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WIENER INDEX OF GRAPHS WITH FIXED NUMBER OF PENDANT OR CUT-VERTICES

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Abstract. The Wiener index of a connected graph is defined as the sum of the distances between all unordered pairs of its vertices. We characterize the graphs which extremize the Wiener index among all graphs on n vertices with k pendant vertices. We also characterize the graph which minimizes the Wiener index over the graphs on n vertices with s cut-vertices.

Keywords: cut-vertex; distance; pendant vertex; unicyclic graph; Wiener index

MSC 2020: 05C05, 05C12, 05C35

1. Introduction

Throughout this paper, graphs are finite, simple, connected and undirected. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, $N_G(v)$ denotes the set of all neighbours of v in G. A vertex of degree one is called a *pendant vertex*. A vertex v of G is called a *cut-vertex* if $G \setminus v$ is disconnected. The distance between two vertices $u, v \in V(G)$, denoted by $d_G(u,v)$ or $d(u,v)$ (if the context is clear), is the number of edges in a shortest path joining u and v. The *eccentricity* of a vertex v, denoted by $e(v)$, is defined as $e(v) = \max\{d(u,v)\colon u \in V(G)\}$. The distance of a vertex $v \in V(G)$, denoted by $D_G(v)$, is defined as $D_G(v) = \sum\limits_{u\in V(G)} d_G(u,v)$. We refer to [18] for undefined notations and terminologies.

The *Wiener index* of G, denoted by $W(G)$, is defined as the sum of distances between all unordered pairs of its vertices, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \frac{1}{2}\sum_{v\in V(G)} D_G(v).$$

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Different names such as *graph distance* (see [6]), *transmission* (see [12]), *total status* (see [3]) and *sum of all distances* (see [7], [21]) have been used to study the graphical invariant $W(G)$. Apparently, the chemist Wiener was the first to point out in 1947 (see [19]) that $W(G)$ is well correlated with certain physio-chemical properties of the organic compound from which G is derived. The *mean distance* (see [5], [20]) or *the average distance* (see [1], [4]) between the vertices is a quantity closely related to $W(G)$. By considering G as an interconnection network connecting many processors, the average distance of G between the nodes of the network is a measure of the average delay for traversing the messages from one node to another.

In mathematical literature, the Wiener index was first studied by Entringer et al. in [6]. This gave an important direction to the researchers to characterize the graphs with extremal Wiener index in certain classes of graphs. In the last 20 years a lot of studies for the optimal graphs associated with Wiener index have been done. For example, characterization of trees with bounded maximum degree (see [9]), with fixed diameter (see [11]), with given degree sequence (see [17], [23]) and characterization of unicyclic graphs with fixed diameter (see [15]), with given girth (see [22]) associated with Wiener index have been studied. Apart from trees and unicyclic graphs, some other classes of graphs are also studied for the characterization of graphs having extremal Wiener index. Wiener index of graphs with fixed maximum degree is studied in [14]. The graphs with maximum and minimum Wiener index among all Eulerian graphs on n vertices are characterized in [8].

Wiener index of unicyclic graphs with fixed number of pendant vertices or cut-vertices is studied in [16]. In this paper, we characterize the graphs having maximum and minimum Wiener index over all connected graphs on n vertices with k pendant vertices. We also obtain the graph which minimizes the Wiener index among all connected graphs on n vertices with s cut-vertices.

1.1. Main results. We first construct some classes of graphs. Let k be a positive integer and let G be a graph. By kG we mean the graph consisting of k copies of G.

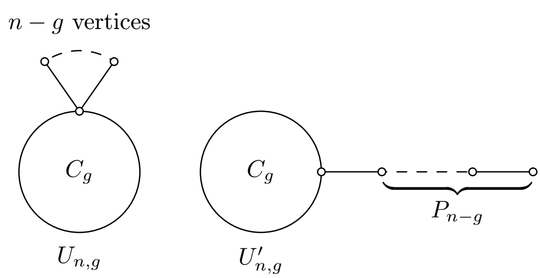

Figure 1. The graphs $U_{n,g}$ and $U'_{n,g}$.

