On the Wiener Index of Graphs with Predetermined Dissociation Number

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Abstract—**In this paper, we focus on the concept of dissociation sets in a graph $G = (V_G, E_G)$, we find the maximum dissociation set by looking for a maximum subset of vertices in the graph such that no edges are connected between any two vertices in the subset. It is the same as the maximum independent set in the graph, but in the definition of dissociation set, it is also allowed to have edges between vertices in the subset, provided that each vertex is connected by at most one edge. The primary objective of this paper is to determine the minimum values of the Wiener indices for all connected graphs with a predetermined order and a specified dissociation number. Specifically, we aim to establish loose lower bounds for the Wiener index among these graphs and identify the corresponding extremal graphs that achieve these lower bounds. Furthermore, we also explore the graphs that attain the maximum Wiener indices for a predetermined order n and a given dissociation number $\varphi \in \{2, \lceil \frac{2n}{3} \rceil, n-1\}$. These results provide valuable insights into the structural properties of graphs with specific dissociation characteristics and their impact on the Wiener index.**

Index Terms—**Connected graphs, Predetermined order and dissociation, Wiener index.**

I. Introduction

We start with some background information on launching the main results, and this section will also give some of the main results.

The graphs under consideration are simple, undirected and connected, see [1] and the references cited therein. For a graph $G = (V_G, E_G)$, V_G is the vertex set and E_G is the edge set. P_n, S_n and K_n represent respectively a path, a star and a complete graph with n vertices. The minimum distance between vertices u and v is written $d_G(u, v)$. Diameter is the maximum distance between any two vertices in the graph, denoted as $diam(G)$. And we call $|V_G|$ the order of G.

We use T denote as a tree. $V(T)$ and $E(T)$ mean the set of vertices and edges of a tree. And a tree is a connected acyclic graph. A pendent vertex is a vertex that is connected to exactly one other vertex. The unique n-vertex trees with two and $n-1$ pendent vertices are called the path and star, respectively, and are denoted by P_n and S_n.

$N_G(v)$ is usually used to represent a graph set of neighbors of a vertex v in G. Specifically, given an undirected graph G and a vertex v in the graph, $N_G(v)$ defined as $N_G(v) = \{u \in V | \{u, v\} \in E\}$. And $N_G[V] := N_G(v) \bigcup \{v\}$ be the closed neighborhood of $v \in V_G$. We use $d_G(V) = |N_G(v)|$ to denote the degree of v. To keep things simple, $G - v$ means delete vertex $v \in V_G$ and $G - uv$ is by deleting edge $uv \in E_G$ in the graph of G. When G_1 and G_2 are connected, we call $G_1 \bigcup G_2$ and when they are attach with each other, we denote as $G_1 \bigvee G_2$. And the connection of k copies of G is kG.

A set of vertices in a graph is termed an independent set if there are no edges linking any two vertices within the set. In other words, an independent set is an edge-free subgraph. A dissociation set is a subset of vertices in a graph that forms an induced subgraph with at most one edge between any two vertices. Unlike an independent set, a dissociation set allows one edge between vertices, but no more than one. The dissociation number $\varphi(G)$ of a graph G is defined as the size of its largest dissociation set, which is a collection of vertices such that no two are adjacent. The matter of determining $\varphi(G)$ was initially proposed by Yannakakis [2] in 1981. Finding the maximal dissociation set is an NP-complete problem.

The Wiener index is an important metric in chemical graph theory for measuring the structural properties of molecules. It is named in honor of the Austrian chemist Harold Wiener [3], who introduced the concept in 1947 to describe the molecular structure of hydrocarbon compounds. Wiener index exhibits a broad spectrum of applications in chemoinformatics, molecular descriptors and graph theory, see [4], [5], [6], [7]. In a undirected and connected graph G, the Wiener index is calculated as the aggregate of the shortest path lengths between every pair of vertices within the graph. The formalization is defined as follows

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

the summation encompasses every pair of vertices in G. The hyper-Wiener index of G, initially presented by Randić [8] in 1993, is characterized by [9]

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V_G} d_G(u, v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V_G} d_G(u, v)^2. \tag{2}$$

In the decades that followed, Plavšić et al. [12] and Ivanciuc et al. [13] proposed another distance-based graph constant, named Harary index, which is is characterized by

$$H(G) = \sum_{\{u,v\} \subseteq V_G} \frac{1}{d_G(u, v)}. \tag{3}$$

In molecular graph theory, Harary index is used to study the structure and properties of molecules, particularly how atoms within a molecule are connected. It can also be applied to assess the robustness and efficiency of networks, where a higher index may indicate a more robust and efficient

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network structure. Subsequently, this invariant has been reformulated as half the sum of the entries within the Harary matrix, it provides a matrix representation of the connectivity of a graph based on the reciprocal of distances between pairs of vertices.

