + \cdots + n_m = n - 1$. Note that any tree with only one branching point is a starlike tree.

If T is a tree of order n with exactly two branching points u_1 and u_2, with $d(u_1) = r$ and $d(u_2) = t$. The orders of $r-1$ components, which are paths, of $T-u_1$ are p_1, ..., p_{r-1}, the order of the component which is not a path of $T - u_1$ is $p_r = n - p_1 - \cdots - p_{r-1} - 1$. The orders of $t - 1$ components, which are paths, of $T - u_2$ are q_1, ..., q_{t-1}, the order of the component which is not a path of $T - u_2$ is $q_t = n - q_1 - \cdots - q_{t-1} - 1$. We denote this tree by $T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$, where $r \leq t$, $p_1 \geq \cdots \geq p_{r-1}$ and $q_1 \geq \cdots \geq q_{t-1}$.

By an elementary computation, we have

$WW(P_n) = \frac{1}{24}(n^4 + 2n^3 - n^2 - 2n)$,

$WW(T(n; n-3, 1, 1)) = \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 72)$,

$WW(T(n; n-4, 2, 1)) = \frac{1}{24}(n^4 + 2n^3 - 25n^2 + 46n + 192)$,

$WW(T(n; 1, 1; 1, 1)) = \frac{1}{24}(n^4 + 2n^3 - 25n^2 + 22n + 168)$,

$WW(T(n; n-5, 3, 1)) = \frac{1}{24}(n^4 + 2n^3 - 37n^2 + 106n + 360)$,

$WW(T(n; n-4, 1, 1, 1)) = \frac{1}{24}(n^4 + 2n^3 - 37n^2 + 82n + 168)$,

$WW(T(n; 1, 1; 2, 1)) = \frac{1}{24}(n^4 + 2n^3 - 37n^2 + 58n + 312)$,

$WW(T(n; n-6, 4, 1)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 190n + 576)$,

$WW(T(n; n-5, 2, 2)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 142n + 480)$,

$WW(T(n; 1, 1; n-5, 1)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 142n + 312)$,

$WW(T(n; 1, 1; 3, 1)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 118n + 504)$,

$WW(T(n; 2, 1; 2, 1)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 94n + 480)$,

$WW(T(n; 1, 1; 1, 1, 1)) = \frac{1}{24}(n^4 + 2n^3 - 49n^2 + 94n + 312)$,

$WW(T(n; n-7, 5, 1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 298n + 840)$,

$WW(T(n; 1, 1; n-6, 1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 226n + 504)$.

Thus, we have

Lemma 3.1 *If* $n \geq 20$, *then* $WW(T(n; n-3, 1, 1)) > WW(T(n; n-4, 2, 1)) > WW(T(n; 1, 1; 1, 1)) > WW(T(n; n-5, 3, 1)) > WW(T(n; n-4, 1, 1, 1)) > WW(T(n; 1, 1; 2, 1)) > WW(T(n; n-6, 4, 1)) > WW(T(n; n-5, 2, 2)) > WW(T(n; 1, 1; n-5, 1)) > WW(T(n; 1, 1; 3, 1)) > WW(T(n; 2, 1; 2, 1)) > WW(T(n; 1, 1; 1, 1, 1)) > WW(T(n; n-7, 5, 1)) > WW(T(n; 1, 1; n-6, 1))$.

By an elementary computation, we have

$WW(T(n; 1, 1; 4, 1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 202n + 744)$,

$WW(T(n; n-5, 2, 1, 1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 202n + 312)$,

$WW(T(n; 2, 1; 3, 1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 154n + 696)$,

$WW(T(n; 1, 1; 2, 2)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 154n + 648)$,

$WW(T(n;2,1;1,1,1)) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 130n + 504)$,

$WW(T(n;n-8,6,1)) = \frac{1}{24}(n^4 + 2n^3 - 73n^2 + 430n + 1152)$,

$WW(T(n;1,1;n-7,1)) = \frac{1}{24}(n^4 + 2n^3 - 73n^2 + 334n + 744)$,

$WW(T(n;n-6,3,2)) = \frac{1}{24}(n^4 + 2n^3 - 73n^2 + 286n + 864)$,

$WW(T(n;n-5,1,1,1,1)) = \frac{1}{24}(n^4 + 2n^3 - 73n^2 + 262n + 168)$,

$WW(T(n;1,1;n-6,2)) = \frac{1}{24}(n^4 + 2n^3 - 85n^2 + 346n + 648)$,

$WW(T(n;n-6,1;1,1,1)) = \frac{1}{24}(n^4 + 2n^3 - 85n^2 + 346n + 312)$,

$WW(T(n;n-7,1;1,1,1)) = \frac{1}{24}(n^4 + 2n^3 - 97n^2 + 454n + 504)$.

