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# Extremal Wiener Index of Trees with All Degrees Odd*

**Hong Lin**
*School of Sciences, Jimei University,*
*Xiamen, Fujian, 361021, P. R. China*
`linhongjm@163.com`

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**Abstract**

The Wiener index of a graph is defined as the sum of distances between all pairs of vertices of the graph. In this paper, we characterize the trees which maximize and minimize the Wiener index among all trees of given order that have only vertices of odd degrees.

## 1 Introduction

All graphs considered in this paper are simple and connected. Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex $v$ in $G$ is the number of edges of $G$ incident with $v$. The distance between vertices $u$ and $v$ of $G$ is denote by $d_G(u, v)$. The Wiener index of a graph $G$ is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) \ . \tag{1}$$

The Wiener index belongs among the oldest graph-based structure descriptors (topological indices). It was first introduced by Wiener [13] and has been extensively studied in many literatures. Numerous of its chemical applications and mathematical properties

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are well studied [1,3,6,8,9,11]. For detailed results on this topic, the readers may referred to [4,5].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. Let $T$ be a tree and $e = uv$ an edge of $T$. Wiener [13] found that the formula (1) is equal to

$$W(T) = \sum_{e \in E(T)} n_{T_1}(e)\, n_{T_2}(e) \tag{2}$$

where $n_{T_1}(e)$ (resp. $n_{T_2}(e)$) is the number of vertices of the component of $T - e$ containing $u$ (resp. $v$). Denote by $K_{1,n-1}$ and $P_n$ the star and the path with $n$ vertices, respectively. Entringer et al. [6] proved the following result which bounds the Wiener index of a tree in term of its order.

**Theorem 1** ([6]). Let $T$ be a tree on $n$ vertices, then

$$(n-1)^2 \leq W(T) \leq \binom{n+1}{3} .$$

The lower bound is achieved if and only if $T \cong K_{1,n-1}$ and the upper bound is achieved if and only if $T \cong P_n$ .

Since every atom has a certain valency, chemists are interested in trees with some restricted degree conditions, having maximal or minimal Wiener index. Fischermann et al. [7] determined the trees which have the minimum Wiener index among all trees of given order and maximum degree. If a graph $G$ has vertices $v_1, v_2, \ldots, v_n$, then the sequence $(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$ is called a degree sequence of $G$. It is well known [2] that a sequence $(d_1, d_2, \ldots, d_n)$ of positive integers is a degree sequence of an $n-$vertex tree if and only if $\sum\limits_{i=1}^{n} d_n = 2(n-1)$. A tree $T$ is called a *caterpillar* if the tree obtained from $T$ by removing all pendent vertices is a path. Shi [10] obtained the following result.

**Theorem 2 ([10]).** Let $(d_1, d_2, \ldots, d_n)$ be a degree sequence with $\sum\limits_{i=1}^{n} d_n = 2(n-1)$, and $T_{max}$ be the tree with maximal Wiener index among all trees which have this particular degree sequence. Then $T_{max}$ is a caterpillar.

Wang [12] and Zhang et al. [14] independently characterized the tree that minimizes the Wiener index among trees of given degree sequences. Recently, by using Theorem 2, Zhang et al. [15] characterized the tree that maximizes the Wiener index among trees of given degree sequences.

In this paper, we continue to study the extremal Wiener index of trees with specific degree conditions. It is well known that every nontrivial tree has at least two vertices of degree one. This motivates the central problem that we consider in this paper.

**Problem A.** Which trees minimize or maximize the Wiener index among all trees of given order that have only vertices of odd degrees?

Since the relation $\sum_{v \in V(G)} d_G(v) = 2|E(G)|$ holds for any graph $G$, it implies that each tree that has only vertices of odd degree must have even number of vertices. Let $\mathcal{T}_{2n}$ be the set of all trees on $2n$ vertices whose vertices are all of odd degrees. Let $F_{2n}$ be the tree shown in Figure 1.