Topological index is mainly used to analyze the nature of molecular structure, to evaluate the chemical and physical properties of compounds, and to solve optimization problems in graph theory [17]. Wiener index is an significant topological index, primarily used to assess molecular transitivity and molecular similarity. The literature extensively explores the mathematical characteristics and applications of the Wiener index, one may be referred to [18], [20].

Numerous researchers have shown interest in determining the loose lower bounds of the Wiener index for all connected graphs. Gutman [21] showed P_n and S_n. Research has demonstrated that similar bounds are applicable to various recently introduced modifications of the Wiener index. Božović Vladimir et al. [24] examined trees of order n with a specified count of vertices possessing the highest degree, and addressed the minimal extremal problem regarding the Wiener index within that category. Shan Zhang et al. [25] identified a subset of unicyclic graphs with a given order n and maximum degree Δ that achieve the minimum Wiener index.

The present article delves into the issue of identifying the minimum and maximum values of Wiener index and this manuscript investigates the matter of determining the extreme graphs that correspond to connected graphs with a predetermined order and dissociation number.

II. Key findings

In this segment, we establish foundational symbols and present the key findings. Let $\mathscr{C}_{n,\varphi}$ (respectively. $\mathscr{B}_{n,\varphi}$, $\mathscr{T}_{n,\varphi}$) represent the set of connected graphs (respectively. bipartite graphs, trees) characterized by a predetermined order n and dissociation number φ.

Introducing an edge to a connected graph reduces its Wiener index. Consequently, it is evident that the minimum Wiener index value and the associated extremal graph among all connected graphs are straightforward.

Theorem 2.1 Let $G \in \mathscr{C}_{n,\varphi}$. Then

$$W(G) \geq \begin{cases} \frac{n(n-1)}{2} + \frac{\varphi(\varphi-2)}{2}, & if\ \varphi\ is\ even; \\ \frac{n(n-1)}{2} + \frac{(\varphi-1)^2}{2}, & if\ \varphi\ is\ odd. \end{cases}$$

with equality holds when

$$G \cong \begin{cases} K_{n-\varphi} \bigvee (\frac{\varphi}{2} K_2), & if\ \varphi\ is\ even; \\ K_{n-\varphi} \bigvee (\frac{\varphi-1}{2} K_2 \bigcup K_1), & if\ \varphi\ is\ odd. \end{cases}$$

Case 1 When $n = 3$, $\varphi = 2$, then $W(G) \geq \frac{3\times 2}{2} + \frac{2\times 0}{2} = 3$ In the extremal graph of $K_1 \bigvee K_2$, $W(G) = d(v_1, v_2) + d(v_1, v_3) + d(v_2, v_3) = 3$;

Case 2 When $n = 4$, $\varphi = 3$, then $W(G) \geq \frac{3\times 4}{2} + \frac{2\times 2}{2} = 8$ In the extremal graph of $K_1 \bigvee (K_2 \bigcup K_1)$, $W(G) = d(v_1, v_2) + d(v_1, v_3) + d(v_1, v_4) + d(v_2, v_3) + d(v_2, v_4) + d(v_3, v_4) = 8$.

The subsequent finding involves determining a broad lower bound for the Wiener index of bipartite graphs with a predetermined order and dissociation number, with the characterization of the corresponding extremal graph.

Theorem 2.2 Let $G \in \mathscr{B}_{n,\varphi} (n \geq 3)$. Then $W(G) \geq n^2 - (\varphi+1)n + \varphi^2$ with equality holding when $G \cong K_{\varphi, n-\varphi}$. The next result characterizes all the tree $T \in \mathscr{T}_{n,\varphi}$ having the minimum Wiener index.

