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On Wiener and Terminal Wiener Indices of Trees*

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Abstract

Heydari [7] presented formulas for the Wiener and terminal Wiener indices of generalized Bethe trees. Unfortunately, these formulas are erroneous. We correct these errors. In addition, we characterize the trees with minimum terminal Wiener index among all the trees of order n and maximum degree Δ.

1 Introduction

There are many molecular structure descriptors until now. The Wiener index is one of the most widely known topological descriptors, which has been much studied in both mathematical and chemical literature (for example, see [2–4]). Throughout this paper, we only consider finite, simple and undirected graphs. Let $G = (V(G), E(G))$ be a simple connected graph of order n with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices v_i and v_j is the minimum number of edges between v_i and v_j and is denoted by

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$d_G(v_i, v_j)$ (or for short $d(v_i, v_j)$). The *Wiener index* of a connected graph G is defined as the sum of distances between all pairs of vertices:

$$W(G) = \sum_{v_i, v_j \subseteq V(G)} d(v_i, v_j) = \frac{1}{2} \sum_{v \in V(G)} d_G(v)$$

where $d_G(v)$ denotes the distance of a vertex v. For trees, Wiener [12] gave a very useful formula:

$$W(G) = \sum_{e \in T} n_1(e) \cdot n_2(e) \tag{1}$$

where $n_1(e)$ and $n_2(e)$ are the number of vertices of two components of $T - e$.

Recently, Smolenski et al. [10] made use of terminal distance matrices to encode molecular structures. Based on these applications, Gutman, Furtula, and Petrović [5] proposed the concept of *terminal Wiener index*, which is defined as the sum of distances between all pairs of pendent vertices of trees:

$$TW(T) = \sum_{1 \leq i < j \leq k} d_T(v_i, v_j)$$

where $d_T(v_i, v_j)$ is the distance of two pendent vertices v_i and v_j. They gave a similar formula for the terminal Wiener index of trees

$$TW(T) = \sum_{e \in T} p_1(e) \cdot p_2(e) \tag{2}$$

where $p_1(e)$ and $p_2(e)$ are the number of pendent vertices in the two components of $T - e$.

For more information on the Wiener and terminal Wiener indices, the readers may refer to the recent papers [8, 9, 11] and the references cited therein.

A generalized Bethe tree (see [7]) is a rooted tree whose vertices at the same level have equal degrees. We agree that the root vertex is at level 1 and T has k levels, and denote the class of generalized Bethe trees of k levels by $\mathcal{B}_k$. *A Bethe tree* $B_{k,d}$ is a rooted tree of k levels in which the root vertex has degree d, the vertices at level $j (2 \leq j \leq k-1)$ have degrees $d+1$, and the vertices at level k are the pendent vertices. A *regular dendrimer tree* $T_{k,d}$ is a generalized Bethe tree of $k+1$ levels with each nonpendent vertex having degree d. So a regular dendrimer tree belongs to $\mathcal{B}_{k+1}$.

The rest of the paper is organized as follows. In Section 2, we present some formulas for the Wiener index of generalized Bethe trees, which correct the errors of [7]. In Section 3, a formula for the terminal Wiener indices of trees is obtained. With the formula, the terminal Wiener index of a generalized Bethe tree is presented, which corrects the errors of [7]. In section 4, the trees with the minimum terminal Wiener index among all the trees of order n and with maximum degree Δ are characterized.

2 Wiener index of generalized Bethe trees

Let $T_1, T_2, \cdots, T_m$ ($m \geq 2$) be trees with disjoint vertex sets and orders $n_1, n_2, \cdots, n_m$. Let $w_i \in V(T_i)$ be the rooted vertex of T_i for $i = 1, 2, \cdots, m$. A tree T on more than two vertices can be regarded as being obtained by joining a new vertex w to each of the vertices $w_1, w_2, \cdots, w_m$. Canfield, Robinson, and Rouvray [1] elaborated a recursive approach for the calculation of the Wiener index of a general tree. Dobrynin, Entringer, and Gutman [2] state this result as the following theorem.

