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On the Wiener Index of Graphs with Given Dissociation Number

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Abstract

For a graph $G = (V_G, E_G)$, a subset $S \subseteq V_G$ is called a dissociation set if the induced subgraph $G[S]$ does not contain P_3 as a subgraph. A maximum dissociation set of G is a dissociation set with the maximum cardinality and its cardinality is called the dissociation number of G. In this paper, among all trees, bipartite graphs and general connected graphs with fixed order and dissociation number, the sharp lower bounds of the Wiener index are determined and the corresponding extremal graphs are characterized, respectively. Furthermore, the graphs having the maximum Wiener indices with fixed order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ are also characterized, respectively.

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1 Introduction

We start with introducing some background information that leads to our main results. Our main results will also be given in this section.

1.1 Background and definitions

All graphs considered in this paper are undirected, simple and connected. Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. The *order* of G is the number of its vertices, which is denoted by $|V_G|$. For a given subset $S \subseteq V_G$, the subgraph of G induced by S is denoted by $G[S]$.

For a vertex $v \in V_G$, let $N_G(v)$ be the set of its neighbors in G and $N_G[v] := N_G(v) \cup \{v\}$ be its closed neighborhood. The *degree* of a vertex v is defined as $d_G(v) := |N_G(v)|$. Subscripts may be omitted when no ambiguity arises. If $d(v) = 1$, then v is called a *pendant vertex* (or a *leaf*) of G, and the unique edge incident to v is called a *pendant edge* of G. A vertex of G is called a *quasi-pendant vertex* if it is adjacent to a pendant vertex in G. An induced path $P_l = v_1v_2 \ldots v_l$ of G is called a *pendant path*, if the degrees satisfy $d(v_2) = d(v_3) = \cdots = d(v_{l-1}) = 2$ and $d(v_1) = 1$ (note there is no requirement on the degree of v_l). The *distance* between two vertices u and v, denoted by $d_G(u, v)$, is the length of a shortest path connecting them. The *diameter* of G, written as $diam(G)$, is the maximum distance between any two vertices of G.

Let $V_1 \subseteq V_G$ and $E_1 \subseteq E_G$. Then $G - V_1, G - E_1$ are the graphs formed from G by deleting the vertices in V_1 and their incident edges, the edges in E_1, respectively. For simplicity, denote $G - \{v\}$ and $G - \{uv\}$ by $G - v$ and $G - uv$, respectively. For two graphs G_1 and G_2, denote by $G_1 \cup G_2$ and $G_1 \vee G_2$ the disjoint union and join of G_1 and G_2, respectively. Furthermore, kG represents the disjoint union of k copies of G. As usual, a path, a star, a complete graph and a complete bipartite graph with order n are denoted as $P_n,\ S_n,\ K_n$ and $K_{a,n-a}$ $(a \geq \frac{n}{2})$, respectively. The vertex of degree $n - 1$ is called the *center* of S_n.

Topological indices are the graph invariants that characterize the structural properties of a graph. They play an important role in graph theory, particularly in chemical graph theory, as these indices are capable of effectively capturing fundamental molecular characteristics such as size and shape [8]. In 1947, Wiener [19] introduced a profound distance-based topological index, namely the *Wiener index* of a graph G, which is defined as

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

Wiener index is a representative topological index in chemical graph theory. It has been successfully applied to predict alkane boiling points and various molecular physical properties.

The study on the Wiener index focuses mainly on the extremal problems and a number of results have been obtained. Gutman [4] showed that P_n (resp. S_n) attains the maximum (resp. minimum) Wiener index among all n-order trees. The extremal problems on the Wiener index among line graphs, connected graphs, circuit and bipartite graphs were also studied, see in [7, 8, 13, 18].

Based on them, researchers became interested in studying the extremal problems of the Wiener index among some graphs with given order and other parameters. The extremal values of the Wiener index among n-order trees with given diameter, number of branching vertices, maximum degree and maximum degree have been determined, and the corresponding extremal graphs characterized, refer to [1, 9, 14, 17]. Chen et al. [3] and Li et al. [11] determined the bounds of the Wiener index and characterized the corresponding extremal graphs among n-order bipartite graphs with given matching number. The study on the Wiener index and its extremal problems also can been seen in a survey [12] and recent researches [10, 22].

In this paper, we focus on studying the extremal problems of the Wiener index among some n-order graphs with given dissociation number.

A subset $S \subseteq V_G$ is called a *dissociation set* if the induced subgraph $G[S]$ does not contain P_3 as a subgraph. A *maximum dissociation set* of G is a dissociation set with the maximum cardinality. The *dissociation number* of G, written as $\varphi(G)$ (or φ for short), is the cardinality of a maximum dissociation set in G. Considerable research progress has focused on extremal problems for graphs with given dissociation sets. Among n-order trees, bipartite graphs and connected graphs with given dissociation number, the extremal problem of the Harary index, the spectral radius and the A_α-index was studied in [5,6,21], respectively. In addition, some researchers focused on investigating the number of maximum dissociation sets, for specific details, refer to [15,16,20].

Motivated by [5,6,21] directly, it is natural and interesting to determine the sharp lower bounds of the Wiener index and characterize the corresponding extremal graphs among n-order connected graphs (resp. bipartite graphs, trees) with given dissociation number. Furthermore, the graphs having the maximum Wiener indices with order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ are also characterized, respectively.

1.2 Main results

In this subsection, we give some basic notation and describe our main results. Let $\mathscr{G}_{n,\varphi}$ (resp. $\mathscr{B}_{n,\varphi}$, $\mathscr{T}_{n,\varphi}$) denote the set of connected graphs (resp. bipartite graphs, trees) with fixed order n and dissociation number φ. Note that the graph is just P_n for the order $n = 1, 2$, we consider that $n \geq 3$ in this paper.

Our first main result determine the minimum value of the Wiener index and characterize the corresponding extremal graph in $\mathscr{G}_{n,\varphi}$.

Theorem 1.1. *Let $G \in \mathscr{G}_{n,\varphi}$. If φ is even, then $W(G) \geq \frac{n^2-n+\varphi^2-2\varphi}{2}$ with equality if and only if $G \cong K_{n-\varphi} \vee \left(\frac{\varphi}{2}K_2\right)$; If φ is odd, then $W(G) \geq \frac{n^2-n+\varphi^2-2\varphi+1}{2}$ with equality if and only if $G \cong K_{n-\varphi} \vee \left(\frac{\varphi-1}{2}K_2 \cup K_1\right)$.*

The following result immediately follows from Theorem 1.1.

Corollary 1.2. *If G is a connected graph of order n with the minimum Wiener index, then $G \cong K_n$.*

Our second result establishes a sharp lower bound on the Wiener index among $\mathscr{B}_{n,\varphi}$. The corresponding extremal graph is also characterized.