Let $S^*_{n,\varphi}$ be a tree with n vertices, constructed by appending two pendent edges to each leaf of $S_{n-\varphi}$ and adding $3\varphi - 2n + 2$ pendent edges to the center vertex of $S_{n-\varphi}$. Denote $\mathbb{S}_{n,\varphi}$ as the set of trees with n vertices, where two pendent edges or a pendent path of length two are attached to each leaf of $S_{n-\varphi}$ and $3\varphi - 2n + 2$ pendent edges are attached to the central vertex of $S_{n-\varphi}$. Clearly, $S^*_{n,\varphi} \in \mathbb{S}_{n,\varphi}$. Fig. 1 gives an example of $S^*_{n,\varphi}$ and $\mathbb{S}_{n,\varphi}$, where each ellipse signifies the addition of two pendent edges or a pendent path of length two to vertices $v_1, v_2, \cdots, v_{n-\varphi-1}$.

Fig. 1. Trees $S^*_{n,\varphi}$ (left) and $\mathbb{S}^*_{n,\varphi}$ (right)

Theorem 2.3 Let $T \in \mathscr{T}_{n,\varphi} (n \geq 3)$. Then $W(T) \geq \frac{1}{2}n^2 - 2n + \frac{1}{2}\varphi^2 + \varphi + \frac{3}{2}$ with equality holds when $T \cong S^*_{n,\varphi}$.

Theorem 2.4 Consider a graph G in $\mathscr{C}_{n,\varphi}$, where $\varphi \in \{2, \lceil \frac{2n}{3} \rceil, n-1\}$.

(i) If $\varphi = \lceil \frac{2n}{3} \rceil$, then $W(G) \leq \binom{n+1}{3} = \frac{n^3-n}{6}$ with equality holds when $G \cong P_n$.

(ii) If $\varphi = 2$, then

$$W(G) \leq \begin{cases} \frac{2n^2-3n}{4}, & if\ n\ is\ even; \\ \frac{2n^2-3n+4}{4}, & if\ n\ is\ odd. \end{cases}$$

with equality holds when $G \cong K_n - M(K_n)$, where $M(K_n)$ is a maximum matching of K_n.

(iii) If $n \geq 3$ and $\varphi = n - 1$, then

$$W(G) \leq \begin{cases} \frac{3n^2-9n+8}{2}, & if\ n\ is\ even; \\ \frac{3n^2-8n+7}{2}, & if\ n\ is\ odd. \end{cases}$$

with equality holds when

$$G \cong \begin{cases} S(1, \frac{n-2}{2}), & if\ n\ is\ even; \\ S(0, \frac{n-1}{2}), & if\ n\ is\ odd. \end{cases}$$

III. Initial findings

In this section, we give few preparatory results for proving the key findings. The subsequent finding is directly inferred from the definition of the dissociation number.

Lemma 3.1 For a simple graph G. It holds that $\varphi(G) - 1 \leq \varphi(G - v) \leq \varphi(G)$ for any vertex $v \in V_G$.

Brešar et al.[26] established a lower bound for the dissociation number in trees, as described subsequently.

Lemma 3.2 ([26]) Consider a tree T with n vertices. It follows that $\varphi(T) \geq \frac{2n}{3}$.

For a graph G, denote $\mathcal{P}(G)$ and $\mathcal{Q}(G)$ as the set of all pendent vertices and quasi-pendent vertices of G. Let $\mathcal{Q}_2(G)$ as the set of all quasi-pendent vertices of degree two in G. The next result by Jing Huang et al. [33] is crucial for proving Theorem 2.3.

Lemma 3.3 ([33]) Consider a graph G of order $n \geq 5$. It is then possible to identify a maximum dissociation set $S(G)$ that encompasses $\mathcal{P}(G) \bigcup \mathcal{Q}_2(G) \subseteq S(G)$.

The next result involve the change of the Wiener index after some graph transformations.

Lemma 3.4 Let G be a simple and connected graph. Then $W(G+uv) < W(G)$ for any $uv \notin E_G$.