Theorem 2.1 ([2]) *Let T be a tree on $n \geq 3$ vertices, whose structure is specified above. Then*

$$W(T) = \sum_{i=1}^{m} \left[W(T_i) + (n - n_i) d_{T_i}(w_i) - n_i^2\right] + n(n-1)$$

where $d_{T_i}(w_i)$ is the sum of distances between w_i and all other vertices of T_i for $1 \leq i \leq m$.

Since a generalized Bethe tree is the very special tree whose vertices have the same degree at the same level, Heydari [7] presented a formula for the Wiener index of generalized Bethe trees. The result can be stated as follows:

Theorem 2.2 ([7]) *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. If d_1 denotes the degree of the rooted vertex, and $d_i + 1$ denotes degree of the vertices on i-th level of B_{k+1} for $1 < i < k$, then the Wiener index of B_{k+1} is computed as follows:*

$$W(B_{k+1}) = \sum_{i=1}^{k} (n_{i+1} - 1)\, m_i\, (n - m_i)$$

where n_{i+1} is the number of vertices on the $(i+1)$-th level of B_{k+1} and m_i is the number of all children vertices lying on one side of the edge where a vertex on the i-th level is adjacent to another vertex on $(i+1)$-th level of B_{k+1} for $1 \leq i \leq k$.

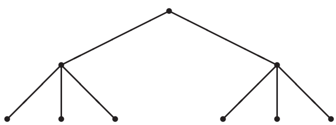

Fig. 1. B_3

Unfortunately, this result is not correct. For example [see Fig. 1]: B_3 is a generalized Bethe tree with 9 vertices. It is easy to see that $k = 2, n_2 = 2, n_3 = 6, m_1 = 4, m_2 = 1$. Using the above formula, we have $W(B_3) = 60$. But actually, the Wiener index of $W(B_3)$ is 88. In here, we present a correct formula for the Wiener index of a generalized Bethe tree.

Theorem 2.3 *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. If d_1 denotes the degree of rooted vertex and $d_i + 1$ denotes the degree of vertices on the i-th level of B_{k+1} for $1 < i \leq k$, then*

$$W(B_{k+1}) = \sum_{i=1}^{k} n_{i+1}\, m_i\, (n - m_i) \tag{3}$$

where $n_{i+1} = d_1 d_2 \cdots d_i$ and $m_i = 1 + \sum\limits_{j=i+1}^{k} \prod_{r=i+1}^{i} d_r$ for $1 \leq i \leq k$.

Proof. Let n_i be the number of vertices on the i-th level of B_{k+1}. Thus $n_1 = 1$ and $n_i = d_1 d_2 d_3 \cdots d_{i-1}$ for $i = 2, 3, \cdots, k+1$. Denote by $|V(B_{k+1})| = n$. Then

$$n = n_1 + n_2 + \cdots + n_{k+1} = 1 + \sum_{i=1}^{k} \prod_{j=1}^{i} d_j \,.$$

Suppose that u on the i-th level of B_{k+1} for $1 \leq i \leq k$ is the parent of v. So all of the children of the vertex v are lying on one side of the edge $e = uv$. Denote by m_i the number of those vertices of the tree. Then

$$m_i = 1 + d_{i+1} + d_{i+1}\, d_{i+2} + \cdots + d_{i+1}\, d_{i+2} \ldots d_k = 1 + \sum_{j=i+1}^{k} \prod_{r=i+1}^{i} d_r$$

for $1 \leq i \leq k$. Obviously, $m_k = 1$. Hence, the number of vertices lying on two sides of e are equal to $n_1(e) = m_i$ and $n_2(e) = n - m_i$, respectively. Since the number of edges of B_{k+1} adjacent to a vertex on the i-th level to another vertex on $(i+1)$-th level of B_{k+1} is equal to n_{i+1}, by using (1), we have

$$W(B_{k+1}) = \sum_{e=E(B_{k+1})} n_1(e) \cdot n_2(e) = \sum_{i=1}^{k} n_{i+1}\, m_i\, (n - m_i)$$

The proof is completed. ∎

By using the correct formula (3), it is easy to check that $W(B_3) = 88$. Obviously, the dendrimer tree $T_{k,d}$ is one of the special generalized Bethe trees.

