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Extremal Wiener Index of Trees with Given Number of Vertices of Even Degree*

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Abstract

The Wiener index of a connected graph is defined as the sum of distances between all pairs of its vertices. In this paper, we characterize the trees which minimize and maximize the Wiener index among all trees with given number of vertices of even degree respectively.

1 Introduction

All graphs considered in this paper are simple, connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A vertex of degree one is called a *pendent vertex*. Let S_n and P_n denote the star and path with n vertices, respectively. The distance of a vertex v, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G. The distance between vertices u and v of G is denoted by $d_G(u, v)$. For other terminologies and notations not defined here we refer the readers to [2]. The Wiener index of a connected graph G is defined as

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

The Wiener index belongs among the oldest graph-based structure descriptors (topological indices) which was first introduced by Wiener [16] and has been extensively studied

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in many literatures. Numerous of its chemical applications and mathematical properties are well studied. For detailed results on this topic, the readers may referred to two surveys by Dobrynin et al. [2] and Gutman et al. [3] and two recent monographs by Gutman and Furtula [8, 9].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. Since every atom has a certain valency, chemists are also in particular interested in trees with some degree restrictions and having maximal or minimal Wiener index. Many researches is devoted to this topics and can be roughly divided into the following groups.

- *Trees with fixed maximum degree*, see [5, 14].

Fischermann et al. [5] characterized the trees which minimize the Wiener index among all trees with the maximum degree Δ. On the other hand, Stevanović [14] determine the trees which maximize the Wiener index among all graphs with the maximum degree Δ.

- *Trees with given number of pendent vertices*, see [1, 4, 12].

The upper bound of the Wiener index of an $n-$vertex tree with exactly k pendent vertices was obtained by Shi [12] and Entringer [4] independently. The lower bound was obtained by Burns and Entringer [1], see also Section 12 of [2].

Let $S(n,m)$ be an $n-$tree obtained from m disjoint paths (each has $\lceil \frac{n-1}{m} \rceil$ or $\lfloor \frac{n-1}{m} \rfloor$ vertices) by attaching one endvertex of each path to a new vertex a. The vertex a is called the *center* of $S(n,m)$. Note that $S(n,2) = P_n$ and $S(n,n-1) = S_n$. The main result of [1] is as follows.

Theorem 1 ([1]). Let T be a tree on n vertices with k pendent vertices, then

$$W(T) \geq W(S(n,k)),$$

with equality if and only if $T = S(n,k)$.

- *Trees with given degree sequence*, see [10, 12, 13, 15, 17, 18].

The degree $deg(v)$ of a vertex v in G is the number of edges of G incident with v. If a graph G has vertices v_1, v_2, ...,v_n, then the sequence $(deg(v_1), deg(v_2), ..., deg(v_n))$ is called a degree sequence of G. It is well known that a sequence $(d_1, d_2, ..., d_n)$ of positive integers is a degree sequence of an $n-$vertex tree if and only if $\sum_{i=1}^{n} d_n = 2(n-1)$. A tree T is called a *caterpillar* if the tree obtained from T by removing all pendent vertices is a path. Shi [12] obtained the following result.

Theorem 2 ([12]). Let $(d_1, d_2, ..., d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_n = 2(n-1)$, and T_{max} be the tree with maximal Wiener index among all trees with this prescribed degree sequence. Then T_{max} is a caterpillar.

Wang [15] and Zhang et al. [17] independently determined the tree that minimizes the Wiener index among trees of given degree sequence through different approaches. But the problem that which tree maximizes the Wiener index among trees of given degree sequence is still open [10, 18]. Very recently, Sills and Wang [13] characterized the maximal Wiener index of chemical trees with prescribed degree sequence by proving the following result, see also [10].

Theorem 3 ([13]). Let $(d_1, ..., d_k, d_{k+1}, ..., d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_n = 2(n-1)$ and $4 \geq d_1 \geq ... \geq d_k > d_{k+1} = ... = d_n = 1$. Let T_{max} be the tree with maximal Wiener index among all trees with this prescribed degree sequence. If $(d_1, d_2, ..., d_k)=(\underbrace{a_s, ..., a_s}_{m_s}, \underbrace{a_{s-1}, ..., a_{s-1}}_{m_{s-1}}, ..., \underbrace{a_1, ..., a_1}_{m_1})$ with $a_s > a_{s-1} > ... > a_1 \geq 2$, then T_{max} can be formed by attaching pendent edges to a path $P = v_1 v_2 ... v_k$ such that

$$(deg(v_1), ..., deg(v_k))=(\underbrace{a_s, ..., a_s}_{l_s}, \underbrace{a_{s-1}, ..., a_{s-1}}_{l_{s-1}}, ..., \underbrace{a_1, ..., a_1}_{m_1}, ..., \underbrace{a_{s-1}, ..., a_{s-1}}_{r_{s-1}}, \underbrace{a_s, ..., a_s}_{r_s}).$$

where $|l_i - r_i| \leq 1$ and $l_i + r_i = m_i$ for $i = 2, ..., s$.