Lemma 3.5 Let G_1 and G_2 be two separate connected graphs with vertex sets V_{G_1} and V_{G_2}, respectively. Denote G as the graph obtained from $G_1 \bigcup G_2$ by joining an edge between v_1 and v_2, and G' as the graph obtained from $G_1 \bigcup G_2$ by identifying vertices v_1 and v_2 and adding a pendent edge at v. Then $W(G) > W(G')$.

The subsequent corollary is derived from Lemma 3.5.

Corollary 3.6 Consider a connected graph G that has $|V_G| \geq 4$. Suppose $v \in \mathcal{Q}_2(G)$ with $N(v) = \{w, u\}$ and $w \in \mathcal{P}(G)$. Then $W(G) > W(G - vw + uw)$.

IV. Proof of Theorem 2.2

Now we present the proof for Theorem 2.2, which we carve all connected bipartite graphs with predetermined order and dissociation number with minimal Wiener index.

Proof. Assuming that $G^\star = (X, Y)$ is a connected bipartite graph with minimal Wiener index in $\mathscr{B}_{n,\varphi}$. Without prejudice to generality, suppose that $|X| \geq |Y|$. Suppose S is a maximal dissociation set for $G^\star$. Afterwards $\varphi = |S| \geq |X|$. By Lemma 3.4, it follows that if $\varphi = |X|$, then $G^\star \cong K_{\varphi,n-\varphi}$. Next suppose that $\varphi > |X|$. Then S can be categorized as $S = X_1 \bigcup Y_2$, where $X_1 \subseteq X$ and $Y_2 \subseteq Y$. Let $X_2 = X \backslash X_1$ and $Y_1 = Y \backslash Y_2$, and let $|X_1| = a$, $|Y_1| = b$, $|X_2| = c$, $|Y_2| = d$. Recognizes that $|X_1 \bigcup Y_2| > |X| \geq |Y|$, then $a > b$ and $c < d$. Since $G^\star$ is a bipartite graph with a minimal Wiener index. So we known that every vertex in X_1 is connected to every vertex in Y_1, every vertex in X_2 is connected to every vertex in Y, and there are as many matching edges as possible between X_1 and Y_2. If $d \geq a$, there will be a set $Y_{21} \subseteq Y_2$ with $|Y_{21}| = a$ such that $G^\star[X_1 \bigcup Y_{21}]$ is a perfect matching.
By some direct computation, we get

$$\begin{aligned} W(G^\star) =& (ab+bc+cd+a) + 2[\binom{a}{2} + \binom{b}{2} + \binom{c}{2} \\ &+ \binom{d}{2} + ac + bd] + 3[a(a-1) + a(d-a)] \\ =& a^2 + b^2 + c^2 + d^2 - \frac{1}{3}(9a + 3b + 3c + 3d) \\ &+ \frac{1}{6}(6ab + 6bc + 6cd + 12bc + 12bd + 18ad). \end{aligned}$$

Another aspect, this is a way to check that

$$\begin{aligned} W(K_{a+d,b+c}) =& (a+d)(b+c) + 2[\binom{a+d}{2} + \binom{b+c}{2}] \\ =& a^2 + b^2 + c^2 + d^2 - (a+b+c+d) \\ &+ \frac{1}{2}(2ab + 4bc + 2cd + 2ac + 2bd + 4ad). \end{aligned}$$

Then

$$W(K_{a+d,b+c}) - W(G^\star) = 2a + (bc - ac - bd - ad). \quad (4)$$

Observe that $n \geq 3$ and $G^\star$ is connected, implying that the maximum of b and c is at least 1.
In view of (4), we get that $W(K_{a+d,b+c}) - W(G^\star) < 0$. If $c \geq 1$, then $d \geq 2$ and thus $W(K_{a+d,b+c}) - W(G^\star) < 0$ immediately follows from (4). All the possible scenarios are generated that $W(K_{a+d,b+c}) < W(G^\star)$, this contradicts the selection of $G^\star$, as $\varphi(K_{a+d,b+c}) = \varphi(G^\star)$. Similarly, there is a paradox when $d < a$. Hence, $G^\star \cong K_{\varphi,n-\varphi}$. Through simple calculations, we know that

$$\begin{aligned} W(K_{\varphi,n-\varphi}) =& \varphi(n-\varphi) + \varphi(\varphi-1) + (n-\varphi)(n-\varphi-1) \\ =& n^2 - (\varphi+1)n + \varphi^2. \end{aligned}$$

So we have $W(K_{\varphi,n-\varphi}) = n^2 - (\varphi+1)n + \varphi^2$ and we are done.