Corollary 2.4 *Let $T_{k,d}$ be a dendrimer tree of $k+1$ levels where degree of the non-pendent vertices is equal to d. Then the Wiener index of $T_{k,d}$ is computed as follows:*

$$W(T_{k,d}) = \frac{d}{(d-2)^3}\left[(d-1)^{2k}\left(kd^2-2(k+1)d+1\right)+2d(d-1)^k-1\right] . \qquad (4)$$

Proof. Since the degree of non-pendent vertices of $T_{k,d}$ is equal to d, we have $n_1 = 1$, $n_i = d(d-1)^{i-2}$ for $2 \le i \le k+1$, $n = 1 + \frac{d((d-1)^k-1)}{d-2}$ and $m_i = 1 + \frac{(d-1)((d-1)^{k-i}-1)}{d-2}$. By (3),

$$\begin{aligned}
W(T_{k,d}) &= \sum_{i=1}^{k} d(d-1)^{i-1}\left[1+\frac{(d-1)\left[(d-1)^{k-i}-1\right]}{d-2}\right]\left[\frac{d((d-1)^k-1)}{d-2}\right. \\
&\quad \left. - \frac{(d-1)[(d-1)^{k-i}-1]}{d-2}\right] \\
&= \sum_{i=1}^{k} d(d-1)^{i-1}\frac{[d-2+(d-1)][(d-1)^{k-i}-1]}{d-2} \times \\
&\quad \frac{[d(d-1)^k-(d-1)^{k-i+1}-1]}{d-2} \\
&= \sum_{i=1}^{k} d(d-1)^{i-1}\frac{(d-1)^{k-i+1}-1}{d-2} \times \frac{d(d-1)^k-(d-1)^{k-i+1}-1}{d-2} \\
&= \frac{d}{(d-2)^2}\sum_{i=1}^{k}[(d-1)^k-(d-1)^{i-1}][d(d-1)^k-(d-1)^{k-i+1}-1] \\
&= \frac{d}{(d-2)^2}\sum_{i=1}^{k}[d(d-1)^{2k}-(d-1)^{2k-i+1}-d(d-1)^{k+i-1}+(d-1)^{i-1}] \\
&= \frac{d}{(d-2)^2}\left[kd(d-1)^{2k}-\sum_{i=1}^{k}(d-1)^{2k-i+1}\right. \\
&\quad \left. -d\sum_{i=1}^{k}(d-1)^{k+i-1}+\sum_{i=1}^{k}(d-1)^{i-1}\right] \\
&= \frac{d}{(d-2)^2}\left[kd(d-1)^{2k}-\frac{(d-1)^{k+1}[(d-1)^k-1]}{d-2}\right. \\
&\quad \left. -\frac{d(d-1)^k[(d-1)^k-1]}{d-2}+\frac{(d-1)^k-1}{d-2}\right] \\
&= \frac{d}{(d-2)^3}\left[(d-1)^{2k}(kd^2-2(k+1)d+1)+2d(d-1)^k-1\right]
\end{aligned}$$

The proof is completed. ■

Corollary 2.5 *The Wiener index of a Bethe tree $B_{k,d}$ is computed as follows:*

$$W(B_{k,d}) = \frac{d^k}{(d-1)^3}\left[(k-1)(d-1)(d^k+1) - 2d(d^{k-1}-1)\right]$$