The next lemma can be obtained directly from the above equalities.

Lemma 3.2 *If $n \geq 20$, then*

(1) $WW(T(n;1,1;n-6,1)) > WW(T(n;1,1;4,1)) > WW(T(n;n-5,2,1,1)) > WW(T(n;2,1;3,1)) > WW(T(n;1,1;2,2)) > WW(T(n;2,1;1,1,1))$;

(2) $WW(T(n;1,1;n-6,1)) > WW(T(n;n-8,6,1)) > WW(T(n;1,1;n-7,1)) > WW(T(n;n-6,3,2)) > WW(T(n;n-5,1,1,1,1)) > WW(T(n;1,1;n-6,2)) > WW(T(n;n-6,1;1,1,1)) > WW(T(n;n-7,1;1,1,1))$.

Lemma 3.3 *If $n \geq 20$ and T is a tree with exactly one branching point of degree $m \geq 5$, then $WW(T) \leq WW(T(n;n-5,1,1,1,1)) < WW(T(n;1,1;n-6,1))$.*

Proof. By hypothesis, $T = T(n;n_1,n_2,...,n_m)$. Without loss of generality, assume $n_1 \geq n_2 \geq \cdots \geq n_m$. We prove the lemma by induction on m.

If $m = 5$, by Proposition 2.1 and Lemma 3.2 it follows that $WW(T) = WW(T(n;n_1,n_2,n_3,n_4,n_5)) \leq WW(T(n;n_1{+}n_5{-}1,n_2,n_3,n_4,1)) \leq WW(T(n;n_1{+}n_4{+}n_5{-}2,n_2,n_3,1,1)) \leq WW(T(n;n_1{+}n_3{+}n_4{+}n_5{-}3,n_2,1,1,1)) \leq WW(T(n;n{-}5,1,1,1,1)) < WW(T(n;1,1;n{-}6,1))$. Thus, this lemma holds for $m = 5$.

If $m \geq 6$, by Proposition 2.1, Lemma 3.2 and the induction hypothesis it follows that $WW(T) = WW(T(n;n_1,n_2,...,n_m)) < WW(T(n;n_1{+}n_m,n_2,...,n_{m-1})) \leq WW(T(n;n-5,1,1,1,1)) < WW(T(n;1,1;n-6,1))$. ∎

Lemma 3.4 *Suppose $n \geq 20$, and T is a tree with only one branching point. If $T \notin \{T(n;n{-}3,1,1),T(n;n{-}4,2,1),T(n;n{-}5,3,1),T(n;n{-}4,1,1,1),T(n;n{-}6,4,1),T(n;n{-}5,2,2),T(n;n-7,5,1)\}$, then $WW(T) < WW(T(n;1,1;n-6,1))$.*

Proof. Suppose the degree of the unique branching point is m, then $T = T(n; n_1, ..., n_m)$. Without loss of generality, assume $n_1 \geq \cdots \geq n_m$. If $m \geq 5$, then the conclusion follows from Lemma 3.3. We consider the next two cases.

Case 1. $m = 3$.

If $n_3 \geq 2$, since $T \neq T(n; n-5, 2, 2)$, then $n_2 \geq 3$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T(n; n_1, n_2, n_3)) \leq WW(T(n; n_1 + n_3 - 2, n_2, 2)) \leq WW(T(n; n-6, 3, 2)) < WW(T(n; 1, 1; n-6, 1))$.

If $n_3 = 1$, since $T \notin \{T(n; n-3, 1, 1), T(n; n-4, 2, 1), T(n; n-5, 3, 1), T(n; n-6, 4, 1), T(n; n-7, 5, 1)\}$, then $n_1 \geq n_2 \geq 6$. By Lemma 3.2 and Proposition 2.1 it follows that $WW(T) \leq WW(T(n; n-8, 6, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 2. $m = 4$. Since $T \neq T(n; n-4, 1, 1, 1)$, then $n_1 \geq n_2 \geq 2$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T(n; n_1, n_2, n_3, n_4)) \leq WW(T(n; n_1 + n_4 - 1, n_2, n_3, 1)) \leq WW(T(n; n_1 + n_3 + n_4 - 2, n_2, 1, 1)) \leq WW(T(n; n-5, 2, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.