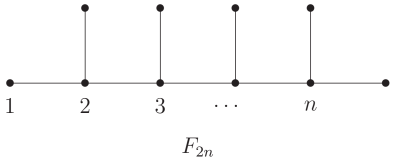


**Fig. 1.** The tree with odd vertex degrees, having greatest Wiener index.

The main result of this paper is as follows which settles Problem A.

**Theorem 3.** Let $T \in \mathcal{T}_{2n}$. Then

$$W(K_{1,2n-1}) \leq W(T) \leq W(F_{2n})$$

the lower bound is achieved if and only if $T \cong K_{1,2n-1}$ and the upper bound is achieved if and only if $T \cong F_{2n}$.

## 2 Proof of Theorem 3

**Proof.** Note that $K_{1,2n-1} \in \mathcal{T}_{2n}$, thus by Theorem 1, we have $W(T) \geq W(K_{1,2n-1})$ with equality if and only if $T \cong K_{1,2n-1}$.

Now we turn to determine the upper bound of $W(T)$. Let $T^*$ be a tree with maximal Wiener index in $\mathcal{T}_{2n}$. Suppose $(d_1, d_2, \ldots, d_{2n})$ is the degree sequence of $T^*$. Let $\mathcal{T}_d$ be the set of all trees with this degree sequence $(d_1, d_2, \ldots, d_{2n})$. Clearly $\mathcal{T}_d$ is a subclass of $\mathcal{T}_{2n}$, so $T^*$ also is a tree with maximal Wiener index in $\mathcal{T}_d$. By Theorem 2, $T^*$ is a caterpillar.

Let $P = y_0 y_1 \ldots y_\ell y_{\ell+1}$ be a longest path in $T^*$. Assume that $T^* \neq F_{2n}$, then there exists a vertex $y_i$ $(1 \le i \le \ell)$ such that $d_{T^*}(y_i) = 2t+1 \ge 5$. Let $y_{i-1}$ , $y_{i+1}$, $u_1$, $u_2$,. . . , $u_{2t-1}$ be the neighbors of $y_i$ .

Now we are going to construct a tree $T' \neq T^*$ such that $T' \in \mathcal{T}_{2n}$ and $W(T') > W(T^*)$. In order to do so, we delete the pendent vertex $u_{2t-1}$ and the edges $y_i u_1$, $y_i u_2$,. . . , $y_i u_{2t-2}$ from $T^*$, split $y_i$ into two adjacent vertices $y_i'$ and $y_i''$ and further join $u_1$, $u_2$,. . . , $u_{2t-3}$ to $y_i'$ and join $u_{2t-2}$ to $y_i''$. The resulting tree is denoted by $T'$. See Figure 2 for an example.

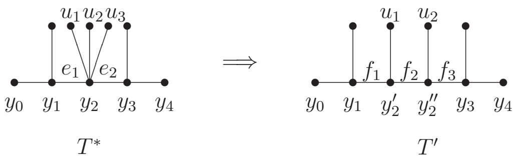


**Fig. 2.** The trees used in the proof of Theorem 3.

Obviously, $T' \in \mathcal{T}_{2n}$. Denote by $e_1$, $e_2$, . . . , $e_{\ell-1}$ and $f_1$, $f_2$, . . . , $f_\ell$ the consecutive edges on the path $P_1 = y_1 \ldots y_i \ldots y_\ell$ of $T^*$ and on the path $P_2 = y_1 \ldots y_i' y_i'', \ldots y_\ell$ of $T'$ from $y_1$ to $y_\ell$, respectively (see Figure 2). Note that $T^*$ has $|E(T^*)| - (\ell-1) = (2n-1) - (\ell-1) = 2n - \ell$ pendent edges and $T'$ has $|E(T')| - \ell = (2n-1) - \ell$ pendent edges. Now by the formula (2) we have