Theorem 1.3. *Let $G \in \mathscr{B}_{n,\varphi}$. Then $W(G) \geq n^2+\varphi^2-n\varphi-n$ with equality if and only if $G \cong K_{\varphi,n-\varphi}$.*

Denote by $S^*_{n,\varphi}$ the tree on n vertices obtained from the star $S_{n-\varphi}$ by attaching exactly two pendant edges to each leaf of $S_{n-\varphi}$ and attaching

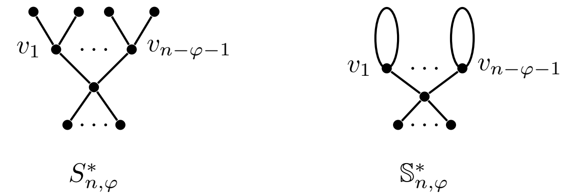

Figure 1. Trees $S^*_{n,\varphi}$ and $\mathbb{S}^*_{n,\varphi}$.

$3\varphi - 2n + 2$ pendant edges to the center of $S_{n-\varphi}$. Let $\mathbb{S}^*_{n,\varphi}$ be the set of n-vertex trees obtained from $S_{n-\varphi}$ by attaching exactly two pendant edges or one pendant path of length two to each leaf of $S_{n-\varphi}$ and then attaching $3\varphi - 2n + 2$ pendant edges to the center of $S_{n-\varphi}$. Obviously, $S^*_{n,\varphi} \in \mathbb{S}^*_{n,\varphi}$. Figure 1 gives an example for $S^*_{n,\varphi}$ and $\mathbb{S}^*_{n,\varphi}$, where the ellipses indicate two pendant edges or one pendant path of length two are attached at vertices $v_1, v_2, \ldots, v_{n-\varphi+1}$.

The next result characterizes all the trees in $\mathscr{T}_{n,\varphi}$ having the minimum Wiener index.

Theorem 1.4. *Let $T \in \mathscr{T}_{n,\varphi}$. Then $W(T) \geq 3n^2 - 2n\varphi - 12n + 8\varphi + 9$ with equality if and only if $T \cong S^*_{n,\varphi}$.*

Let $S(\ell_1, \ell_2)$ be the tree obtained by attaching ℓ_1 pendant edges and ℓ_2 pendant paths of length two to an isolated vertex, respectively. Denote by $T_1(s_1, t_1)$ the tree obtained from P_4 by attaching one pendant edge and s_1 pendant paths of length two to one leaf of P_4, and then attaching t_1 pendant paths of length two to another leaf of P_4. Let $T_2(s_2, t_2)$ be the tree obtained from P_4 by attaching s_2 and t_2 pendant paths of length two to the two leaves of P_4, respectively. Figure 2 gives an example for $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$. Obviously, the orders of $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$ are $\ell_1 + 2\ell_2 + 1, 2s_1 + 2t_1 + 5$ and $2s_2 + 2t_2 + 4$, respectively.

Our last result characterizes all the graphs in $\mathscr{G}_{n,\varphi}$ for $\varphi = 2$ (resp. $\left\lceil \frac{2}{3}n \right\rceil, n-2, n-1$) having the maximum Wiener indices.

Theorem 1.5. *Let G be a graph in $\mathscr{G}_{n,\varphi}$, where $\varphi \in \{2, \left\lceil \frac{2}{3}n \right\rceil, n-2, n-1\}$.*

(i) *If $\varphi = \left\lceil \frac{2}{3}n \right\rceil$, then $W(G) \leq \binom{n+1}{3}$ with equality if and only if $G \cong P_n$.*

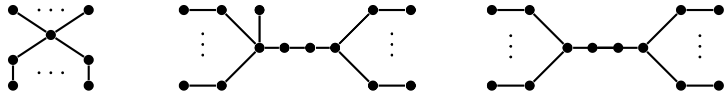

Figure 2. Graphs $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$

(ii) *If* $\varphi = 2$, *then* $W(G) \leq \frac{n^2}{2}$ *for even* n, *while* $W(G) \leq \frac{n^2-1}{2}$ *for odd* n. *The equalities hold if and only if* $G \cong K_n - M(K_n)$, *where* $M(K_n)$ *is a maximum matching of* K_n.

(iii) *If* $\varphi = n - 1$, *then* $W(G) \leq \frac{3n^2-9n+8}{2}$ *with equality if and only if* $G \cong \left(1, \frac{n-2}{2}\right)$ *for even* n*; while* $W(G) \leq \frac{3n^2-8n+5}{2}$ *with equality if and only if* $G \cong \left(0, \frac{n-1}{2}\right)$ *for odd* n.

(iv) *If* $n \geq 6$ *and* $\varphi = n - 2$, *then* $W(G) \leq \frac{3n^2-5n-8}{2} + 12 \left\lfloor \frac{n-4}{4} \right\rfloor \left\lceil \frac{n-4}{4} \right\rceil$ *with equality if and only if* $G \cong T_2\left(\left\lfloor \frac{n-4}{4} \right\rfloor, \left\lceil \frac{n-4}{4} \right\rceil\right)$ *for even* n*; while* $W(G) \leq \frac{3n^2-6n-3}{2} + 6\left\lceil \frac{n-5}{4} \right\rceil \left(1 + 2\left\lfloor \frac{n-5}{4} \right\rfloor\right)$ *with equality if and only if* $G \cong T_1\left(\left\lfloor \frac{n-5}{4} \right\rfloor, \left\lceil \frac{n-5}{4} \right\rceil\right)$ *for odd* n.

The remainder of this paper is organized as follows: In Section 2, we review some definitions and preliminary results. In Sections 3-6, we give proofs for Theorem 1.1, 1.3, 1.4 and 1.5, respectively. In the last section, we propose some problems for future studies.

2 Preliminary results

In this section, we give some preliminary results, which will be used to prove our main results. The following result immediately follows from the definition of dissociation number.

Lemma 2.1. *Let* G *be a simple graph. Then* $\varphi(G) - 1 \leq \varphi(G - v) \leq \varphi(G)$ *for any* $v \in V_G$.

Brešar et al. [2] gave a beautiful lower bound on the dissociation number of a tree, as shown below.

Lemma 2.2 ([2])**.** *Let* T *be a tree with* n *vertices. Then* $\varphi(T) \geq \frac{2n}{3}$.

For a graph G, denote by $\mathcal{P}(\mathcal{G})$ (resp. $\mathcal{Q}(G)$) the set of all pendant vertices (resp. quasi-pendant vertices) of G. In particular, let $\mathcal{Q}_2(G)$ be the set of all quasi-pendant vertices of degree 2 in G. Huang et al. [6] obtained an important property of the maximum dissociation set of G.