Proof. Since the degrees of the non-pendent vertices of $B_{k,d}$ are equal to $d+1$, except the rooted vertex whose degree is d, we have $n_1 = 1$, $n_{i+1} = d^i$ for $1 \le i \le k-1$, $n = \frac{d^k-1}{d-1}$ and $m_i = \frac{d^{k-i}-1}{d-1}$. By (3), we get

$$\begin{aligned} W(B_{k,d}) &= \sum_{i=1}^{k-1} d^i \frac{d^{k-i}-1}{d-1}\left(\frac{d^k-1}{d-1} - \frac{d^{k-i}-1}{d-1}\right) \\ &= \frac{d^k}{(d-1)^2}\sum_{i=1}^{k-1}(d^k - d^{k-i} - d^i + 1) \\ &= \frac{d^k}{(d-1)^2}\left[(k-1)(d^k+1) - \sum_{i=1}^{k-1} d^{k-i} - \sum \_i = 1^{k-1} d^i\right] \\ &= \frac{d^k}{(d-1)^2}\left[(k-1)(d^k+1) - \frac{2d(d^{k-1}-1)}{d-1}\right] \\ &= \frac{d^k}{(d-1)^3}\left[(k-1)(d-1)(d^k+1) - 2d(d^{k-1}-1)\right]. \end{aligned}$$

The proof is completed. ■

3 Terminal Wiener index of trees

In this section, we consider the terminal Wiener index of trees. For a tree T with order $n \ge 3$ with rooted w, let $T_1, T_2, \cdots, T_m$ $(m \ge 2)$ be components of $T - w$ with orders $n_1, n_2, \cdots, n_m$, respectively, where w_i is adjacent to the vertex w in T and is the rooted vertex in T_i. Let l be the number of pendent vertices in T and l_i $(1 \le i \le m)$ be the number of pendent vertices in T_i. Clearly, $l_1 + l_2 + \cdots + l_m = l$. We present a formula for computing the terminal Wiener index of a tree by the terminal Wiener index of subtrees.

Theorem 3.1 *Let T be a tree with order $n \ge 3$, whose structure is described as above. Then*

$$TW(T) = \sum_{i=1}^{m}\left[TW(T_i) + (l - l_i)d'_{T_i}(w_i) - l_i^2\right] + l^2 \tag{5}$$

where $d'_{T_i}(w_i)$ is the sum of distances between w_i and all other pendent vertices of T_i for $1 \le i \le m$.

Proof. Let x_{ij} $(1 \leq j \leq l_i)$ be the pendent vertices in $T_i (1 \leq i \leq m)$. Then

$$
\begin{aligned}
TW(T) &= \sum_{i=1}^{m} TW(T_i) + \sum_{k=1}^{l_2} \sum_{h=1}^{l_1} d(x_{1h}, x_{2k}) + \sum_{k=1}^{l_3} \sum_{h=1}^{l_1} d(x_{1h}, x_{3k}) + \cdots \\
&+ \sum_{k=1}^{l_m} \sum_{h=1}^{l_1} d(x_{1h}, x_{mk}) + \sum_{k=1}^{l_3} \sum_{h=1}^{l_2} d(x_{2h}, x_{3k}) + \cdots + \sum_{k=1}^{l_m} \sum_{h=1}^{l_2} d(x_{2h}, x_{mk}) \\
&+ \cdots + \sum_{k=1}^{l_m} \sum_{h=1}^{l_{m-1}} d(x_{(m-1)h}, x_{mk}) \\
&= \sum_{i=1}^{m} TW(T_i) + \sum_{i=2}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_1} d(x_{1h}, x_{ik}) + \sum_{i=3}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_2} d(x_{2h}, x_{ik}) \\
&+ \cdots + \sum_{i=m-1}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_{m-2}} d(x_{(m-2)h}, x_{ik}) + \sum_{k=1}^{l_m} \sum_{h=1}^{l_{m-1}} d(x_{(m-1)h}, x_{mk})
\end{aligned}
$$