- *Trees with all degrees odd*, see [6, 7, 11].

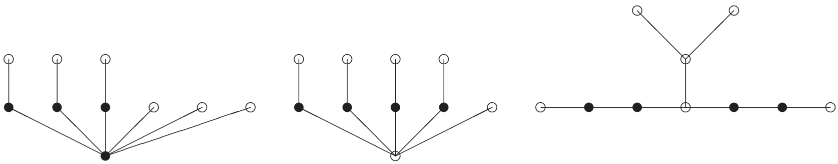
Note that the set of all trees $\mathbb{T}$ can be partitioned into

$$\mathbb{T} = \mathbb{OT} \cup \mathbb{ET},$$

where $\mathbb{OT}$ is the set of trees with all degrees odd and $\mathbb{ET}$ is the set of trees possess some vertices of even degree. In [11], the present author characterized the trees which maximize and minimize the Wiener index among trees of given order in the class $\mathbb{OT}$ respectively. An ordering of trees by their smallest Wiener indices in this category was obtained by Furtula, Gutman and Lin [6]. In [7], Furtula further determined the trees with the second up to seventeenth greatest Wiener indices in this category and obtained some interesting recurrence equations for Wiener index of some trees. Above researches focused on the determination the extremal Wiener index of trees in the class $\mathbb{OT}$. It is natural to consider the similar extremal problems within the class $\mathbb{ET}$.

To fill this gap, it is worthwhile to investigate the extremal Wiener index of trees within the class $\mathbb{ET}$ with some specific restrictions. A general restriction is to require all

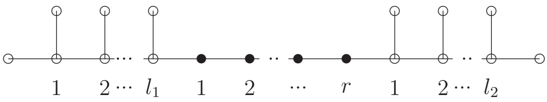
$n-$vertex trees in $\mathbb{ET}$ possessing the same number of vertices of even degree. This leads us to consider the set of all $n-$vertex trees with exactly $r(\geq 1)$ vertices of even degree, which will be denoted by $\mathbb{ET}_{n,r}$. Since the relation $\sum_{v\in V(G)} deg(v) = 2|E(G)|$ holds for any graph G, it implies that n and r have the same parity. Different trees in the class $\mathbb{ET}_{n,r}$ may have different numbers of pendent vertices. See Figure 1 for an example.



$S(10,6)$ 6 pendent vertices $S(10,5)$ 5 pendent vertices T 4 pendent vertices

Fig. 1 Trees in $\mathbb{ET}_{10,4}$ with different numbers of pendent vertices.

Note that the vertex set of the tree $S(n,m)$ consists of m pendent vertices, a center of degree m and $n-m-1$ vertices of degree two. So if two integers n and r have the same parity, then the degree of the center of the tree $S(n,n-r)$ will be even, and hence $S(n,n-r) \in \mathbb{ET}_{n,r}$. Let $E(n,r)$ be the $n-$vertex tree shown in Figure 2, clearly $E(n,r) \in \mathbb{ET}_{n,r}$.



$E(n,r)$

$n \equiv r \pmod 2$, $\quad l_1 + l_2 = \frac{n-r-2}{2}$, $\quad |l_1 - l_2| \leq 1$

Fig. 2 The tree $E(n,r)$

The main work of the present paper (Theorem 4 stated below) is to find, by virtue of Theorem 1, Theorem 2 and Theorem 3, the upper and lower bounds of Wiener index of trees in the class $\mathbb{ET}_{n,r}$ respectively. Clearly the path P_n is the unique element in $\mathbb{ET}_{n,n-2}$. So in the following we only consider the class $\mathbb{ET}_{n,r}$ with $r < n-2$.

Theorem 4. Let $T \in \mathbb{ET}_{n,r}$, where $1 \leq r < n-2$ and $n \equiv r \pmod 2$. Then

$$W(S(n, n-r)) \leq W(T) \leq W(E(n,r)),$$

with left equality if and only if $T = S(n, n-r)$ and with right equality if and only if $T = E(n,r)$.

The rest of this paper is organized as follows. In Section 2, we provide some useful results which will help to prove our main result. We close this paper in Section 3 by proving Theorem 4 and proposing some new problems for research.

2 Preliminaries

First we will prove the following result on comparing the Wiener index of trees $S(n,m)$ with different value m.