Lemma 2.3 ([6]). *Let G be a graph with order $n \geq 5$. Then there exists a maximum dissociation set $S(G)$ such that $\mathcal{P}(G) \cup \mathcal{Q}_2(G) \subseteq S(G)$.*

By the definition of the Wiener index, the following lemma is obvious.

Lemma 2.4. *Let G be a simple connected graph. Then $W(G+uv) < W(G)$ for any $uv \notin E_G$.*

The next conclusion involve the change of the Wiener index after a graph transformation.

Lemma 2.5. *Let G_1 and G_2 be two vertex-disjoint connected graphs with $v_i \in V_{G_i}$ and $|V_{G_i}| \geq 2$ for $i = 1, 2$. Denote by G the graph obtained from $G_1 \cup G_2$ by adding an edge between v_1 and v_2, and G' the graph obtained from $G_1 \cup G_2$ by identifying vertices v_1 and v_2 (the new vertex is labeled by v) and attaching a pendant edge at v. Then $W(G') < W(G)$.*

Proof. By the construction of the graph G and the definition of the Wiener index, we have

$$\begin{aligned}
W(G) &= \sum_{x,y \in V_{G_1}} d_G(x,y) + \sum_{x,y \in V_{G_2}} d_G(x,y) + \sum_{x \in V_{G_1}, y \in V_{G_2}} d_G(x,y) \\
&= W(G_1) + W(G_2) + d_G(v_1,v_2) + \sum_{x \in V_{G_1} \setminus \{v_1\}} d_G(x,v_2) \\
&\quad + \sum_{y \in V_{G_2} \setminus \{v_2\}} d_G(v_1,y) + \sum_{x \in V_{G_1} \setminus \{v_1\}, y \in V_{G_2} \setminus \{v_2\}} d_G(x,y) \\
&= W(G_1) + W(G_2) + 1 + \sum_{x \in V_{G_1} \setminus \{v_1\}} (d_{G_1}(x,v_1) + 1) \\
&\quad + \sum_{y \in V_{G_2} \setminus \{v_2\}} (1 + d_{G_2}(v_2,y)) + \sum_{x \in V_{G_1} \setminus \{v_1\}, y \in V_{G_2} \setminus \{v_2\}} (d_{G_1}(x,v_1) \\
&\quad + 1 + d_{G_2}(v_2,y)).
\end{aligned}$$

Recall the definition of the graph G' and let v_0 be the pendant vertex attached at v. One has

$$\begin{aligned} W(G') &= \sum_{x,y\in V_{G_1}} d_{G'}(x,y) + \sum_{x,y\in V_{G_2}} d_{G'}(x,y) + d_{G'}(v_0,v) \\ &\quad + \sum_{x\in V_{G_1}\setminus\{v_1\},y\in V_{G_2}\setminus\{v_2\}} d_{G'}(x,y) + \sum_{x\in V_{G'}\setminus\{v,v_0\}} d_{G'}(v_0,x) \\ &= W(G_1)+W(G_2)+1+\sum_{x\in V_{G_1}\setminus\{v_1\},y\in V_{G_2}\setminus\{v_2\}} (d_{G_1}(x,v_1) \\ &\quad + d_{G_2}(v_2,y)) + \sum_{x\in V_{G_1}\setminus\{v_1\}} (d_{G_1}(x,v_1)+1) \\ &\quad + \sum_{y\in V_{G_2}\setminus\{v_2\}} (d_{G_2}(v_2,y)+1). \end{aligned}$$

Thus, together with the fact that $|V_{G_i}| \geq 2$ for $i = 1, 2$, we get

$$W(G) - W(G') = \sum_{x\in V_{G_1}\setminus\{v_1\},y\in V_{G_2}\setminus\{v_2\}} 1 = (|V_{G_1}|-1)(|V_{G_2}|-1) > 0,$$

which implies $W(G') < W(G)$. This completes the proof. ■

The following result immediately follows from Lemma 2.5.

Corollary 2.6. *Let G be a connected graph with $|V_G| \geq 4$. Assume $v \in \mathcal{Q}_2(G)$ with $N(v) = \{w, u\}$ and $w \in \mathcal{P}(G)$. Then $W(G) > W(G-vw+uw)$.*

3 Proof of Theorem 1.1

In this section, we give the proof for Theorem 1.1.

Proof of Theorem 1.1. Let $S \subseteq V_G$ be a maximum dissociation set of G and denote $S' = V_G \setminus S$. Note that $G \in \mathscr{G}_{,\varphi}$. Clearly, $|S| = \varphi,\ |S'| = n - \varphi$. By Lemma 2.4, the induced subgraph $G[S'] \cong K_{n-\varphi}$ and each vertex in S is adjacent to each vertex in S'. Again by Lemma 2.4, we can also get $G[S] \cong \left(\frac{\varphi}{2}K_2\right)$ if φ is even; while $G[S] \cong \left(\frac{\varphi-1}{2}K_2 \cup K_1\right)$ otherwise. Thus, $G \cong K_{n-\varphi} \vee \left(\frac{\varphi}{2}K_2\right)$ if φ is even; while $G \cong K_{n-\varphi} \vee \left(\frac{\varphi-1}{2}K_2 \cup K_1\right)$ otherwise. Our result holds. ■

4 Proof of Theorem 1.3

In this section, we give the proof for Theorem 1.3.

Proof of Theorem 1.3. Assume $G^\star$ is in $\mathscr{B}_{,\varphi}$ with the minimum Wiener index, whose vertex set can be partitioned into two disjoint vertex classes X and Y. Without loss of generality, assume that $|X| \geq |Y|$. Obviously, $|X| \geq \frac{n}{2}$. Thus, $\varphi \geq |X| \geq \frac{n}{2}$ since X is a dissociation set of G. So we only need to consider that $\varphi \geq \frac{n}{2}$ in the following. Let S be a maximum dissociation set of $G^\star$. Clearly, $\varphi = |S| \geq |X|$.

If $\varphi > |X|$, then X is not a maximum dissociation set of $G^\star$. Thus, S can be partitioned as $S = X_1 \cup Y_2$ with $X_1 \subseteq X$ and $Y_2 \subseteq Y$. Denote $X_2 = X \setminus X_1,\ Y_1 = Y \setminus Y_2$ and let $|X_1| = a, |Y_1| = b, |X_2| = c,\ |Y_2| = d$. Since $\varphi = |S| = |X_1 \cup Y_2| > |X| \geq |Y|$, one has $a > b$ and $c < d$.