V. Proof of Theorem 2.3

Now we give the proof of Theorem 2.3, we establish a loose lower bound on the Wiener index of a tree with predetermined order and dissociation number and the extremal tree which satisfy the upper bound is also characterized. We complete this proof by first giving some key conclusions.

Gutman [21] gave that if G is an acyclic molecular graph with n vertices, then it follows $W(S_n) \leq W(G) \leq W(P_n)$. And Dobrynin et al. [27] shown that the best known of a large number of trees close combinatorial expressions for W are $W(P_n) = \binom{n+1}{3}$ and $W(S_n) = (n-1)^2$. These formulas have been first reported in [29] in 1976.

Lemma 5.1 ([21],[27]) Let $T \in \mathscr{T}_n$. Then $(n-1)^2 \leq W(T) \leq \binom{n+1}{3}$. The left-hand equivalence is true exclusively when T is isomorphic to S_n, and the right-hand equivalence is true exclusively when T is isomorphic to P_n.

Lemma 5.2 ([33]) Let $T \in \mathscr{T}_{n,\varphi}(n \geq 3)$ and $\triangle(T)$ be the maximum degree of T. Then $\triangle(T) \leq 2\varphi - n + 1$.

Now we will give the proof of Theorem 2.3. In this Theorem, we determine the loose lower bound of the Wiener index in $\mathscr{T}_{n,\varphi}$ and give the corresponding extremal tree.

Proof of Theorem 2.3 We continue the proof using mathematical induction on the variable n. If $\varphi = n-1$, then Lemma 5.1 gives $W(T) \geq (n-1)^2$ with equality holds when $T \cong S_n \cong S^*_{n,n-1}$. When $3 \leq n \leq 9$, it is obviously that $W(T) \geq \frac{1}{2}n^2 - 2n + \frac{1}{2}\varphi^2 + \varphi + \frac{3}{2}$ and the equality holds if and only if $T \cong S^*_{n,\varphi}$. Subsequently, we presume that the outcome is valid for every tree of order smaller than n and dissociation number $\varphi \leq n-2$.

Choose $T \in \mathscr{T}_{n,\varphi}(n \geq 10, \varphi \leq n-2)$ where $W(T)$ is maximized to its greatest extent. Let $P_k = v_1v_2v_3v_4\cdots v_k$ be a diametral path of T. Consequently, according to Lemma 3.1, it can be deduced that $\varphi(T - v_1) \in \{\varphi, \varphi - 1\}$. We continue the proof by considering the following cases.

Case 1 $\varphi(T - v_1) = \varphi - 1$. As a result of Lemma 5.2, we have that $\triangle(T - v_1) \leq 2\varphi - n$. Then

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

The equality in (5) holds when $d_{T-v_1}(v_2)=\triangle(T-v_1)=2\varphi-n$ and $d_{T-v_1}(v,v_2)=2$ for any $v\notin N_{T-v_1}[v_2]$. By Lemma 5.2, we have (5) holds when $T-v_1\cong S^*_{n-1,\varphi-1}$ with $d_{T-v_1}(v_2)=2\varphi-n$.

The induction hypothesis together with (5) yields

$$\begin{aligned}W(T)=&W(T-v_1)+\sum_{v\in V_{T-v_1}}d_T(v,v_1)\\=&W(T-v_1)+\sum_{v\in V_{T-v_1}}d_{T-v_1}(v,v_2)+1\\\geq&\frac{1}{2}(n-1)^2-2(n-1)+\frac{1}{2}(\varphi-1)^2\\&+(\varphi-1)+\frac{3}{2}+4n-2\varphi-5\\\geq&\frac{1}{2}n^2-2n+\frac{1}{2}\varphi^2+\varphi+\frac{3}{2}.\end{aligned}\tag{6}$$

The equality in (6) holds when $T-v_1\cong S^*_{n-1,\varphi-1}$ with $d_{T-v_1}(v_2)=\triangle(T-v_1)=2\varphi-n$. According to Lemma 3.2, we know that $\varphi(T)\geq\frac{2n}{3}$. Then $2\varphi-n\geq\frac{n}{3}>3$, implying (6) holds with equality if and only if $T\cong S^*_{n,\varphi}$.