Since the sum of distances between pendent vertices in each T_i and T_j can be calculated, i.e.,

$$\sum_{k=1}^{l_j} \sum_{h=1}^{l_i} d(x_{ih}, x_{jk}) = l_j d'_{T_i}(w_i) + l_i d'_{T_j}(w_j) + 2 l_i l_j$$

and $l^2 = (l_1 + l_2 + \cdots + l_m)^2 = \sum_{i=1}^{m} l_i^2 + 2 \sum\_1 \leq i < j \leq m l_i l_j$, then we have

$$
\begin{aligned}
TW(T) &= \sum_{i=1}^{m} TW(T_i) + (l_2 + l_3 + \cdots + l_m) d'_{T_1}(w_1) + (l_1 + l_3 + \cdots + l_m) d'_{T_2}(w_2) \\
&+ \cdots + (l_1 + l_2 + \cdots + l_{m-1}) d'_{T_m}(w_m) + 2 \sum_{1 \leq i < j \leq m} l_i l_j \\
&= \sum_{i=1}^{m} TW(T_i) + (l - l_1) d'_{T_1}(w_1) + (l - l_2) d'_{T_2}(w_2) + \cdots \\
&+ (l - l_m) d'_{T_m}(w_m) + l^2 - \sum_{i=1}^{m} l_i^2 \\
&= \sum_{i=1}^{m} [TW(T_i) + (l - l_i) d'_{T_i}(w_i) - l_i^2] + l^2 \ .
\end{aligned}
$$

By this the proof is finished. ■

With (5), the formulas for the terminal Wiener index of generalized Bethe trees, Bethe trees $B_{k,d}$, and $T_{k,d}$ are obtained, which correct the errors of [7].

Theorem 3.2 *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. Then*

$$TW(B_{k+1}) = \prod_{i=1}^{k} d_i \times \left(k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j+1} \right) . \tag{6}$$

Proof. The pendent vertices of the generalized Bethe tree B_{k+1} are located on the final level of the tree. Let n' be the number of pendent vertices of B_{k+1}, then $n' = d_1 d_2 \cdots d_k$. Suppose that $e = uv$ is an edge of B_{k+1}, and u is the parent of v on the i-th level of B_{k+1} for $1 \leq i \leq k$. Let m'_i and m''_i be the number of pendent vertices of B_{k+1}, lying on the two sides of e. Then $m'_i = d_{i+1} d_{i+2} \cdots d_k$ and $m''_i = n' - d_{i+1} d_{i+2} \cdots d_k$ for $1 \leq i \leq k-1$. Obviously, $m'_k = 1$ and $m''_k = n' - 1$. Since we have mentioned in Theorem 2.2 that n_{i+1}, which stands for the number of edges where adjacent a vertex on the i-th level to another vertex on the $(i+1)$-th level of B_{k+1}, is equal to $d_1 d_2 \cdots d_i$ for $1 \leq i \leq k+1$, by using (2), we have

$$\begin{aligned}
TW(B_{k+1}) &= \sum_{e \in E(B_{k+1})} p_1(e) \cdot p_2(e) \\
&= \sum_{i=1}^{k-1} n_{i+1} m'_i m''_i + n' m'_k m''_k \\
&= \sum_{i=1}^{k-1} n_{i+1} d_{i+1} d_{i+2} \cdots d_k (n' - d_{i+1} d_{i+2} \cdots d_k) + n'(n'-1) \\
&= \sum_{i=1}^{k-1} d_1 d_2 \cdots d_i d_{i+1} d_{i+2} \cdots d_k (d_1 d_2 \cdots d_k - d_{i+1} d_{i+2} \cdots d_k) \\
&+ d_1 d_2 \cdots d_k (d_1 d_2 \cdots d_k - 1) \\
&= (k-1) \left(\prod_{i=1}^{k} d_i \right)^2 - \prod_{i=1}^{k} d_i \sum_{i=1}^{k-1} d_{i+1} d_{i+2} \cdots d_k + \prod_{i=1}^{k} d_i \left(\prod_{i=1}^{k} d_i - 1 \right) \\
&= \prod_{i=1}^{k} d_i \times \left[(k-1) \left(\prod_{i=1}^{k} d_i \right) + \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} d_{i+1} d_{i+2} \cdots d_k \right] \\
&= \prod_{i=1}^{k} d_i \times \left(k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j+1} \right)
\end{aligned}$$