We denote the cycle on g vertices by C_g. For $3 \leqslant g \leqslant n-1$, let $U_{n,g}$ be the graph obtained by attaching $n-g$ pendant vertices at one vertex of the cycle C_g and $U'_{n,g}$ be the graph obtained by joining an edge between a pendant vertex of the path P_{n-g} and a vertex of C_g, see Figure 1. Note that $U_{n,n-1} \cong U'_{n,n-1}$.

Let $\mathfrak{H}_{n,k}$ denote the class of all connected graphs on n vertices with k pendant vertices. Let $\mathfrak{T}_{n,k}$ be the subclass of $\mathfrak{H}_{n,k}$ containing all trees on n vertices with k pendant vertices.

The path $[v_1v_2\dots v_n]$ on n vertices is denoted by P_n. For positive integers k, l, d with $n = k+l+d$, let $T(k,l,d)$ be the tree obtained by taking the path P_d and adding k pendant vertices adjacent to v_1 and l pendant vertices adjacent to v_d. Note that $T(1,1,d)$ is a path on $d+2$ vertices.

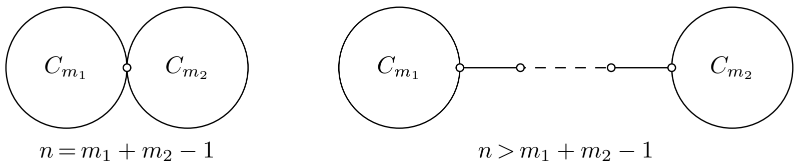

Figure 2. The graphs $C^n_{m_1,m_2}$.

We define a specific subclass of graphs in $\mathfrak{H}_{n,0}$ as follows. Let m_1, m_2 and n be positive integers with $m_1, m_2 \geqslant 3$ and $n \geqslant m_1+m_2-1$. If $n > m_1+m_2-1$, take a path on $n-(m_1+m_2)+2$ vertices and identify one pendant vertex of the path with a vertex of C_{m_1} and another pendant vertex with a vertex of C_{m_2}. If $n = m_1+m_2-1$, then identify one vertex of C_{m_1} with a vertex of C_{m_2}. We denote this graph by $C^n_{m_1,m_2}$, see Figure 2.

In this paper, we prove the following results:

Theorem 1.1. *Let $0 \leqslant k \leqslant n-2$ and let $G \in \mathfrak{H}_{n,k}$. Then:*

(i) *For $2 \leqslant k \leqslant n-2$, $W(G) \leqslant W(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k))$ and equality happens if and only if $G = T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$. Furthermore,*

$$W\Big(T\Big(\Big\lfloor\frac{k}{2}\Big\rfloor, \Big\lceil\frac{k}{2}\Big\rceil, n-k\Big)\Big) = \begin{cases} \binom{n-k+1}{3} + \frac{k^2}{4}(n-k+3) \\ \qquad + \frac{k}{2}((n-k)^2+n-k-2) & \text{if } k \text{ is even,} \\ \binom{n-k+1}{3} + \frac{k^2-1}{4}(n-k+3) \\ \qquad + \frac{k}{2}((n-k)^2+n-k-2)+1 & \text{if } k \text{ is odd.} \end{cases}$$

(ii) *For* $k = 1$, $W(G) \leqslant W(U'_{n,3})$ *and equality holds if and only if* $G = U'_{n,3}$. *Furthermore,*

$$W(U'_{n,3}) = \frac{n^3 - 7n + 12}{6}.$$

(iii) *For* $k = 0$ *and* $n \geqslant 7$, $W(G) \leqslant W(C^n_{3,3})$ *and equality holds if and only if* $G = C^n_{3,3}$. *Furthermore,*

$$W(C^n_{3,3}) = \frac{n^3 - 13n + 24}{6}.$$

For $0 \leqslant k \leqslant n-3$ and $n \geqslant 4$, let K^k_n be the graph obtained by adding k pendant vertices to one vertex of the complete graph K_{n-k}.