There exist at least two pendent vertices when $\varphi\leq n-3$, and the distance between them is 4, contradicting to the fact that v_1 lies on a diameter path of T. So $T\ncong S^*_{n,\varphi}$ and then $W(T)>\frac{1}{2}n^2-2n+\frac{1}{2}\varphi^2+\varphi+\frac{3}{2}=W(S^*_{n,\varphi})$, this leads to a contradiction with the selection of T. Therefore, $\varphi=n-2$ and $W(T)\geq n^2-3n+\frac{3}{2}$ with equality when $T\cong S^*_{n,n-2}$.

Case 2 $\varphi(T-v_1)=\varphi$. Consequently, there is a maximal dissociation set, denoted as $S(T)$, for which $v_1\notin S(T)$. According to Lemma 3.3, we get $d(v_2\leq 3)$ and thus $d(v_2=3)$ by Corollary 3.6. Suppose that w is the sole vertex within $N(v_2)\backslash\{v_1,v_3\}$. Put $T':=T-v_1-v_2-w$. Then $T'\in\mathscr{T}_{n-3,\varphi-2}$. In the same way as Case 1, we get

$$\begin{aligned}\sum_{v\in V_{T'}}d_{T'}(v,v_3)+2\leq&2+3d_{T'}(v_3)+4(n-d_{T'}(v_3)-4)\\=&4n-d_{T'}(v_3)-12\\\geq&5n-2\varphi-12.\\\sum_{v\in V_{T'}}d_{T'}(v,v_3)+1\leq&1+2d_{T'}(v_3)+3(n-d_{T'}(v_3)-4)\\=&3n-d_{T-v_1}(v_2)-5\\\geq&4n-2\varphi-11.\end{aligned}\tag{7}$$

Each equality in (7) holds when $T'\cong S^*_{n-3,\varphi-2}$ with $d_{T'}(v_3)=\triangle(T')=2\varphi-n$ and $d_{T'}(v,v_3)=2$ for any $v\notin N_{T'}[v_3]$. The induction hypothesis together with (7) yields

$$\begin{aligned}W(T)=&W(T')+\sum_{v\in V_{T'}}d_T(v,v_1)+\sum_{v\in V_{T'}}d_T(v,v_2)\\=&W(T')+\sum_{v\in V_{T'}}d_{T'}(v,v_3)+\sum_{v\in V_{T'}}d_{T'}(v,v_3)+3\\\geq&\frac{1}{2}(n-3)^2-2(n-3)+\frac{1}{2}(\varphi-2)^2+(\varphi-2)\\&+\frac{3}{2}+(5n-2\varphi-12)+(4n-2\varphi-11)\\\geq&\frac{1}{2}n^2-2n+\frac{1}{2}\varphi^2+\varphi+\frac{3}{2}.\end{aligned}\tag{8}$$

The equality in (8) holds when $T'\cong S^*_{n-3,\varphi-2}$ with $d_{T'}(v_3)=2\varphi-n>3$, which means (8) holds when $T\cong S^*_{n,\varphi}$.

That is the end of proof.

VI. Proof of Theorem 2.4

Now we present the proof for Theorem 2.4, by which we characterize all the graphs with order n and dissociation number $\varphi\in\{2,\lceil\frac{2n}{3}\rceil,n-1\}$ having the maximum Wiener indices.

The following result shows as the preliminary to show Theorem 2.4.

Lemma 6.1 ([27]) Consider G as a connected graph comprising n vertices. Then

$$W(G)\leq\binom{n+1}{3}$$

with equality holds when $G\cong P_n$.

Now we will give the proof for Theorem 2.4.

Proof of Theorem 2.4.

(i) Based on Lemma 6.1, we know that $W(G)\leq\binom{n+1}{3}$ with equality holds when $G\cong P_n$, and $\varphi(P_n)=\lceil\frac{2n}{3}\rceil$.