Recall that $G^\star$ is in $\mathscr{B}_{,\varphi}$ with the minimum Wiener index. By Lemma 2.4, it is easy to get that each vertex in Y_1 is adjacent to each vertex in X and each vertex in Y_2 is adjacent to each vertex in X_2. Moreover, since $S = X_1 \cup Y_2$ is a maximum dissociation set of $G^\star$, the induced subgraph $G^\star[S]$ just contains P_2 or P_1 as a subgraph. Combining with Lemma 2.4, we get there are as many matching edges as possible between X_1 and Y_2. Thus, $G^\star[S] \cong dP_2 \cup (a-d)P_1$ if $a \geq d$, while $G^\star[S] \cong aP_2 \cup (d-a)P_1$ if $a < d$.

If $a \geq d$, then $G^\star[S] \cong dP_2 \cup (a-d)P_1$ and there exists a set $X_{11} \subseteq X_1$ with $|X_{11}| = d$ such that $G^\star[X_{11} \cup Y_2]$ is a perfect matching. Note that $n \geq 3$ and $G^\star$ is connected. It is easy to get that $\max\{b, c\} \geq 1$. Now we proceed our proof by distinguishing the following three cases.

Case 1. $b \geq 1,\ c \geq 1$. Obviously, the distance is 1 for vertex pairs between X and Y_1, between X_2 and Y_2, and for those pairs connected by the matching edges between X_{11} and Y_2. The vertex pairs with distance 2 are those internal to X and those internal to Y. The distance is 3 for vertex pairs between X_{11} and Y_2 that are not linked by any matching edge, and for those pairs between $X \setminus X_{11}$ and Y_2. By the definition of $W(G^\star)$, one has

$$W(G^\star) \;=\; (ab + bc + cd + d) + 2\left[\binom{a}{2} + \binom{b}{2} + \binom{c}{2} + \binom{d}{2} + ac + bd\right]$$

$$
\begin{aligned}
&+3\left[d(d-1)+d(a-d)\right]\\
=\ & (a^2+b^2+c^2+d^2)+(ab+2ac+3ad+bc+2bd+cd)\\
&-(a+b+c+3d).
\end{aligned}
$$

Moreover, it is routine to check that

$$
\begin{aligned}
W(K_{a+d,b+c}) &= (a+d)(b+c)+2\left[\binom{a+d}{2}+\binom{b+c}{2}\right]\\
&= (a^2+b^2+c^2+d^2)+(ab+ac+2ad+2bc+bd+cd)\\
&\quad -(a+b+c+d).
\end{aligned}
$$

Therefore,

$$
W(K_{a+d,b+c})-W(G^\star)=d(2-a-b)+c(b-a). \tag{1}
$$

Recall that $b\geq 1,\ c\geq 1,\ a>b$ and $c<d$, one has $d\geq 2$ and $a\geq 2$. $W(K_{a+d,b+c})-W(G^\star)<0$ immediately follows from (1), contradicting the choice of $G^\star$.

Case 2. $b\geq 1,\ c=0$. Obviously, the distance is 1 for vertex pairs between X_1 and Y_1 and for those pairs connected by the matching edges between X_{11} and Y_2. The distance is 2 for vertex pairs between Y_1 and Y_2 and for those internal to X_1 and Y_1. The distance is 3 for vertex pairs between X_{11} and Y_2 that are not linked by any matching edge, and for those pairs between $X\setminus X_{11}$ and Y_2. The distance between any two vertices within Y_2 is 4. Thus,

$$
\begin{aligned}
W(G^\star)=&(ab+d)+2\left[\binom{b}{2}+\binom{a}{2}+bd\right]+3[d(d-1)+d(a-d)]+4\binom{d}{2}\\
=&(b^2+a^2+2d^2)+(ab+2bd+3ad)-(b+a+4d).
\end{aligned}
$$

Recall that $c=0$, one has

$$
W(K_{a+d,b+c})=W(K_{a+d,b})=(a^2+b^2+d^2)+(ab+bd+2ad)-(a+b+d)
$$

and $W(K_{a+d,b+c}) - W(G^\star) = d(3-b-a-d)$. Note that $a > b \geq 1$ and $d > c = 0$, we get $d \geq 1$ and $a \geq 2$. Thus, $W(K_{a+d,b}) - W(G^\star) < 0$, contradicting the choice of $G^\star$.

Case 3. $b = 0,\ c \geq 1$. Since $G^\star$ is a connected bipartite graph, thus $|X_1| = |X_{11}| = d$. In this case, the distance between any two vertices within X_1 is 4. By a similar way, we can get

$$\begin{aligned} W(G^\star) &= (cd+d) + 2\left[\binom{c}{2} + \binom{d}{2} + cd\right] + 3d(d-1) + 4\binom{d}{2} \\ &= c^2 + 6d^2 + 3cd - 5d - c \end{aligned}$$

and

$$W(K_{a+d,b+c}) = W(K_{2d,c}) = c^2 + 4d^2 + 2dc - 2d - c.$$

In view of $a \geq d$ and $d > c \geq 1$, we get $a \geq d \geq 2$. Thus,

$$W(K_{a+d,b+c}) - W(G^\star) = -2d^2 - cd + 3d = -d(2d+c-3) < 0,$$

contradicting the choice of $G^\star$.

If $a < d$, by a similar way, we can get a contradiction. Therefore, $\varphi = |X|$. Clearly, X is a maximum dissociation set of $G^\star$ and by Lemma 2.4 one has $G^\star \cong K_{\varphi,n-\varphi}$. By direct calculation, we have $W(K_{\varphi,n-\varphi}) = n^2 + \varphi^2 - n\varphi - n$, our result holds. ■

5 Proof of Theorem 1.4

In this section, we prove Theorem 1.4. First, we need some crucial results.

Lemma 5.1 ([4]). *Let $T \in \mathscr{T}_n$. Then $(n-1)^2 \leq W(T) \leq \binom{n+1}{3}$. The left equality holds if and only if $T \cong S_n$, whereas the right equality holds if and only if $T \cong P_n$.*

Lemma 5.2 ([6]). *Let $T \in \mathscr{T}_{n,\varphi}$ $(n \geq 3)$ and $\Delta(T)$ be the maximum degree of T. Then $\Delta(T) \leq 2\varphi - n + 1$ with equality if and only if $T \in \mathbb{S}^*_{n,\varphi}$.*

Then, we are ready to give the proof for Theorem 1.4.

Proof of Theorem 1.4. Note that $T \in \mathscr{T}_{n,\varphi}$ and $n \geq 3$. It is easy to get $\varphi \leq n-1$. If $\varphi = n-1$, then Lemma 5.1 gives $W(T) \geq (n-1)^2$ with equality if and only if $T \cong S_n$. Note that $S_n \cong S^*_{n,n-1}$, our result holds.

Now we consider that $\varphi \leq n-2$. We proceed by induction on n. If $3 \leq n \leq 9$, then it is straightforward to check that $W(T) \geq 3n^2 - 2n\varphi - 12n + 8\varphi + 9$ and the equality holds if and only if $T \cong S^*_{n,\varphi}$, as desired. In the following, we assume that the result holds for each tree with order less than n and consider the tree of order n.