Theorem 1.2. *Let* $0 \leqslant k \leqslant n-2$ *and let* $G \in \mathfrak{H}_{n,k}$. *Then:*

(i) *For* $0 \leqslant k \leqslant n-3$, $W(K^k_n) \leqslant W(G)$ *and equality holds if and only if* $G = K^k_n$. *Furthermore,*

$$W(K^k_n) = \binom{n-k}{2} + k^2 + 2k(n-k-1).$$

(ii) *For* $k = n-2$, $W(T(1, n-3, 2)) \leqslant W(G)$ *and equality holds if and only if* $G = T(1, n-3, 2)$. *Furthermore,*

$$W(T(1, n-3, 2)) = n^2 - n - 2.$$

Let $T_{n,k} \in \mathfrak{T}_{n,k}$ be the tree that has a vertex v of degree k and $T_{n,k} \setminus v = rP_{q+1} \cup (k-r)P_q$, where $q = \lfloor \frac{n-1}{k} \rfloor$ and $r = n - 1 - kq$. Here, we have $0 \leqslant r < k$.

Theorem 1.3. *Let* $2 \leqslant k \leqslant n-2$ *and* $T \in \mathfrak{T}_{n,k}$. *Then* $W(T_{n,k}) \leqslant W(T)$ *and equality holds if and only if* $T = T_{n,k}$.

Let $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ be the set of all connected graphs on n vertices and s cut-vertices. For $2 \leqslant m \leqslant n$, let $v_1, v_2, \ldots, v_m$ be the vertices of a complete graph K_m. For $i = 1, 2, \ldots, m$ consider the paths P_{l_i} such that $l_1 + l_2 + \ldots + l_m = n$. Identify a pendant vertex of the path P_{l_i} with the vertex v_i, for $i = 1, 2, \ldots, m$, to obtain a graph on n vertices and denote it by $K^n_m(l_1, l_2, \ldots, l_m)$.

Theorem 1.4. *Let* $0 \leqslant s \leqslant n-3$ *and* $i, j \in \{1, 2, \ldots, n-s\}$. *Then the graph* $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ *with* $|l_i - l_j| \leqslant 1$ *has the minimum Wiener index over* $\mathfrak{C}_{n,s}$.

In the next section we will discuss some results related to Wiener index of graphs which are useful to prove our main theorems.

2. Preliminaries

We start this section with the following lemma.

Lemma 2.1. *Let G be a graph and $u, v \in V(G)$ are nonadjacent. Let G' be the graph obtained from G by joining the vertices u and v by an edge. Then $W(G') < W(G)$.*

It follows from Lemma 2.1 that among all connected graphs on n vertices, the Wiener index is minimized by the complete graph K_n and maximized by a tree. Among all trees on n vertices, the Wiener index is minimized by the star $K_{1,n-1}$ and maximized by the path P_n, see [18], Theorem 2.1.14. It is easy to determine the Wiener index of the following graphs, see [18]:
(i) $W(K_n) = \binom{n}{2}$,
(ii) $W(P_n) = \binom{n+1}{3}$,
(iii) $W(K_{1,n-1}) = (n-1)^2$.
The Wiener index of the cycle C_n is (see [12],Theorem 5)

$$W(C_n) = \begin{cases} \frac{1}{8}n^3 & \text{if } n \text{ is even,} \\ \frac{1}{8}n(n^2-1) & \text{if } n \text{ is odd.} \end{cases} \tag{2.1}$$

Also for $u \in V(C_n)$

$$D_{C_n}(u) = \begin{cases} \frac{n^2}{4} & \text{if } n \text{ is even,} \\ \frac{n^2-1}{4} & \text{if } n \text{ is odd.} \end{cases} \tag{2.2}$$

The following lemma is very useful.

Lemma 2.2 ([2], Lemma 1.1)**.** *Let G be a graph and u be a cut-vertex in G. Let G_1 and G_2 be two subgraphs of G with $G = G_1 \cup G_2$ and $V(G_1) \cap V(G_2) = \{u\}$. Then*

$$W(G) = W(G_1) + W(G_2) + (|V(G_1)| - 1)D_{G_2}(u) + (|V(G_2)| - 1)D_{G_1}(u).$$

Corollary 2.3. *Let G and H be two connected graphs having at least 2 vertices each. Let $u, v \in V(G)$ and $w \in V(H)$. Let G_1 and G_2 be the graphs obtained from G and H by identifying the vertex w of H with the vertices u and v of G, respectively. If $D_G(v) \geqslant D_G(u)$, then $W(G_2) \geqslant W(G_1)$ and equality happens if and only if $D_G(v) = D_G(u)$.*