The proof is completed. ■

From Theorem 3.2, we can get the terminal Wiener index of $T_{k,d}$.

Corollary 3.3 *Let $T_{k,d}$ be a dendrimer tree of $k+1$ levels where the degrees of the non-pendent vertices are equal to d. Then the terminal Wiener index of $T_{k,d}$ is computed as follows:*

$$TW(T_{k,d}) = d(d-1)^{k-1}\left[kd(d-1)^{k-1} + \frac{1-(d-1)^k}{d-2}\right]$$

Proof. Since the degrees of the non-pendent vertices of $T_{k,d}$ are equal to d, it is easy to see that d_1 is equal to d and n_i is equal to $d-1$ for $2 \leq i \leq k$. Then

$$n' = \prod_{i=1}^{k} d_i = d(d-1)^{k-1}$$

and

$$\begin{aligned} \sum \_i = 1^{k-1} \prod_{j=1}^{i} d_{k-j+1} &= \sum_{i=1}^{k-1} d_{i+1}d_{i+2}\cdots d_k \\ &= \sum_{i=1}^{k-1}(d-1)^{k-i} \\ &= \frac{(d-1)[(d-1)^{k-1}-1]}{d-2} \ . \end{aligned}$$

By using (6), we have

$$\begin{aligned} TW(T_{k,d}) &= d(d-1)^{k-1}\left[kd(d-1)^{k-1} - 1 - \frac{(d-1)[(d-1)^{k-1}-1]}{d-2}\right] \\ &= d(d-1)^{k-1}\left[kd(d-1)^{k-1} + \frac{1-(d-1)^k}{d-2}\right] \ . \end{aligned}$$

The proof is completed. ■

Corollary 3.4 *Let $B_{k,d}$ be a Bethe tree of k levels. Then*

$$TW(B_{k,d}) = \frac{d^{k-1}}{d-1}[d^{k-1}(kd-k-d)+1] \ .$$

Proof. Since $B_{k,d}$ is a Bethe tree of level k, we replace k in formula (6) by $k-1$. According to the definition of the Bethe tree $B_{k,d}$, it is easy to see that $\prod_{i=1}^{k-1} d_i = d^{k-1}$ and

$$\begin{aligned} \sum_{i=1}^{k-2}\prod_{j=1}^{i} d_{k-j} &= \sum_{i=1}^{k-2} d_{i+1}d_{i+2}\cdots d_{k-1} \\ &= \sum_{i=1}^{k-2} d^{k-i-1} = \frac{d[d^{k-2}-1]}{d-1}. \end{aligned}$$

By using (6), we have

$$\begin{aligned} TW(B_{k,d}) &= d^{k-1}\left[(k-1)d^{k-1}-1-\frac{d(d^{k-2}-1)}{d-1}\right] \\ &= d^{k-1}\left[(k-1)d^{k-1}-\frac{d^{k-1}-1}{d-1}\right] \\ &= \frac{d^{k-1}}{d-1}[(k-1)(d-1)d^{k-1}-d^{k-1}+1] \\ &= \frac{d^{k-1}}{d-1}[d^{k-1}(kd-k-d)+1] \ . \end{aligned}$$

The proof is completed. ■

4 Terminal Wiener index versus maximum degree in trees

Let $\mathcal{T}(n,\Delta)$ denote the set of all trees of order n with maximum degree Δ. In this section, we characterize the trees with the minimum terminal Wiener index in $\mathcal{T}(n,\Delta)$.