Choose $T \in \mathscr{T}_{n,\varphi}$ $(n \geq 10)$ such that $W(T)$ is as small as possible. Let $P_k = v_1v_2v_3v_4\cdots v_k$ be a diametral path of T. Then it follows from Lemma 2.1 that $\varphi(T-v_1) \in \{\varphi, \varphi-1\}$. We proceed by distinguishing the following two cases to complete the proof.

Case 1. $\varphi(T-v_1) = \varphi-1$. It follows from Lemma 5.2 that $\Delta(T-v_1) \leq 2(\varphi-1)-(n-1)+1 = 2\varphi-n$. Therefore,

$$\begin{aligned}\sum_{v\in V_{T-v_1}} d_T(v,v_1) &= \sum_{v\in V_{T-v_1}} (d_{T-v_1}(v,v_2)+1)\\ &\geq 1+2d_{T-v_1}(v_2)+3(n-d_{T-v_1}(v_2)-2)\\ &= 3n-5-d_{T-v_1}(v_2)\\ &\geq 4n-2\varphi-5. \qquad (2)\end{aligned}$$

The equality in (2) holds if and only if $d_{T-v_1}(v_2) = \Delta(T-v_1) = 2\varphi-n$ and $d_{T-v_1}(v,v_2) = 2$ for any $v \notin N_{T-v_1}[v_2]$. Again by Lemma 5.2, (**??**) with equality if and only if $T-v_1 \cong S^*_{n-1,\varphi-1}$ and $d_{T-v_1}(v_2) = 2\varphi-n$.

The induction hypothesis together with (2) yields

$$\begin{aligned}W(T) &= W(T-v_1) + \sum_{v\in V_{T-v_1}} d_T(v,v_1)\\ &\geq 3(n-1)^2-2(n-1)(\varphi-1)-12(n-1)+8(\varphi-1)+9\\ &\quad +(4n-2\varphi-5)\\ &= 3n^2-12n-2n\varphi+8\varphi+9. \qquad (3)\end{aligned}$$

The equality in (3) holds if and only if $T-v_1 \cong S^*_{n-1,\varphi-1}$ and $d_{T-v_1}(v_2) = \Delta(T-v_1) = 2\varphi-n$. Note that $\varphi \geq \frac{2}{3}n$ by Lemma 2.2. Then $2\varphi-n \geq \frac{n}{3} > 3$, implying (3) holds with equality if and only if $T \cong S^*_{n,\varphi}$.

Furthermore, we may obtain $\varphi = n-2$ in this case. Indeed, if $\varphi \leq n-3$, then there exist at least two pendant vertices such that the distance between them is 4, contradicting the fact that v_1 lies on a diametral path of T. So $T \ncong S^*_{n,\varphi}$ and then $W(T) > 3n^2 - 12n - 2n\varphi + 8\varphi + 9 = W(S^*_{n,\varphi})$, contradicting the choice of T. Thus, $\varphi = n-2$ and $W(T) \geq 3n^2 - 12n - 2n\varphi + 8\varphi + 9$ with equality if and only if $T \cong S^*_{n,n-2}$, as desired.

Case 2. $\varphi(T - v_1) = \varphi$. Then there exists a maximum dissociation set, say $S(T)$, such that $v_1 \notin S(T)$. If $v_2 \notin S(T)$, then there will exist a dissociation set $S'(T) = S(T) \bigcup \{v_1\}$, such that $|S'(T)| > |S(T)|$, contradicting the choice of $S(T)$. Therefore, $v_2 \in S(T)$.

Now we prove that $d(v_2) = 3$. On the one hand, if $d(v_2) \geq 4$, then we may assume $\{x, y\} \subseteq N(v_2) \setminus \{v_1, v_3\}$. Recall that $P_k = v_1 v_2 v_3 v_4 \cdots v_k$ is a diametral path of T, it is obvious that both x and y are pendant vertices. Since $v_2 \in S(T)$, at most one of x and y belongs to $S(T)$. Without loss of generality, we may assume $y \notin S(T)$. Combining with Lemma 2.3, we can find a dissociation set $S''(T) = (S(T) - \{v_2\}) \bigcup \{y, v_1\}$, such that $|S''(T)| > |S(T)|$, which is also a contradiction. On the other hand, if $d(v_2) = 2$, then let $T' = T - v_1v_2 + v_1v_3$. It is easy to check T' is also in $\mathscr{T}_{n,\varphi-2}$ and by Corollary 2.6 one has $W(T') < W(T)$, a contradiction. Thus, $d(v_2) = 3$.

Assume that w is the unique vertex in $N(v_2) \setminus \{v_1, v_3\}$. By Lemma 2.3, there exists a maximum dissociation set $\bar{S}(T)$ satisfying $|\bar{S}(T)| = |S(T)|$ and $v_1, w \in \bar{S}(T)$, $v_2 \notin \bar{S}(T)$. Put $T'' = T - v_1 - v_2 - w$. Clearly, $\bar{S}(T) \setminus \{v_1, w\}$ is a maximum dissociation set of T''. Thus, $T'' \in \mathscr{T}_{n-3,\varphi-2}$. By a similar way as the proof of Case 1, we get

$$\begin{aligned} \sum_{v \in V_{T''}} d_T(v, v_1) &= \sum_{v \in V_{T''}} (d_{T''}(v, v_3) + 2) \\ &\geq 2 + 3d_{T''}(v_3) + 4(n - 4 - d_{T''}(v_3)) \\ &= 4n - d_{T''}(v_3) - 14 \\ &\geq 5n - 2\varphi - 14 \qquad (4) \end{aligned}$$

and

$$\begin{aligned}\sum_{v\in V_{T''}} d_T(v,v_2) &= \sum_{v\in V_{T''}} (d_{T''}(v,v_3)+1)\\ &\geq 1+2d_{T''}(v_3)+3(n-4-d_{T''}(v_3))\\ &= 3n-d_{T''}(v_3)-11\\ &\geq 4n-2\varphi-11. \end{aligned}\tag{5}$$

The equality in (4) and (5) holds if and only if $T'' \cong S^*_{n-3,\varphi-2}$ with $d_{T''}(v_3)=\Delta(T'')=2(\varphi-2)-(n-3)+1=2\varphi-n$ and $d_{T''}(v,v_3)=2$ for any $v\notin N_{T''}[v_3]$. Clearly, $d_T(v_1,v_2)=d_T(w,v_2)=1$ and $d_T(v_1,w)=2$. The induction hypothesis together with (4) and (5) yields

$$\begin{aligned}W(T) &= W(T'')+\sum_{v\in V_{T''}} d_T(v,v_1)+\sum_{v\in V_{T''}} d_T(v,w)+\sum_{v\in V_{T''}} d_T(v,v_2)\\ &\quad +d_T(v_1,v_2)+d_T(w,v_2)+d_T(v_1,w)\\ &\geq 3(n-3)^2-12(n-3)-2(n-3)(\varphi-2)+8(\varphi-2)+9\\ &\quad +2(5n-2\varphi-14)+(4n-2\varphi-11)+4\\ &= 3n^2-12n-2n\varphi+8\varphi+9. \end{aligned}\tag{6}$$

The equality in (6) holds if and only if $T''\cong S^*_{n-3,\varphi-2}$ with $d_{T''}(v_3)=\Delta(T'')=2\varphi-n>3$, which implies $T\cong S^*_{n,\varphi}$.