P r o o f. By Lemma 2.2,

$$W(G_1) = W(G) + W(H) + (|V(G)| - 1)D_H(w) + (|V(H)| - 1)D_G(u)$$

and

$$W(G_2) = W(G) + W(H) + (|V(G)| - 1)D_H(w) + (|V(H)| - 1)D_G(v).$$

So

$$W(G_2) - W(G_1) = (|V(H)| - 1)(D_G(v) - D_G(u))$$

and the result follows. □

Let G be a connected graph on $n \geqslant 2$ vertices and $v \in V(G)$. For $l, k \geqslant 1$, let $G_{k,l}$ be the graph obtained from G by attaching two new paths $P\colon vv_1v_2\ldots v_k$ and $Q\colon vu_1u_2\ldots u_l$ at v, where $u_1, u_2, \ldots, u_l$ and $v_1, v_2, \ldots, v_k$ are distinct new vertices. By $G_{0,l}$ we mean attaching a path of length l at v. Let $\widetilde{G}_{k,l}$ be the graph obtained from $G_{k,l}$ by removing the edge $\{v_{k-1}, v_k\}$ and adding the edge $\{u_l, v_k\}$. Observe that the graph $\widetilde{G}_{k,l}$ is isomorphic to the graph $G_{k-1,l+1}$. We say that $\widetilde{G}_{k,l}$ is obtained from $G_{k,l}$ by *grafting* an edge.

Consider the path $P_n\colon v_1v_2\ldots v_n$ on n vertices with v_i adjacent to v_{i-1} and v_{i+1} for $2 \leqslant i \leqslant n-1$. Then for $i = 1, 2, \ldots, n$,

$$D_{P_n}(v_i) = D_{P_n}(v_{n-i+1}) = \frac{(n-i)(n-i+1) + i(i-1)}{2}.$$

So, if n is odd, then

$$\begin{aligned} D_{P_n}(v_1) > D_{P_n}(v_2) > \ldots > D_{P_n}(v_{(n+1)/2}) \\ < D_{P_n}(v_{(n+3)/2}) < \ldots < D_{P_n}(v_{n-1}) < D_{P_n}(v_n) \end{aligned}$$

and if n is even, then

$$\begin{aligned} D_{P_n}(v_1) > D_{P_n}(v_2) > \ldots > D_{P_n}(v_{n/2}) \\ = D_{P_n}(v_{(n+2)/2}) < \ldots < D_{P_n}(v_{n-1}) < D_{P_n}(v_n). \end{aligned}$$

The next result follows from the above observation and Corollary 2.3.

Corollary 2.4 ([11], Lemma 2.4). *If* $1 \leqslant k \leqslant l$, *then* $W(G_{k-1,l+1}) > W(G_{k,l})$.

The following result compares the Wiener index of two graphs, where one is obtained from the other by moving one component from a vertex to another vertex.

Lemma 2.5 ([10], Lemma 2.4)**.** *Let H, X and Y be three connected pairwise vertex disjoint graphs having at least 2 vertices each. Suppose $u, v \in V(H)$ with $u \neq v$, $x \in V(X)$ and $y \in V(Y)$. Let G be the graph obtained from H, X and Y by identifying u with x and v with y, respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices u, x, y and let G_2^* be the graph obtained from H, X, Y by identifying vertices v, x, y, see Figure 3. Then $W(G_1^*) < W(G)$ or $W(G_2^*) < W(G)$.*

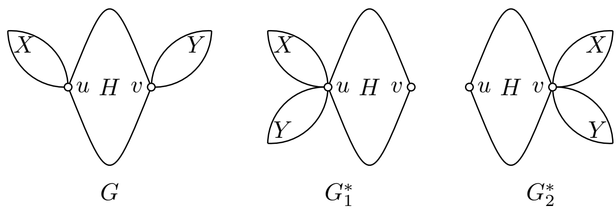

Figure 3. Movement of a component from one vertex to another.