Lemma 1. $W(S(n,2)) > W(S(n,3)) > ... > W(S(n,n-2)) > W(S(n,n-1))$.

Proof. It suffices to prove that if $r \leq n-2$, then $W(S(n,r)) > W(S(n,r+1))$.

Assume that the center of $S(n,r)$ is a. Since $r \leq n-2$, therefore $S(n,r) \neq S_n$, and hence we can choose a pendent vertex, say v of $S(n,r)$ such that $d_{S(n,r)}(a,v) \geq 2$. Let u be the unique neighbor of v. Now by deleting the edge uv and joining v to a, we can get another $n-$vertex tree T' with exactly $r+1$ pendent vertices. See Figure 3 for an example.

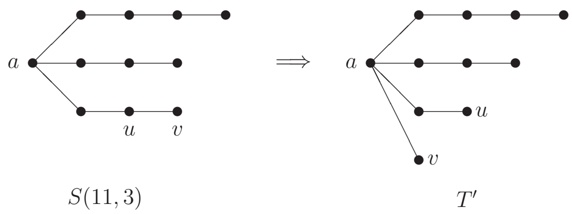


Fig. 3 Two trees $S(11,3)$ and T'.

It is easily checked that

$$\begin{aligned} W(S(n,r)) - W(T') &= d_{S(n,r)}(v) - d_{T'}(v) \\ &= [|V(S(n,r))| - d_{S(n,r)}(a,v)][d_{S(n,r)}(a,v) - 1] - [d_{S(n,r)}(a,v) - 1] \\ &= [|V(S(n,r))| - d_{S(n,r)}(a,v) - 1][d_{S(n,r)}(a,v) - 1] \\ &\geq |V(S(n,r))| - d_{S(n,r)}(a,v) - 1 \quad (\text{Since } d_{S(n,r)}(a,v) \geq 2.) \geq 1 \ . \end{aligned}$$

On the other hand, since T' has $r+1$ pendent vertices, from Theorem 1 it follows that $W(T') \geq W(S(n, r+1))$. Therefore $W(S(n,r)) > W(S(n,r+1))$, as required. □

For a graph G and a vertex $v \in V(G)$, the set of the neighbors of v is denoted by $N_G(v)$. The following result is contained in the proof of Theorem 3 of [11].

Lemma 2. Let T be a caterpillar with the longest path $P = y_0y_1...y_ly_{l+1}$. If there exists a vertex y_i $(1 \leq i \leq l)$ such that $N_T(y_i) = \{y_{i-1}, y_{i+1}, u_1, u_2, ..., u_{2t+1}\}$, where $t \geq 1$, suppose T' is the tree obtained from T by deleting the pendent vertex u_{2t+1} and the edges y_iu_1, y_iu_2,..., y_iu_{2t}, splitting y_i into two adjacent vertices y_i' and y_i'', joining u_1, u_2,... , u_{2t-1} to y_i' and joining u_{2t} to y_i'', then $W(T') > W(T)$.

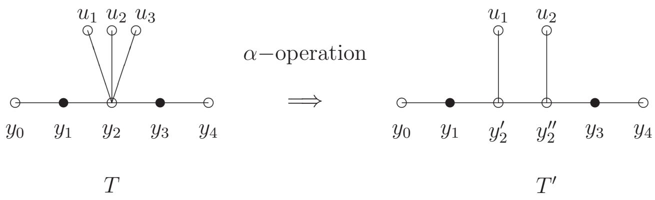


Fig. 4 Two trees T and T'.

For convenience of the subsequent discussion, such a transfer operation introduced in Lemma 2 will be called a $\alpha-$*operation*. It is easy to see that if a caterpillar $T \in \mathbb{ET}_{n,r}$ contains a vertex of degree $2t+1 \geq 5$, where $t \geq 2$, then by a $\alpha-$operation, one can get another caterpillar $T' \in \mathbb{ET}_{n,r}$ with $W(T') > W(T)$, see Figure 4 for an example.

Lemma 3. Let T be a caterpillar with the longest path $P = y_0y_1...y_ly_{l+1}$. If there exists a vertex y_i $(1 \leq i \leq l)$ such that $N_T(y_i) = \{y_{i-1}, y_{i+1}, u_1, u_2, ..., u_{2t}\}$, where $t \geq 1$, suppose T' is the tree obtained from T by deleting the edges y_iu_1, y_iu_2,..., y_iu_{2t} and joining u_1, u_2,... , u_{2t} to y_0, then $W(T') > W(T)$.