$$
\begin{aligned}
W(T^*) &= \sum_{e \in E(T^*)} n_{T^*1}(e)\, n_{T^*2}(e) \\
&= \sum_{e \textit{ is a pendent edge}} n_{T^*1}(e)\, n_{T^*2}(e) + \sum_{e \textit{ is not a pendent edge}} n_{T^*1}(e)\, n_{T^*2}(e) \\
&= (2n-\ell)(2n-1) + \sum_{k=1}^{\ell-1} n_{T^*1}(e_k)\, n_{T^*2}(e_k) \qquad (3)
\end{aligned}
$$

and

$$
\begin{aligned}
W(T') &= \sum_{e \in E(T')} n_{T'1}(e)\, n_{T'2}(e) \\
&= \sum_{e \textit{ is a pendent edge}} n_{T'1}(e)\, n_{T'2}(e) + \sum_{e \textit{ is not a pendent edge}} n_{T'1}(e)\, n_{T'2}(e) \\
&= (2n-\ell-1)(2n-1) + \sum_{k=1}^{\ell} n_{T'1}(f_k)\, n_{T'2}(f_k)\ . \qquad (4)
\end{aligned}
$$

It is easily checked that $n_{T^*1}(e_j)\, n_{T^*2}(e_j) = n_{T'1}(f_j)\, n_{T'2}(f_j)$ holds for any $j \in \{1, 2, \ldots, i-1\}$ and $n_{T^*1}(e_r)\, n_{T^*2}(e_r) = n_{T'1}(f_{r+1})\, n_{T'2}(f_{r+1})$ holds for any $r \in \{i, i+1, \ldots, \ell-1\}$. Now from (3) and (4), we arrive at

$$
\begin{aligned}
& W(T') - W(T^*) \\
& = n_{T'1}(f_i)\, n_{T'2}(f_i) - (2n-1) \\
& = n_{T'1}(f_i)\, n_{T'2}(f_i) - n_{T'1}(f_i) - n_{T'2}(f_i) + 1 \quad (\text{Since } n_{T'1}(f_i) + n_{T'2}(f_i) = 2n.) \\
& = [n_{T'1}(f_i) - 1][n_{T'2}(f_i) - 1] > 0\,. \quad (\text{Since } n_{T'1}(f_i) > 1\,, n_{T'2}(f_i) > 1\,.)
\end{aligned}
$$

But this contradicts to the choice of $T^*$. ■

While Problem A is settled, it is also natural to consider the analogous questions for general graphs with other degree restrictions. Denote by $\mathcal{O}_{2n}$ the set of graphs on $2n$ vertices whose vertices are all of odd degree. Denote by $\mathcal{E}_n$ the set of connected graphs on $n$ vertices whose vertices are all of even degree. An *Euler tour* of $G$ is a closed walk that traverses each edge of $G$ exactly once. A graph is *Eulerian* if it contains an Euler tour. It is well known [2] that $\mathcal{E}_n$ is the set of all Eulerian graphs on $n$ vertices. The following problem is worthwhile to study.

**Problem B.** Characterize the graphs with maximal Wiener index in $\mathcal{O}_{2n}$ and in $\mathcal{E}_n$, respectively.

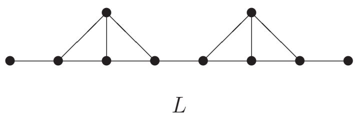


**Fig. 3.** A 10-vertex graph whose Wiener index exceeds the Wiener index of the tree $F_{10}$.

Although $\mathcal{T}_{2n} \subset \mathcal{O}_{2n}$ and $F_{2n}$ is the unique graph with maximal Wiener index in $\mathcal{T}_{2n}$, we remark that $F_{2n}$ may not be the graph with maximal Wiener index in $\mathcal{O}_{2n}$. For an example, let $L$ be the graph shown in Figure 3. Then $L \in \mathcal{O}_{10}$. A straightforward calculation gives that $W(L) = 125 > W(F_{10}) = 121$. Settling Problem B seems to be difficult.

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