This completes the proof of this lemma. ∎

Lemma 3.5 *Suppose $n \geq 20$, and $T = T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$. If $t \geq 5$, then $WW(T) < WW(T(n; n-5, 1, 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.*

Proof. By Proposition 2.3, Lemmas 3.2-3.3 it follows that $WW(T) < WW(T(n; q_1, ..., q_{t-1}, n - q_1 - \cdots - q_{t-1} - 1)) \leq WW(T(n; n-5, 1, 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$. ∎

Lemma 3.6 *Suppose $n \geq 20$, and $T = T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$. If $t = r = 4$, then $WW(T) < WW(T(n; 1, 1; n-6, 1))$.*

Proof. By hypothesis, $T = T(n; p_1, p_2, p_3; q_1, q_2, q_3)$. Without loss of generality, suppose that $p_1 + p_2 + p_3 \geq q_1 + q_2 + q_3$. We consider the next cases.

Case 1. $p_1 + p_2 + p_3 \geq 4$. By Proposition 2.1 we have $WW(T) < WW(T(n; p_1, p_2, p_3, n - p_1 - p_2 - p_3 - 1)) \leq WW(T(n; p_1 + p_3 - 1, p_2, 1, n - p_1 - p_2 - p_3 - 1)) \leq WW(T(n; p_1 + p_2 + p_3 - 2, 1, 1, n - p_1 - p_2 - p_3 - 1))$. Note that $p_1 + p_2 + p_3 - 2 \geq 2$ and $n - p_1 - p_2 - p_3 - 1 \geq q_1 + q_2 + q_3 > 2$, then $WW(T(n; p_1 + p_2 + p_3 - 2, 1, 1, n - p_1 - p_2 - p_3 - 1)) \leq WW(T(n; n-5, 2, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$ follows from Proposition 2.1 and Lemma 3.2.

Case 2. $p_1 + p_2 + p_3 = 3$. Then, $q_1 + q_2 + q_3 = 3$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) < WW(T(n; 2, 1; 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$. ∎

Lemma 3.7 *Suppose* $n \geq 20$*, and* $T = T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$ *with* $t = 4$*,* $r = 3$*. If* $T \neq T(n; 1, 1; 1, 1, 1)$*, then* $WW(T) < WW(T(n; 1, 1; n-6, 1))$*.*

Proof. By hypothesis, $T = T(n; p_1, p_2; q_1, q_2, q_3)$. Two cases should be considered as follows.

Case 1. $q_1+q_2+q_3 \geq 4$. By Proposition 2.1, we have $WW(T) < WW(T(n; q_1, q_2, q_3, n-q_1-q_2-q_3-1)) \leq WW(T(n; q_1+q_3-1, q_2, 1, n-q_1-q_2-q_3-1)) \leq WW(T(n; q_1+q_2+q_3-2, 1, 1, n-q_1-q_2-q_3-1))$. Note that $n-q_1-q_2-q_3-1 \geq p_1+p_2 \geq 2$ and $q_1+q_2+q_3-2 \geq 2$, by Proposition 2.1 and Lemma 3.2 it follows that $WW(T(n; q_1+q_2+q_3-2, 1, 1, n-q_1-q_2-q_3-1)) \leq WW(T(n; n-5, 2, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 2. $q_1+q_2+q_3 = 3$. Since $T \neq T(n; 1, 1; 1, 1, 1)$, then $3 \leq p_1+p_2 \leq n-5$. We divide the proof into four subcases.

Subcase 1. $3 \leq p_1+p_2 \leq 6$. By Proposition 2.1, it follows that $WW(T) \leq WW(T(n; p_2+p_1-1, 1; 1, 1, 1))$. Recall that $n \geq 20$, by Propositions 2.2 and Lemma 3.2 we have $WW(T(n; p_2+p_1-1, 1; 1, 1, 1)) \leq WW(T(n; 2, 1; 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 2. $7 \leq p_1+p_2 \leq n-7$. This implies that $n-p_1-p_2-1 \geq 6$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) < WW(T(n; p_1, p_2, n-p_1-p_2-1)) \leq WW(T(n; p_2+p_1-1, 1, n-p_1-p_2-1)) \leq WW(T(n; n-8, 6, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 3. $p_1+p_2 = n-6$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) \leq WW(T(n; n-7, 1; 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 4. $p_1+p_2 = n-5$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) \leq WW(T(n; n-6, 1; 1, 1, 1)) < WW(T(n; 1, 1; n-6, 1))$.