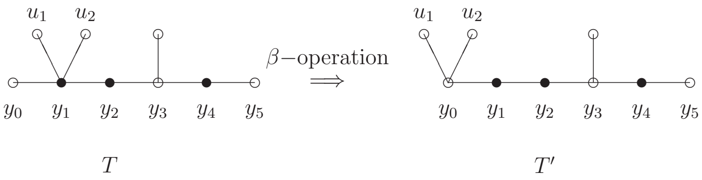


Fig. 5 Two trees T and T'.

Proof. Let T_{u_1} be the tree obtained from T by deleting the vertices u_2, ..., u_{2t} and let T'_{u_1} be the tree obtained from T' by deleting the vertices u_2, ..., u_{2t}.

It is easily verified that $W(T') - W(T) = 2t[d_{T'_{u_1}}(u_1) - d_{T_{u_1}}(u_1)] > 0$. $\square$

For convenience of the subsequent discussion, such a transfer operation introduced in Lemma 3 will be called a *$\beta-$operation.* It is easy to see that if a caterpillar $T \in \mathbb{ET}_{n,r}$ contains a vertex of degree $2t \geq 4$, where $t \geq 2$, then by a $\beta-$operation, one can get another caterpillar $T' \in \mathbb{ET}_{n,r}$ with $W(T') > W(T)$, see Figure 5 for an example.

3 Proof of Theorem 4

Proof. Assume that T has exactly t pendent vertices, since $T \in \mathbb{ET}_{n,r}$, $t \leq n - r$. We distinguish two cases.

Case 1. $t < n - r$.

By Theorem 1, we have

$$W(T) \geq W(S(n,t)),$$

with equality if and only if $T = S(n,t)$.

On the other hand, since $t < n - r$, by Lemma 1 we have

$$W(S(n,t)) > W(S(n,t+1)) > ... > W(S(n,n-r)) .$$

So in this case, $W(T) > W(S(n,n-r))$.

Case 2. $t = n - r$.

If so, directly by Theorem 1, we can get

$$W(T) \geq W(S(n,n-r)),$$

with equality if and only if $T = S(n,n-r)$.

So we conclude that $W(T) \geq W(S(n, n-r))$ with equality if and only if $T = S(n, n-r)$.

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

We can further claim that T^* possesses only vertices of degree 1, 2 and 3.

Otherwise, if T^* contains a vertex v of degree $p \geq 4$, according to Lemma 2 and Lemma 3, by using a $\alpha-$operation if p is odd or a $\beta-$operation if p is even, we can get another tree $T' \in \mathbb{ET}_{n,r}$ with $W(T') > W(T^*)$, but this contradicts to the choice of T^*.

Consequently, T^* is a chemical tree with exactly r vertices of degree 2, now from the relation $\sum\limits_{v \in V(T^*)} deg(v) = 2|E(T^*)| = 2n-2$, one can find that the degree sequence of T^* is $(\underbrace{3, ..., 3}_{\frac{n-r-2}{2}}, \underbrace{2, ..., 2}_{r}, \underbrace{1, ..., 1}_{\frac{n-r+2}{2}})$.

Since T^* is the tree with maximal Wiener index among all trees with this prescribed degree sequence, from Theorem 3 it follows that $T^* = E(n, r)$. This completes the proof of this theorem. $\square$

Let $\mathbb{EG}_{n,r}$ be the set of all $n-$vertex graphs with exactly $r(\geq 1)$ vertices of even degree, where $n \equiv r \pmod 2$. In the end of the paper, we leave the following problems which might be worthwhile to study.

- Order the trees in $\mathbb{ET}_{n,r}$ with the smallest or greatest Wiener indices.
- Characterize the graphs with maximal and minimal Wiener index in $\mathbb{EG}_{n,r}$, respectively.

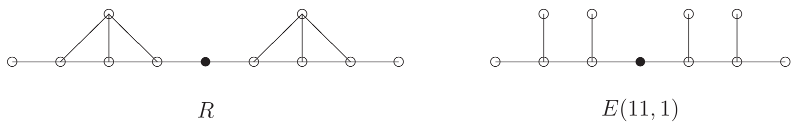


Fig. 6 Two graphs R and $E(11, 1)$.

Although $\mathbb{ET}_{n,r} \subset \mathbb{EG}_{n,r}$ and $E(n, r)$ is the unique tree with maximal Wiener index in $\mathbb{ET}_{n,r}$, we remark that $E(n, r)$ may not be the graph with maximal Wiener index in

$\mathbb{EG}_{n,r}$. For an example, let R be the graph shown in Figure 6, then $R \in \mathbb{EG}_{11,1}$. A straightforward calculation gives that $W(R) = 174 > W(E(11,1)) = 168$.

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