Corollary 2.6. *Let G be a connected graph on $n \geqslant 2$ vertices and let $u, v \in V(G)$. For $n_1, n_2 \geqslant 0$, let $G_{uv}(n_1, n_2)$ be the graph obtained from G by attaching n_1 pendant vertices at u and n_2 pendant vertices at v. If $n_1, n_2 \geqslant 1$, then*

$$W(G_{uv}(n_1+n_2, 0)) < W(G_{uv}(n_1, n_2)) \text{ or } W(G_{uv}(0, n_1+n_2)) < W(G_{uv}(n_1, n_2)).$$

In [22], the authors have proved the following in Lemma 2.6:

Let G_0 be a connected graph of order $n_0 > 1$ and $u_0, v_0 \in V(G_0)$ be two distinct vertices in G_0. $P_s = u_1 u_2 \ldots u_s$ and $P_t = v_1 v_2 \ldots v_t$ are two paths of order s and t, respectively. Let G be the graph obtained from G_0, P_s and P_t by adding edges $u_0 u_1$, $v_0 v_1$. Suppose that $G_1 = G - u_0 u_1 + v_t u_1$ and $G_2 = G - v_0 v_1 + u_s v_1$. Then either $W(G) < W(G_1)$ or $W(G) < W(G_2)$ holds.

If we take $G_0 = P_{n_0}$ and u_0 and v_0 as two distinct pendant vertices of G_0, then $G_0 \cong G_1 \cong G_2$. So, $W(G_0) = W(G_1) = W(G_2)$ and hence the statement is not true. In the following result, we give a proof of the corrected version of it.

Lemma 2.7. *Let G be a connected graph on $n \geqslant 3$ vertices and $u, v \in V(G)$. For $l, k \geqslant 1$, let $G_{uv}^p(l, k)$ be the graph obtained from G by identifying a pendant vertex of the path P_l with u and identifying a pendant vertex of the path P_k with v. Suppose $l, k \geqslant 2$. If G is not the u-v path and $D_G(u) \geqslant D_G(v)$, then*

$$W(G_{uv}^p(l+k-1, 1)) > W(G_{uv}^p(l, k)).$$

P r o o f. First consider the graph $G^p_{u,v}(l,1)$ as H and let w be the pendant vertex of H corresponding to P_l. Then by Lemma 2.2,

$$W(G^p_{u,v}(l,k)) = W(H) + W(P_k) + (|V(H)|-1)D_{P_k}(v) + (k-1)D_H(v)$$

and

$$W(G^p_{u,v}(l+k-1,1)) = W(H) + W(P_k) + (|V(H)|-1)D_{P_k}(w) + (k-1)D_H(w).$$

As $D_{P_k}(v) = D_{P_k}(w)$, we get

$$W(G^p_{u,v}(l+k-1,1)) - W(G^p_{u,v}(l,k)) = (k-1)(D_H(w) - D_H(v)).$$

Now

$$D_H(w) = D_{P_{l-1}}(w) + (l-1)|V(G)| + D_G(u)$$

and

$$D_H(v) = D_G(u) + (l-1)(d_G(u,v)+1) + D_{P_{l-1}}(u'),$$

where u' is the vertex on the path P_l adjacent to u. Since $D_{P_{l-1}}(w) = D_{P_{l-1}}(u')$,

$$D_H(w) - D_H(v) = (l-1)(|V(G)| - d_G(u,v) - 1) + D_G(u) - D_G(v).$$

As $l \geqslant 2$ and G is not the u-v path, $(l-1)(|V(G)| - d_G(u,v) - 1) > 0$. Hence, the result follows from the given condition $D_G(u) \geqslant D_G(v)$. □

The Wiener index of $U_{n,g}$ and $U'_{n,g}$ is useful for our results and can be found in [22], see Theorem 1.1.

$$(2.3)\quad W(U_{n,g}) = \begin{cases} \dfrac{g^3}{8} + (n-g)\Big(\dfrac{g^2}{4} + n - 1\Big) & \text{if } g \text{ is even,} \\ \dfrac{g(g^2-1)}{8} + (n-g)\Big(\dfrac{g^2-1}{4} + n - 1\Big) & \text{if } g \text{ is odd,} \end{cases}$$

$$(2.4)\quad W(U'_{n,g}) = \begin{cases} \dfrac{g^3}{8} + (n-g)\Big(\dfrac{n^2+ng+3g-1}{6} - \dfrac{g^2}{12}\Big) & \text{if } g \text{ is even,} \\ \dfrac{g(g^2-1)}{8} + (n-g)\Big(\dfrac{n^2+ng+3g-1}{6} - \dfrac{g^2}{12} - \dfrac{1}{4}\Big) & \text{if } g \text{ is odd.} \end{cases}$$