By combining the above arguments, the result follows. ∎

Lemma 3.8 *Suppose* $n \geq 20$*, and* $T = T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$ *with* $t = 3$*,* $r = 3$*. If* $T \notin \{T(n; 1, 1; 1, 1), T(n; 1, 1; 2, 1), T(n; 1, 1; n-5, 1), T(n; 1, 1; 3, 1), T(n; 2, 1; 2, 1), T(n; 1, 1; n-6, 1)\}$*, then* $WW(T) < WW(T(n; 1, 1; n-6, 1))$*.*

Proof. By hypothesis, $T = T(n; p_1, p_2; q_1, q_2)$. Without loss of generality, suppose $q_1+q_2 \geq p_1+p_2$. Since $T \notin \{T(n; 1, 1; 1, 1), T(n; 1, 1; 2, 1), T(n; 2, 1; 2, 1)\}$, then $4 \leq q_1+q_2 \leq n-4$. We consider the next cases.

Case 1. $q_1+q_2 = 4$. Then, $2 \leq p_1+p_2 \leq 4$. Two subcases occur as follows.

Subcase 1. $p_1+p_2 = 2$. Since $T \neq T(n; 1, 1; 3, 1)$, then $T = T(n; 1, 1; 2, 2)$. By Lemma 3.2, $WW(T(n; 1, 1; 2, 2)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 2. $3 \leq p_1 + p_2 \leq 4$. By Propositions 2.1-2.2 and Lemma 3.2, we have $WW(T) \leq WW(T(n; p_1, p_2; 3, 1)) \leq WW(T(n; 2, 1; 3, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 2. $5 \leq q_1 + q_2 \leq 6$. By Propositions 2.1-2.3 and Lemma 3.2, it follows that $WW(T) \leq WW(T(n; 1, 1; q_1, q_2)) \leq WW(T(n; 1, 1; q_1+q_2-1, 1)) \leq WW(T(n; 1, 1; 4, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 3. $7 \leq q_1 + q_2 \leq n-7$. Then, $n - q_1 - q_2 - 1 \geq 6$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) < WW(T(n; q_1, q_2, n - q_1 - q_2 - 1)) \leq WW(T(n; q_1 + q_2 - 1, 1, n - q_1 - q_2 - 1)) \leq WW(T(n; n-8, 6, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 4. $q_1 + q_2 = n - 6$. By Proposition 2.1, Proposition 2.3 and Lemma 3.2 it follows that $WW(T) \leq WW(T(n; p_1, p_2; n-7, 1)) \leq WW(T(n; 1, 1; n-7, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Case 5. $q_1+q_2 = n-5$. By Proposition 2.1, it follows that $WW(T) \leq WW(T(n; p_1, p_2; n-6, 1))$. Since $T \neq T(n; 1, 1; n-6, 1)$, by Proposition 2.3 we have $WW(T) < WW(T(n; 1, 1; n-6, 1))$.

Case 6. $q_1 + q_2 = n - 4$. This implies that $p_1 = p_2 = 1$. Since $T \neq T(n; 1, 1; n-5, 1)$, then $q_1 \geq q_2 \geq 2$. By Proposition 2.1 and Lemma 3.2, we have $WW(T) = WW(T(n; 1, 1; q_1, q_2)) \leq WW(T(n; 1, 1; n-6, 2)) < WW(T(n; 1, 1; n-6, 1))$.

This completes the proof. ∎

Lemma 3.9 *Suppose $n \geq 20$, and T is a tree of order n with exactly three branching points, then $WW(T) < WW(T(n; 1, 1; n-6, 1))$.*

Proof. Let u_1, u_2, u_3 be the three branching points of T. Let u_1 be an in-branching point and u_2, u_3 be two out-branching points. Now suppose $d(u_1) = m$, T_1, ..., T_m be the components of $T - u_1$ and let they be paths except T_{m-1}, T_m, where the order of T_i is n_i for $1 \leq i \leq m$. By the definition of T it follows that $u_2 \in V(T_{m-1})$ and $u_3 \in V(T_m)$, which implies that $n_{m-1} \geq 3$ and $n_m \geq 3$. Without loss of generality, we suppose $n_{m-1} \geq n_m$. The next cases should be taken into account.

Case 1. $n_1 + n_2 + \cdots + n_{m-2} \geq 2$. Note that $n_{m-1} \geq n_m \geq 3$, by Proposition 2.1 and Lemma 3.2 it follows that $WW(T) < WW(T(n; n_{m-1}, n_m, n_1 + \cdots + n_{m-2})) \leq WW(T(n; n-6, 3, 2)) < WW(T(n; 1, 1; n-6, 1))$.