This completes the proof. ■

6 Proof of Theorem 1.5

In this section, we prove Theorem 1.5. First, we give some necessary preliminaries.

Lemma 6.1 ([8]). *Let G be a connected graph with n vertices. Then $\binom{n}{2}\leq W(G)\leq\binom{n+1}{3}$. The left equality holds if and only if $T\cong K_n$, whereas the right equality holds if and only if $T\cong P_n$.*

Lemma 6.2. *If $s_2\geq t_2\geq 1$, then $W(T_2(s_2+1,t_2-1))<W(T_2(s_2,t_2))$.*

Proof. Note that $T_2(s_2,t_2)$ can be obtained from $T_2(s_2,t_2-1)$ by attaching a pendant path of length two to the vertex of degree t_2, whereas $T_2(s_2+1,t_2-1)$ can be obtained from $T_2(s_2,t_2-1)$ by attaching a pendant path of length two to the vertex of degree s_2+1. Then

$$\begin{aligned} & W(T_2(s_2+1,t_2-1))-W(T_2(s_2,t_2)) \\ = \; & [(2+3(s_2+1)+4(s_2+1)+5+6(t_2-1)+7(t_2-1)) \\ & +(1+2(s_2+1)+3(s_2+1)+4+5(t_2-1)+6(t_2-1))] \\ & -[(2+3t_2+4t_2+5+6s_2+7s_2)+(1+2t_2+3t_2+4+5s_2+6s_2)] \\ = \; & 12(t_2-s_2-1)<0, \end{aligned}$$

which implies $W(T_2(s_2+1,t_2-1))<W(T_2(s_2,t_2))$, as desired. ■

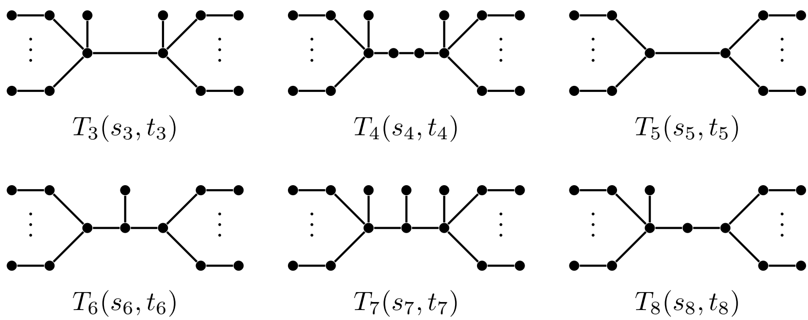

Figure 3. Tree $T_i(s_i,t_i)$ $(3\le i\le 8)$.

Let $T_3(s_3,t_3)$ (resp. $T_4(s_4,t_4)$) be the tree obtained from P_4 (resp. P_6) by attaching s_3 (resp. s_4) and t_3 (resp. t_4) pendant paths of length two to the two quasi-pendant vertices of P_4 (resp. P_6), respectively. Let $T_5(s_5,t_5)$ (resp. $T_6(s_6,t_6)$) be the tree obtained from P_2 (resp. S_4) by attaching s_5 (resp. s_6) and t_5 (resp. t_6) pendant paths of length two to two leaves of P_2 (resp. S_4), respectively. Let $T_7(s_7,t_7)$ be the tree obtained from $S(1,2)$ by attaching s_7 and t_7 pendant paths of length two to the two quasi-pendant vertices with degree 2 of $S(1,2)$, respectively. Let $T_8(s_8,t_8)$ be the tree obtained from P_3 by attaching one pendant edge and s_8 pendant paths of length two to one leaf of P_3, and then attaching t_8 pendant paths of length two to another leaf of P_3. Figure 3 gives an example for $T_i(s_i, t_i)$ $(3 \leq i \leq 8)$. Obviously, $|V_{T_i(s_i,t_i)}| = 2s_i+2t_i+4$ for $i \in \{3, 6, 8\}$, $|V_{T_i(s_i,t_i)}| = 2s_i+2t_i+6$ for $i \in \{4, 7\}$ and $|V_{T_5(s_5,t_5)}| = 2s_5 + 2t_5 + 2$.

Lemma 6.3. *If* $(s_4, t_4) \neq (0, 0)$, *then*

$$W(T_4(s_4, t_4)) < \max\{W(T_2(s_4, t_4 + 1)), W(T_2(s_4 + 1, t_4))\}.$$

Proof. If $s_4 \geq t_4$, then $s_4 \geq 1$ and direct calculation yields

$$\begin{aligned} & W(T_4(s_4, t_4)) - W(T_2(s_4, t_4 + 1)) \\ = \ & [1 + 2(s_4 + 1) + 3(s_4 + 1) + 4 + 5(t_4 + 1) + 6t_4] \\ & -[1 + 2 + 3(t_4 + 1) + 4(t_4 + 1) + 5 + 6s_4 + 7s_4] \\ = \ & 4(t_4 - 2s_4) < 0, \end{aligned}$$

which implies $W(T_4(s_4, t_4)) < W(T_2(s_4, t_4 + 1))$.

Otherwise, $s_4 < t_4$. Clearly, $t_4 \geq 1$ and similarly we get $W(T_4(s_4, t_4)) < W(T_2(s_4 + 1, t_4))$. This completes the proof. ■

Lemma 6.4. *If* $\min\{s_5, t_5\} \geq 1$ *and* $(s_5, t_5) \neq (1, 1)$, *then*

$$W(T_5(s_5, t_5)) < \begin{cases} W(T_2(s_5 - 1, t_5)), & \text{if } s_5 \geq 2; \\ W(T_2(s_5, t_5 - 1)), & \text{if } t_5 \geq 2, \end{cases}$$