We next calculate the Wiener index of some other trees, which we need for the extremal bounds in some of our results. Let $S_{d,k}$ be the tree obtained by identifying a pendant vertex of the path P_d with the central vertex of the star $K_{1,k}$. By using Lemma 2.2, it is easy to see that

$$(2.5)\qquad W(S_{d,k}) = \binom{d+1}{3} + k^2 + (d-1)k + \frac{d(d-1)k}{2}.$$

Using the value of $W(S_{d,k})$ and $W(K_{1,l})$ in Lemma 2.2, we get

$$W(T(l,k,d)) = \binom{d+1}{3} + l^2 + k^2 + \frac{(d^2+d-2)(k+l)}{2} + (d+1)kl. \tag{2.6}$$

For $l \geqslant 2$ and $q \geqslant 1$, let T_l^q be the tree on $lq+1$ vertices with l pendant vertices having one vertex v of degree l and $T_l^q - v = lP_q$ (l copies of P_q). Note that T_1^q is the path P_{q+1}. Then

$$D_{T_l^q}(v) = l + 2l + \ldots + ql = \frac{lq(q+1)}{2}. \tag{2.7}$$

Now by Lemma 2.2,

$$\begin{aligned} W(T_l^q) &= W(T_{l-1}^q) + W(T_1^q) + (l-1)qD_{T_1^q}(v) + qD_{T_{l-1}^q}(v) \\ &= W(T_{l-1}^q) + \binom{q+2}{3} + (l-1)q^2(q+1). \end{aligned}$$

Solving this recurrence relation we get

$$W(T_l^q) = l\binom{q+2}{3} + \frac{q^2l(q+1)(l-1)}{2}. \tag{2.8}$$

3. Proofs of Theorem 1.1, Theorem 1.2 and Theorem 1.3

We first recall three known results related to Wiener index of graphs.

Theorem 3.1 ([13], Theorem 4)**.** *For $2 \leqslant k \leqslant n-2$, the tree $T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$ uniquely maximizes the Wiener index over $\mathfrak{T}_{n,k}$.*

Theorem 3.2 ([22], Corollary 1.2)**.** *Among all unicyclic graphs on $n > 4$ vertices, the graph $U'_{n,3}$ uniquely maximizes the Wiener index.*

Theorem 3.3 ([12], Theorem 5)**.** *Let G be a two connected graph with n vertices. Then $W(G) \leqslant W(C_n)$ and equality holds if and only if $G = C_n$.*

We now compare the Wiener index of the graphs $C_{3,3}^n$ and C_n.

Lemma 3.4. *For $n \geqslant 6$, $W(C_n) \leqslant W(C_{3,3}^n)$ and equality happens if and only if $n = 6$.*

P r o o f. By (2.4), we have $W(U'_{n,3}) = \frac{1}{6}(n^3 - 7n + 12)$. If u is the pendant vertex of $U'_{n,3}$, then

$$D_{U'_{n,3}}(u) = D_{P_{n-2}}(u) + 2(n-2) = \frac{(n-3)(n-2)}{2} + 2n - 4 = \frac{n^2 - n - 2}{2}.$$

For $n \geqslant 6$, let u be the cut-vertex common to C_3 and $U'_{n-2,3}$ of $C^n_{3,3}$. Then by Lemma 2.2,

$$\begin{aligned} (3.1)\quad W(C^n_{3,3}) &= W(C_3) + W(U'_{n-2,3}) + 2D_{U'_{n-2,3}}(u) + 2(n-3), \\ &= 3 + \frac{(n-2)^3 - 7(n-2) + 12}{6} + (n-2)^2 - (n-2) - 2 + 2n - 6 \\ &= \frac{n^3 - 13n + 24}{6}. \end{aligned}$$