Case 2. $n_1 + n_2 + \cdots + n_{m-2} = 1$. Then, $m = 3$ and $n_1 = 1$. Four subcases should be considered.

Subcase 1. $n_3 \geq 6$. Thus, $n_2 \geq 6$. By Proposition 2.1 and Lemma 3.2 it follows that $WW(T) < WW(T(n; n_2, n_3, 1)) \leq WW(T(n; n-8, 6, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 2. $n_3 = 5$. Then, $n_2 = n - n_1 - n_3 - 1 = n - 7$. By Proposition 2.3 and Lemma 3.2 it follows that $WW(T) < WW(T(n; 1, 1; n-7, 1)) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 3. $n_3 = 4$. Then, $n_2 = n - n_1 - n_3 - 1 = n - 6$. By Proposition 2.3 it follows that $WW(T) < WW(T(n; 1, 1; n-6, 1))$.

Subcase 4. $n_3 = 3$. By Proposition 2.3 it follows that $WW(T) \leq WW(T_D)$, which is shown in Fig. 4. By an elementary computation, we have $WW(T_D) = \frac{1}{24}(n^4 + 2n^3 - 61n^2 + 154n + 480)$. Thus, $WW(T_D) < WW(T(n; 1, 1; n-6, 1))$.

The result follows by combining the above arguments. ∎

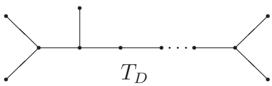

Fig. 4.

Lemma 3.10 *Suppose $n \geq 20$, and T is a tree of order n with k branching points. If $k \geq 3$, then $WW(T) < WW(T(n; 1, 1; n-6, 1))$.*

Proof. We prove the lemma by induction on k. By Lemma 3.9, it is true for $k = 3$.

Let $k \geq 4$, and T be a tree of order n with k branching points. Then T must have an out-branching point, and by Proposition 2.3, $WW(T) < WW(T_C)$, where T_C has $k-1$ branching points. Thus, $WW(T_C) < WW(T(n; 1, 1; n-6, 1))$ follows from the induction hypothesis. This completes the proof. ∎

Lemma 3.11 [14] *Let T be a tree of order n, then $WW(T) \leq WW(P_n)$. Moreover, the equality holds if and only if $T = P_n$.*

Let $\mathcal{T}(n)$ be the set of trees of order n. By combining Lemmas 3.1-3.11, we can conclude that

Theorem 3.1 *Suppose $n \geq 20$ and $T \in \mathcal{T}(n) \setminus \{P_n, T(n; n-3, 1, 1), T(n; n-4, 2, 1), T(n; 1, 1; 1, 1), T(n; n-5, 3, 1), T(n; n-4, 1, 1, 1), T(n; 1, 1; 2, 1), T(n; n-6, 4, 1), T(n; n-5, 2, 2), T(n; 1, 1; n-5, 1), T(n; 1, 1; 3, 1), T(n; 2, 1; 2, 1), T(n; 1, 1; 1, 1, 1), T(n; n-7, 5, 1), T(n; 1, 1; n-6, 1)\}$, then $WW(P_n) > WW(T(n; n-3, 1, 1)) > WW(T(n; n-4, 2, 1)) > WW(T(n; 1, 1; 1, 1))$*

$> WW(T(n;n-5,3,1)) > WW(T(n;n-4,1,1,1)) > WW(T(n;1,1;2,1)) > WW(T(n;n-6,4,1)) > WW(T(n;n-5,2,2)) > WW(T(n;1,1;n-5,1)) > WW(T(n;1,1;3,1)) > WW(T(n;2,1;2,1)) > WW(T(n;1,1;1,1,1)) > WW(T(n;n-7,5,1)) > WW(T(n;1,1;n-6,1)) > WW(T)$.

4 The ordering of the smallest hyper-Wiener indices of trees

The *first Zagreb index* $M_1(G)$ is defined as [16]:

$$M_1(G) = \sum_{v \in V} d(v)^2,$$

it is also an important topological index and has been closely correlated with many chemical and mathematical properties [17-19]. In [19], it has been proved that

Lemma 4.1 [19] *Let G be a connected (n,m) graph, then $M_1(G) \leq m \cdot max\{d(v)+m(v) : v \in V\}$, where $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.*

With the help of Lemma 4.1, we have

Lemma 4.2 *Let T be a tree of order n, then*

$$M_1(T) \leq \max\{(n-1)(\Delta + \frac{n-1}{\Delta}), \frac{(n-1)(n+3)}{2}\}.$$

Proof. By Lemma 4.1, we only need to prove that $\max\{d(v) + m(v) : v \in V\} \leq \max\{\Delta + \frac{n-1}{\Delta}, 2 + \frac{n-1}{2}\}$. Suppose $\max\{d(v) + m(v) : v \in V\}$ occurs at the vertex u. Two cases arise $d(u) = 1$, or $2 \leq d(u) \leq \Delta$.