Proof. Obviously, s_5 or $t_5 \geq 2$. If $s_5 \geq 2$, then by direct calculation one has

$$\begin{aligned} W(T_5(s_5, t_5)) &= (2s_5 + 2t_5 + 1) + 2\left[2s_5 + 2t_5 + \binom{s_5}{2} + \binom{t_5}{2}\right] \\ &\quad +3[s_5(s_5 - 1) + t_5(t_5 - 1) + s_5 + t_5 + s_5t_5] \\ &\quad +4\left[\binom{t_5}{2} + \binom{s_5}{2} + 2s_5t_5\right] + 5s_5t_5 \\ &= 6t_5^2 + 6s_5^2 + 3s_5 + 3t_5 + 16s_5t_5 + 1 \end{aligned}$$

and

$$\begin{aligned} W(T_2(s_5-1,t_5)) &= [2(s_5-1)+2t_5+3]+2\left[s_5-1+t_5+\binom{s_5}{2}\right. \\ &\quad \left.+\binom{t_5+1}{2}+2\right]+3[(s_5-1)(s_5-2)+t_5(t_5-1) \\ &\quad +2(s_5-1)+2t_5+1]+4\left[\binom{t_5}{2}+\binom{s_5-1}{2}\right. \\ &\quad +2(s_5-1)+2t_5]+5[s_5-1+t_5+(s_5-1)t_5] \\ &\quad +6[2(s_5-1)t_5]+7(s_5-1)t_5 \\ &= 6t_5^2+6s_5^2+7s_5-5t_5+24s_5t_5-3. \end{aligned}$$

Thus,

$$\begin{aligned} W(T_2(s_5-1,t_5))-W(T_5(s_5,t_5)) &= 4s_5-8t_5+8s_5t_5-4 \\ &= 4(s_5-1)(2t_5+1) \\ &> 0, \end{aligned}$$

that is, $W(T_5(s_5,t_5)) < W(T_2(s_5-1,t_5))$.

By a similar way, we can get $W(T_5(s_5,t_5)) < W(T_2(s_5,t_5-1))$ when $t_5 \geq 2$. This completes the proof. ■

Then, we give the proof for Theorem 1.5.

Proof of Theorem 1.5. (i) It immediately follows from Lemma 6.1 and $\varphi(P_n) = \lceil \frac{2}{3}n \rceil$.

(ii) Let $G \in \mathscr{G}_{n,2}$ be the graph having the maximum Wiener index. Then G does not contain $3K_1$ or $K_2 \cup K_1$ as an induced subgraph, which implies $d_{\bar{G}}(v) \leq 1$ for every $v \in V_G$, where $\bar{G}$ is the complement graph of G. That is to say, $E_{\bar{G}}$ is a matching of K_n. Combining with Lemma 2.4, we get $G \cong K_n - M(K_n)$, where $M(K_n)$ is a maximum matching of K_n. Some direct calculations yield that $W(K_n - M(K_n)) = \frac{n^2}{2}$ if n is even and $W(K_n - M(K_n)) = \frac{n^2-1}{2}$ otherwise. Thus, (ii) holds.

(iii) Let $G \in \mathscr{G}_{n,n-1}$ $(n \geq 3)$ be a graph having the maximum Wiener index and let $S = S_1 \cup S_2$ be a maximum dissociation set of G such that

$G[S_1]$ is a perfect matching and S_2 is an independent set. Assume that $V_G = \{v_1, v_2, \ldots, v_n\}$ and $S = V_G \setminus \{v_1\}$. Then $S_2 \subseteq N(v_1) \cap \mathcal{P}(G)$ since G is connected.

If there exist two vertices, say v_{n-1} and v_n, such that $\{v_{n-1}, v_n\} \subseteq S_2$, then we put $G' = G - v_1v_{n-1} + v_nv_{n-1}$ and get $G' \in \mathscr{G}_{n,n-1}$ by Lemma 2.3. In view of Corollary 2.6, we have $W(G') > W(G)$, contradicting the choice of G. Therefore, $|S_2| \leq 1$. Note that G is connected, and together with Lemma 2.4, we conclude that just one edge connects v_1 to each connected component of $G[S_1]$. This implies $G \cong S\left(1, \frac{n-2}{2}\right)$ if n is even and $G \cong S\left(0, \frac{n-1}{2}\right)$ if n is odd, where $S(\ell_1, \ell_2)$ is the graph shown in Figure 2. Some simple calculation gives $W(S\left(1, \frac{n-2}{2}\right)) = \frac{3n^2-9n+8}{2}$ and $W(S\left(0, \frac{n-1}{2}\right)) = \frac{3n^2-8n+5}{2}$. Thus, (iii) holds.

(iv) Let G be a graph in $\mathscr{G}_{n,n-2}$ $(n \geq 6)$ having the maximum Wiener index and let $S = S_1 \cup S_2$ be a maximum dissociation set of G such that $G[S_1]$ is a perfect matching and S_2 is an independent set. Assume that $V_G = \{v_1, v_2, \ldots, v_n\}$ and $S = V_G \setminus \{v_1, v_2\}$. If $|N(v_1) \setminus \{v_2\}| = 0$, then v_1 is a leaf, we can find a dissociation set $S' = S \bigcup \{v_1\}$ with $|S'| = |S| + 1$, contradicting the choice of S. Thus, $|N(v_1) \setminus \{v_2\}| \geq 1$. Similarly, one may also get $|N(v_2) \setminus \{v_1\}| \geq 1$.

Now we prove that $|N(v_1) \cap N(v_2)| \leq 1$. Indeed, if $|N(v_1) \cap N(v_2)| \geq 2$, then we assume $\{v_3, v_4\} \subseteq N(v_1) \cap N(v_2)$. If either v_3 or v_4 is in S_1, we may assume, without loss of generality, that $v_4 \in S_1$ and let $G' = G - v_1v_3$. Clearly, S is also a maximum dissociation set of G'. Otherwise, both v_3 and v_4 are in S_2. Since G is connected and $n \geq 6$, there exists a vertex, say $v_5 \in S \setminus \{v_3, v_4\}$, such that $v_5 \in N(v_1) \cup N(v_2)$. Without loss of generality, we assume $v_5 \in N(v_1)$. We also let $G' = G - v_1v_3$ and it is easy to get S is also a maximum dissociation set of G' since $\{v_4, v_5\} \subseteq N(v_1)$. Thus, $G' \in \mathscr{G}_{n,n-2}$ and one has $W(G') > W(G)$ by Lemma 2.4, a contradiction.

So $|N(v_1) \cap N(v_2)| \leq 1$ and there are at least $|S_2| - 1$ leaves in S_2. If $|S_2| \geq 4$, by the pigeonhole principle at least two pendant vertices are adjacent to some $v_i (i \in \{1, 2\})$. By Corollary 2.6, one has a graph in $\mathscr{G}_{n,n-2}$ with a larger Wiener index, a contradiction. Thus, $|S_2| \leq 3$.

When n is even, one has $|S_2| \in \{0, 2\}$. We proceed by distinguishing the following two cases to complete the proof.

Case 1. $N(v_1) \cap N(v_2) = \emptyset$. By Corollary 2.6, we may get at most one vertex in S_2 is adjacent to v_1 (resp. v_2).