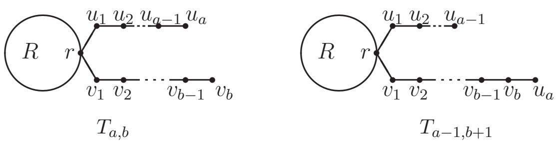

Fig. 2. $T_{a,b}$ and $T_{a-1,b+1}$

In order to prove our main result, we introduce a tree transformation. Let $T_{a,b}$ and $T_{a-1,b+1}$ be the trees depicted in Fig. 2, where $b > a \geq 1$ are integers and R is a rooted tree with root r and at least two vertices. Gutman, Vukičević, and Petrović proved

Lemma 4.1 ([6]) *Let $b > a \geq 1$. Then*

$$W(T_{a,b}) < W(T_{a-1,b+1}) \ .$$

However, the above result is not true for terminal Wiener index. In fact,

Lemma 4.2 *If $b > a > 1$, then*

$$TW(T_{a,b}) = TW(T_{a-1,b+1}) \ .$$

Proof. Suppose that there are k pendent vertices of R which are labeled by $x_1, x_2, \cdots, x_k$. Then

$$\begin{aligned} TW(T_{a,b}) &= \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + \sum_{i=1}^{k} d(x_a,x_i) + \sum_{i=1}^{k} d(v_b,x_i) + a + b \\ &= \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + 2\sum_{i=1}^{k} d(r,x_i) + (a+b)k + a + b \end{aligned}$$

and

$$\begin{aligned} TW(T_{a-1,b+1}) &= \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + \sum_{i=1}^{k} d(u_{a-1},x_i) + \sum_{i=1}^{k} d(x_a,x_i) + a + b \\ &= \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + 2\sum_{i=1}^{k} d(r,x_i) + (a+b)k + a + b \ . \end{aligned}$$

It is easy to see that $TW(T_{a,b}) = TW(T_{a-1,b+1})$. ■

Lemma 4.3 *If $b > a = 1$, then*

$$TW(T_{a,b}) > TW(T_{a-1,b+1}) \ .$$

Proof. Suppose that there are k pendent vertices of R, labeled by $x_1, x_2, \cdots, x_k$. Then

$$TW(T_{a,b}) = \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + 2\sum_{i=1}^{k} d(r,x_i) + (b+1)k + b + 1$$

and

$$TW(T_{a-1,b+1}) = \sum_{1\le x_i<x_j\le k} d(x_i,x_j) + \sum_{i=1}^{k} d(r,x_i) + (b+1)k \ .$$

So $TW(T_{a,b}) - TW(T_{a-1,b+1}) = \sum_{i=1}^{k} d(r,x_i) + b + 1 > 0$. ■

A tree is said to be *starlike* of degree k if exactly one of its vertices has degree greater than two, and its degree is equal to $k \ge 3$.

Theorem 4.4 *If T is a tree in $\mathcal{T}(n,\Delta)(\Delta \ge 3)$, then*

$$TW(T) \ge (n-1)(\Delta - 1)$$

with equality if and only if T is starlike of order n with the maximum degree Δ.

Proof. Since $T \in \mathcal{T}(n, \Delta)$, there exists at least one vertex labeled by v such that $d(v) = \Delta$. So there are Δ branches of $T - v$. If T is not a starlike tree, there exist some branches of T at v that are not paths. Hence by Lemmas 4.2 and 4.3, there exists a starlike tree T_1 of order n with the maximum degree Δ such that $TW(T) > TW(T_1)$. Moreover, any two starlike trees of order n with the maximum degree Δ have the same terminal Wiener index, equal to $(n-1)(\Delta-1)$. Hence the proof is completed. ■

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