Case 1. $d(u) = 1$. Suppose that $N(u) = w$. Since $m(u) = d(w) \leq \Delta$, thus $d(u) + m(u) \leq 1 + \Delta \leq \Delta + \frac{n-1}{\Delta}$, the result follows.

Case 2. $2 \leq d(u) \leq \Delta$. If $n \leq 4$, the conclusion clearly follows. If $n \geq 5$, note that

$$m(u) = \sum_{v \in N(u)} d(v)/d(u) \leq \frac{n-1}{d(u)},$$

then $d(u) + m(u) \leq d(u) + \frac{n-1}{d(u)}$. Let $f(x) = x + \frac{n-1}{x}$, where $x \in [2, \Delta]$.

It is easy to see that $f'(x) = 1 - \frac{n-1}{x^2}$. Let $a = n - 1$. We consider the next two subcases.

Subcase 1. $2 \le \sqrt{a} \le \Delta$. Then, $f'(x) \le 0$ for $x \in [2, \sqrt{a}]$, and $f'(x) \ge 0$ for $x \in [\sqrt{a}, \Delta]$. Thus, $f(x) \le \max\{f(2), f(\Delta)\}$ for $x \in [2, \Delta]$.

Subcase 2. $\sqrt{a} > \Delta$. When $x \in [2, \Delta]$, since $f'(x) < 0$, then $f(x) \le f(2)$.

Recall that $2 \le d(u) \le \Delta$, thus

$$d(u) + m(u) \le d(u) + \frac{n-1}{d(u)} \le \max\{\Delta + \frac{n-1}{\Delta}, 2 + \frac{n-1}{2}\}.$$

By combining the above discussion, this completes the proof. ∎

In [9], a relation between $WW(G)$ and $M_1(G)$ is reported as follows

Lemma 4.3 [9] *Let G be a connected (n, m) graph, which does not contain triangles and/or quadrangles. Then, $WW(G) \ge 3n(n-1) - \frac{3}{2}M_1(G) - 2m$.*

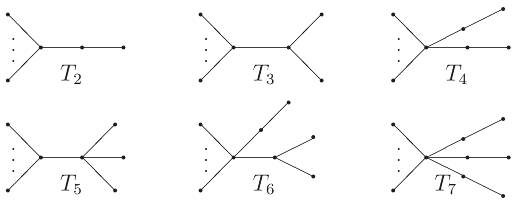

Fig. 5. The trees $T_2, ..., T_7$.

Let $T_1 = K_{1,n-1}$, and $T_2, ..., T_7$ be the trees of order $n \ge 17$ as shown in Fig. 5. By an directly calculation, we have $WW(T_1) = \frac{1}{2}(3n^2 - 7n + 4)$, $WW(T_2) = \frac{1}{2}(3n^2 - n - 14)$, $WW(T_3) = \frac{1}{2}(3n^2 + 5n - 44)$, $WW(T_4) = \frac{1}{2}(3n^2 + 5n - 30)$, $WW(T_5) = \frac{1}{2}(3n^2 + 11n - 86)$, $WW(T_6) = \frac{1}{2}(3n^2 + 11n - 58)$, $WW(T_7) = \frac{1}{2}(3n^2 + 11n - 44)$.

As shown in the next theorem, $T_1, ..., T_7$ is the trees with the first up to seventh smallest hyper-Wiener indices among $\mathcal{T}(n)$, where $n \ge 17$.

Theorem 4.1 *Suppose $n \ge 17$ and $T \in \mathcal{T}(n) \backslash \{T_1, T_2, T_3, T_4, T_5, T_6, T_7\}$, then $WW(T) > WW(T_7) > WW(T_6) > WW(T_5) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.*

The proof of Theorem 4.1 needs the following Lemmas

Lemma 4.4 *If T is a tree of order n $(n \ge 17)$ with $\Delta \le n-7$, then $WW(T) > WW(T_7)$.*