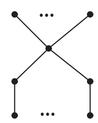

Fig. 2. Graphs $S(l_1,l_2)$

(ii) Let $G\in\mathscr{C}_{n,2}$ be the graph having the maximum Wiener index. When G lacks $3K_1$ or $K_2\bigcup K_1$ as its inducer graph, it follows that $d_{\overline{G}}(v)\leq 1$ for all $v\in V_G$, with $\overline{G}$ being the complement of G. Thus, $E_{\overline{G}}$ constitutes a matching in K_n. By integrating Lemma 3.4, we deduce that $G\cong K_n-M(K_n)$, which $M(K_n)$ represents the maximum matching in K_n. By some direct calculations, we get that $W(K_n-M(K_n))=\frac{2n^2-3n}{4}$ if n is even, while $W(K_n-M(K_n))=\frac{2n^2-3n+4}{4}$ if n is odd.

(iii) Let $G\in\mathscr{C}_{n,n-1}(n\geq 3)$ be the graph with the maximal Wiener index, and let S be a maximal dissociation set of G partitioned into $S=S_1\cup S_2$, such that $G[S_1]$ forms a perfect matching and S_2 is an independent set. Suppose that $V_G=\{v_1,v_2,\cdots,v_n\}$ and $S=V_G\backslash\{v_1\}$. Then $S_2\subseteq N(v_1)\cap\mathcal{P}(G)$.

Denote v_{n-1} and v_n as two vertices, such that $\{v_{n-1},v_n\}\subseteq S_2$, then put $G'=G-v_1v_{n-1}+v_nv_{n-1}$ and thus $G'\in\mathscr{C}_{n,n-1}$ by Lemma 3.3. According to Corollary 3.6, we have $W(G')>W(G)$, contradicting to the choice of G. Therefore, $|S_2|\leq 1$. Then we can know that

$$G\cong\begin{cases}S(1,\frac{n-2}{2}), & if\ n\ is\ even;\\S(0,\frac{n-1}{2}), & if\ n\ is\ odd.\end{cases}$$

where $S(l_1,l_2)$ is the graph as shown in Figure 2. Now we will give a simple calculation about $W(S(1,\frac{n-2}{2}))$ and $W(S(0,\frac{n-1}{2}))$.

$$
\begin{aligned}
W(S(1,\frac{n-2}{2})) =& 1+2\cdot\frac{n-2}{2}+3\cdot\frac{n-2}{2}+\frac{n-2}{2}\\
&+2\cdot\frac{n-2}{2}+\frac{n-2}{2}\\
&+(2+3+3+4)(\frac{n-4}{2}+\frac{n-6}{2}\\
&+\cdots+1)\\
=& 1+9\cdot\frac{n-2}{2}+12\cdot\frac{n^2-6n+8}{8}\\
=& \frac{3n^2-9n+8}{2}.
\end{aligned}
$$

$$
\begin{aligned}
W(S(0,\frac{n-1}{2})) =& \frac{n-1}{2}+2\cdot\frac{n-1}{2}+\frac{n-1}{2}\\
&+(2+3+3+4)(\frac{n-3}{2}+\frac{n-5}{2}\\
&+\cdots+1)\\
=& 4\cdot\frac{n-1}{2}+12\cdot\frac{n^2-4n+3}{8}\\
=& \frac{3n^2-8n+7}{2}.
\end{aligned}
$$

VII. Final observations

Brualdi and Solheid [10] introduced a renowned question that has since become a classic in the field of spectral graph theory.

In this paper, we focus on a specific set of graphs G within the collections $\mathscr{C}_{n,\varphi}$, $\mathscr{B}_{n,\varphi}$ and $\mathscr{T}_{n,\varphi}$ that satisfy certain criteria. Our primary goal is to determine the minimum and maximum Wiener indices for these graphs and to identify the extremal graphs that achieve these values.

The first three theorems provide a comprehensive characterization of all connected graphs with the minimal Wiener indices among those with a predetermined order and dissociation number. The final theorem addresses the graphs with a predetermined order n and dissociation number $\varphi \in \{2, \lceil\frac{2n}{3}\rceil, n-1\}$ that attain the maximal Wiener indices.

Overall, our work provides a detailed analysis of the Wiener indices for graphs within these specific sets, offering insights into both the minimal and maximal values and the corresponding extremal structures.

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