If $|S_2| = 2$ and $v_1 \in N(v_2)$, then by Lemma 2.4 one has $G \cong T_3(s_3, t_3)$ with $s_3 + t_3 = \frac{n-4}{2}$. If $s_3 = t_3 = 0$, then $n = 4$, a contradiction with $n \geq 6$. If $s_3 = 0,\ t_3 \neq 0$ or $s_3 \neq 0,\ t_3 = 0$, then $\varphi = n - 1$, which is also a contradiction with $G \in \mathscr{G}_{n,n-2}$. Thus, $\min\{s_3, t_3\} \geq 1$. By Lemma 2.5, we have $W(G) < W(T_2(s_3, t_3))$. Note that $T_2(s_3, t_3)$ is also in $\mathscr{G}_{n,n-2}$, there is a contradiction.

If $|S_2| = 2$ and $v_1 \notin N(v_2)$, then $G \cong T_4(s_4, t_4)$ with $s_4 + t_4 = \frac{n-6}{2}$. Furthermore, if $(s_4, t_4) = (0, 0)$, then $n = 6$ and $G \cong T_2(0, 1)$, our result holds. If $(s_4, t_4) \neq (0, 0)$, then by Lemma 6.3 one has $W(G) < \max\{W(T_2(s_4, t_4 + 1)), W(T_2(s_4 + 1, t_4))\}$, which implies a contradiction since both $T_2(s_4, t_4 + 1)$ and $T_2(s_4 + 1, t_4)$ are in $\mathscr{G}_{n,n-2}$.

If $|S_2| = 0$ and $v_1 \in N(v_2)$, then $G \cong T_5(s_5, t_5)$ with $s_5 + t_5 = \frac{n-2}{2}$. It is easy to check that $\min\{s_5, t_5\} \geq 1$ since $G \in \mathscr{G}_{n,n-2}$. In addition, if $s_5 = t_5 = 1$, then $G \cong T_2(0, 1)$, our result holds. If $(s_5, t_5) \neq (1, 1)$, then by Lemma 6.4, we get $W(G) < W(T_2(s_5 - 1, t_5))$ when $s_5 \geq 2$, while $W(G) < W(T_2(s_5, t_5 - 1))$ when $t_5 \geq 2$, which is a contradiction since both $T_2(s_5 - 1, t_5)$ and $T_2(s_5, t_5 - 1)$ are in $\mathscr{G}_{n,n-2}$.

If $|S_2| = 0$ and $v_1 \notin N(v_2)$, then $G \cong T_2(s_2, t_2)$ with $s_2 + t_2 = \frac{n-4}{2}$. Therefore, $G \cong T_2\left(\left\lfloor \frac{n-4}{4} \right\rfloor, \left\lceil \frac{n-4}{4} \right\rceil\right)$ by Lemma 6.2, our result holds.

Case 2. $|N(v_1) \cap N(v_2)| = 1$. In this case, we obtain $v_1 \notin N(v_2)$. Otherwise, $G - v_1v_2$ is also in $\mathscr{G}_{n,n-2}$ with $W(G - v_1v_2) > W(G)$ by Lemma 2.4, a contradiction.

If $|S_2| = 0$, then $G \cong T_6(s_6, t_6)$ with $(s_6, t_6) \neq (0, 0)$ and $s_6 + t_6 = \frac{n-4}{2}$. By Lemma 2.5 one has $W(G) < W(T_2(s_6, t_6))$, which is a contradiction since $T_2(s_6, t_6) \in \mathscr{G}_{n,n-2}$.

If $|S_2| = 2$ and $N(v_1) \cap N(v_2) \subseteq S_1$. By Corollary 2.6, there is at most one vertex in S_2 that adjacent to v_1 or v_2. Recall that $G \in \mathscr{G}_{n,n-2}$, one has $G \cong T_7(s_7, t_7)$ with $(s_7, t_7) \neq (0, 0)$ and $s_7 + t_7 = \frac{n-6}{2}$. Again by Lemma 2.5, $W(G) < W(T_4(s_7, t_7))$. Note that $T_4(s_7, t_7) \in \mathscr{G}_{n,n-2}$, a contradiction.

If $|S_2| = 2$ and $N(v_1) \cap N(v_2) \subseteq S_2$, then $G \cong T_8(s_8, t_8)$ with $t_8 \geq 1$ and $s_8 + t_8 = \frac{n-4}{2}$. Similarly, $G \cong T_2(0, t_8)$ for $s_8 = 0$ and $W(G) < W(T_2(s_8, t_8))$ for $s_8 \geq 1$, a contradiction.

By direct calculation, we have

$$W(T_2(s_2,t_2)) = \frac{3n^2-5n-8}{2} + 12\left\lfloor \frac{n-4}{4} \right\rfloor \left\lceil \frac{n-4}{4} \right\rceil.$$

Therefore, (iv) holds for even n.

When n is odd, by a similar discussion as the proof above, we can also get (iv) holds. This completes the proof. ■

7 Concluding remarks

Inspired by [5] and [21], it's natural to consider the following interesting problem:

Problem 1. *Extremal problems for the distance spectral radius of graphs with given order and dissociation number.*

Problem 2. *For a set* $\mathbb{G}$ *of graphs satisfying some certain conditions, determine* $\min\{W(G) \mid G \in \mathbb{G}\}$ *and* $\max\{W(G) \mid G \in \mathbb{G}\}$*, and characterize the extreme graphs which achieve the minimum or maximum value.*

In this paper we focus on Problem 2 for $\mathbb{G} \in \{\mathscr{G}_{n,\varphi}, \mathscr{B}_{n,\varphi}, \mathscr{T}_{n,\varphi}\}$. Theorem 1.1 (resp. Theorem 1.3, Theorem 1.4) characterizes all the connected graphs (resp. bipartite graphs, trees) having the minimum Wiener indices among all connected graphs (resp. bipartite graphs, trees) with given order and dissociation number. Theorem 1.5 determines the graphs with fixed order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ having the maximum Wiener indices.

It is nature to extend this study through examining the following extreme graphs:

- Let $G \in \mathscr{G}_{n,\varphi}$ be the graph having the maximum Wiener index with $\varphi > \frac{2}{3}n$. Then G is a tree.
- trees with fixed order n and dissociation number φ_1 having the maximum Wiener indices, where $\lceil \frac{2}{3}n \rceil < \varphi_1 < n-2$;
- connected bipartite graphs with fixed order n and dissociation number φ_2 having the maximum Wiener indices, where $\lceil \frac{n}{2} \rceil < \varphi_2 < n-2$;

- graphs with fixed order n and dissociation number φ_3 having the maximum Wiener indices, where $2 < \varphi_3 < n - 2$.

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