Proof. Let $f(x) = x + \frac{n-1}{x}$, where $x \in [2, n-7]$. By the proof of Lemma 4.2, we can conclude that $f(x) \leq \max\{n - 7 + \frac{n-1}{n-7}, 2 + \frac{n-1}{2}\}$. Recall that $2 \leq \Delta \leq n - 7$, then by Lemma 4.2 it follows that

$$M_1(T) \leq \max\{(n-1)(n-7) + \frac{(n-1)^2}{n-7}, \frac{(n-1)(n+3)}{2}\}.$$

Bearing Lemma 2.4 and $n \geq 17$ in mind, we have

$$WW(T) \geq min\{\frac{3n^2 + 14n - 17}{2} - \frac{3(n-1)^2}{2(n-7)}, \frac{9n^2 - 26n + 17}{4}\} > \frac{3n^2 + 11n - 44}{2} = WW(T_7).$$

This completes the proof of this lemma. ∎

A graph $G' = (V', E')$ is called an *induced subgraph* of $G = (V, E)$ if $V' \subseteq V$ and $uv \in E'$ if and only if $uv \in E$. Suppose $n \geq 17$ and T is a tree of order n with $\Delta \geq n-6$, let u_0 denote the center of the unique star $K_{1,\Delta}$ of T ($K_{1,\Delta}$ is an induced subgraph of T), and $\kappa(T) = max\{d(u_0, v), v \in V(T)\}$. Clearly, $\kappa(T) = 1$ if and only if $T = K_{1,n-1}$.

Let H_t and F_t be the trees of order t as shown in Fig. 6.

Fig. 6. The trees H_t and F_t.

Lemma 4.5 *If T is a tree of order n ($n \geq 17$) with $\Delta = n-6$, then $WW(T) > WW(T_7)$.*

Proof. We divide the proof in to the next two cases.

Case 1. $\kappa(T) \geq 3$. Then T contains H_{n-3} as an induced subgraph. Let $\{v_1, v_2, v_3\} = V(T) \backslash V(H_{n-3})$, and v_0 be the vertex such that $d(u_0, v_0) = 3$ in H_{n-3} (see Fig. 6). It is easy to see that $\gamma(T, 1) = n - 1$. Note that $d(v_i, u_0) \geq 2$, and either $d(u_0, v_i) \geq 3$ or $d(v_0, v_i) \geq 3$ holds for $1 \leq i \leq 3$, then

$$\begin{aligned} WW(T) &= \frac{1}{2}\sum_{s\geq 1} s(s+1)\gamma(T, s) \\ &\geq n - 1 + 6 \cdot (3(n-7) + 3) + \frac{1}{2}\sum_{s\geq 2} s(s+1)\gamma(H_{n-3}, s) \\ &= n - 1 + 3(2 + \binom{n-6}{2}) + 6(4n - 24) + 10(n-7) \\ &= \frac{3n^2 + 31n - 292}{2} \end{aligned}$$

$$
\begin{aligned}
&> \frac{3n^2+11n-44}{2} \\
&= WW(T_7).
\end{aligned}
$$

Case 2. $\kappa(T)=2$. Then T contains F_{n-4} as an induced subgraph. Let $\{v_1,v_2,v_3,v_4\} = V(T)\backslash V(F_{n-4})$, and v_0 be the vertex such that $d(u_0,v_0)=2$ in F_{n-4} (see Fig. 6). It is easy to see that $\gamma(T,1)=n-1$. Note that $d(v_i,u_0)=2$, and $d(v_i,v_0)\geq 2$ holds for $1\leq i\leq 4$. Moreover, bearing in mind that $d(v_i,v_j)\geq 2$ holds for $1\leq i<j\leq 4$, then

$$
\begin{aligned}
WW(T) &= \frac{1}{2}\sum_{s\geq 1} s(s+1)\gamma(T,s) \\
&\geq n-1+3\cdot(4+4+6)+6\cdot 4(n-7)+\frac{1}{2}\sum_{s\geq 2} s(s+1)\gamma(F_{n-4},s) \\
&= n-1+3(15+\binom{n-6}{2})+6\cdot 5(n-7) \\
&= \frac{3n^2+23n-206}{2} \\
&> \frac{3n^2+11n-44}{2} \\
&= WW(T_7).
\end{aligned}
$$

By combining the above discussion, the result follows. ∎

Lemma 4.6 *If T is a tree of order n ($n\geq 17$) with $\Delta=n-5$, then $WW(T)>WW(T_7)$.*

Proof. We consider the next two cases.

Case 1. $\kappa(T)\geq 3$. Then T contains H_{n-2} as an induced subgraph. Clearly, $\gamma(T,1)=n-1$. Let $\{v_1,v_2\}=V(T)\backslash V(H_{n-2})$. Note that $d(v_i,u_0)\geq 2$ holds for $1\leq i\leq 2$, then

$$
\begin{aligned}
WW(T) &= \frac{1}{2}\sum_{s\geq 1} s(s+1)\gamma(T,s) \\
&\geq n-1+3\cdot 2+6\cdot 2(n-6)+\frac{1}{2}\sum_{s\geq 2} s(s+1)\gamma(H_{n-2},s) \\
&= n-1+3(4+\binom{n-5}{2})+6(3n-17)+10(n-6) \\
&= \frac{3n^2+25n-212}{2} \\
&> \frac{3n^2+11n-44}{2} \\
&= WW(T_7).
\end{aligned}
$$

Case 2. $\kappa(T) = 2$. Then T contains F_{n-3} as an induced subgraph. Let $\{v_1, v_2, v_3\} = V(T)\backslash V(F_{n-3})$, and v_0 be the vertex such that $d(u_0, v_0) = 2$ in F_{n-3} (see Fig. 6). It is easy to see that $\gamma(T, 1) = n - 1$. Note that $d(v_i, u_0) = 2$, and $d(v_i, v_0) \geq 2$ holds for $1 \leq i \leq 3$. Moreover, bearing in mind that $d(v_i, v_j) \geq 2$ holds for $1 \leq i < j \leq 3$, then

$$\begin{aligned}
WW(T) &= \frac{1}{2}\sum_{s\geq 1} s(s+1)\gamma(T, s) \\
&\geq n - 1 + 3 \cdot (3 + 3 + 3) + 6 \cdot 3(n - 6) + \frac{1}{2}\sum_{s\geq 2} s(s+1)\gamma(F_{n-3}, s) \\
&= n - 1 + 3(10 + \binom{n-5}{2}) + 6 \cdot 4(n - 6) \\
&= \frac{3n^2 + 17n - 140}{2} \\
&> \frac{3n^2 + 11n - 44}{2} \\
&= WW(T_7).
\end{aligned}$$

By combining the above arguments, the result follows. ∎

Lemma 4.7 *Let T be a tree of order n ($n \geq 17$) with $\Delta = n - 4$. If $T \notin \{T_5, T_6, T_7\}$, then $WW(T) > WW(T_7)$.*

Proof. Note that T_5, T_6, T_7 are the all trees with $\Delta = n - 4$ and $\kappa = 2$, since $T \notin \{T_5, T_6, T_7\}$, then $\kappa(T) \geq 3$. This implies that T contain H_{n-1} as an induced subgraph. It is easy to see that $\gamma(T, 1) = n - 1$. Let $\{v_1\} = V(T)\backslash V(H_{n-1})$. Note that $d(v_1, u_0) \geq 2$, then

$$\begin{aligned}
WW(T) &= \frac{1}{2}\sum_{s\geq 1} s(s+1)\gamma(T, s) \\
&\geq n - 1 + 3 \cdot 1 + 6 \cdot (n - 5) + \frac{1}{2}\sum_{s\geq 2} s(s+1)\gamma(H_{n-1}, s) \\
&= n - 1 + 3(3 + \binom{n-4}{2}) + 6(2n - 9) + 10(n - 5) \\
&= \frac{3n^2 + 19n - 132}{2} \\
&> \frac{3n^2 + 11n - 44}{2} \\
&= WW(T_7).
\end{aligned}$$

This completes the proof of this lemma. ∎

Lemma 4.8 *Let T be a tree of order n ($n \geq 17$) with $\Delta = n - 3$. If $T \notin \{T_3, T_4\}$, then $WW(T) > WW(T_7)$.*

Proof. Note that T_3, T_4 are the all trees with $\Delta = n - 3$ and $\kappa = 2$, since $T \notin \{T_3, T_4\}$, then $\kappa(T) = 3$. This implies that $T \cong H_n$. By directly computation, we have

$$WW(T) = WW(H_n) = \frac{3n^2 + 13n - 70}{2} > \frac{3n^2 + 11n - 44}{2} = WW(T_7).$$

This completes the proof of this lemma. ∎

Lemma 4.9 [14] *Let T be a tree of order n, then $WW(T) \geq WW(T_1)$. Moreover, the equality holds if and only if $T = T_1$.*

Proof for Theorem 4.1. By the values of $WW(T_2), WW(T_3), \cdots, WW(T_7)$ and $n \geq 17$, it is easy to see that $WW(T_2) < WW(T_3) < \cdots < WW(T_7)$. Recall that T_1 and T_2 are the all trees of order n with $n - 2 \leq \Delta \leq n - 1$, then Theorem 4.1 follows from Lemmas 4.4-4.9. ∎

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