By (2.1) and (3.1), we have

$$W(C^n_{3,3}) - W(C_n) = \begin{cases} \dfrac{n(n^2-52)}{24} + 4 & \text{if } n \text{ is even,} \\ \dfrac{n(n^2-49)}{24} + 4 & \text{if } n \text{ is odd.} \end{cases}$$

Hence, the result follows. □

Lemma 3.5. *Let $m_1, m_2 \geqslant 3$ be two integers and let $n = m_1 + m_2 - 1$. Then $W(C_n) > W(C^n_{m_1,m_2})$.*

P r o o f. Let v be the vertex of degree 4 in $C^n_{m_1,m_2}$. First suppose n is even. Then one of m_1 or m_2 is odd and the other is even. Without loss of generality, suppose m_1 is odd and m_2 is even. Then by Lemma 2.2, (2.1) and (2.2) we have

$$\begin{aligned} W(C^n_{m_1,m_2}) &= W(C_{m_1}) + W(C_{m_2}) + (m_2-1)D_{C_{m_1}}(v) + (m_1-1)D_{C_{m_2}}(v) \\ &= \frac{m_1^3 - m_1}{8} + \frac{m_2^3}{8} + (m_2-1)\frac{m_1^2-1}{4} + (m_1-1)\frac{m_2^2}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_1^2m_2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2 - m_1 - 2m_2 + 2) \end{aligned}$$

and

$$\begin{aligned} W(C_n) &= \frac{1}{8}(m_1 + m_2 - 1)^3 \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 3m_1^2m_2 + 3m_1m_2^2 - 3m_1^2 - 3m_2^2 - 6m_1m_2 + 3m_1 + 3m_2 - 1). \end{aligned}$$

The difference is

$$\begin{aligned} W(C_n) - W(C^n_{m_1,m_2}) &= \frac{1}{8}(m_1^2 m_2 + m_1 m_2^2 - m_1^2 - m_2^2 - 6m_1m_2 + 4m_1 + 5m_2 - 3) \\ &= \frac{1}{8}((m_2-1)m_1^2 + (m_1-1)m_2^2 + 4m_1 + 5m_2 - 6m_1m_2 - 3). \end{aligned}$$

An easy calculation gives

$$\begin{aligned} W(C_n) - W(C^n_{m_1,m_2}) &= \frac{1}{4}m_2(m_2-2) > 0 & \text{if } m_1 = 3, \\ W(C_n) - W(C^n_{m_1,m_2}) &\geqslant \frac{1}{8}(3(m_1-m_2)^2 + 4m_1 + 5m_2 - 3) > 0 & \text{if } m_1 \geqslant 5. \end{aligned}$$

Now suppose n is odd. Then there are two possibilities.

Case 1: Both m_1 and m_2 are even.

$$\begin{aligned} W(C^n_{m_1,m_2}) &= W(C_{m_1}) + W(C_{m_2}) + (m_2-1)D_{C_{m_1}}(v) + (m_1-1)D_{C_{m_2}}(v) \\ &= \frac{m_1^3}{8} + \frac{m_2^3}{8} + (m_2-1)\frac{m_1^2}{4} + (m_1-1)\frac{m_2^2}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_2m_1^2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2), \\ W(C_n) &= W(C_{m_1+m_2-1}) = \frac{1}{8}((m_1+m_2-1)^3 - (m_1+m_2-1)) \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 3m_1^2m_2 + 3m_1m_2^2 - 3m_1^2 - 3m_2^2 - 6m_1m_2 + 2m_1 + 2m_2). \end{aligned}$$

The difference is

$$\begin{aligned} W(C_n) - W(C^n_{m_1,m_2}) &= \frac{1}{8}((m_1-1)m_2^2 + (m_2-1)m_1^2 - 6m_1m_2 + 2m_1 + 2m_2) \\ &\geqslant \frac{1}{8}(3(m_1-m_2)^2 + 2m_1 + 2m_2) > 0. \end{aligned}$$

Case 2: Both m_1 and m_2 are odd.

$$\begin{aligned} W(C^n_{m_1,m_2}) &= \frac{m_1^3 - m_1}{8} + \frac{m_2^3 - m_2}{8} + (m_2-1)\frac{m_1^2-1}{4} + (m_1-1)\frac{m_2^2-1}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_2m_1^2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2 - 3m_1 - 3m_2 + 4) \end{aligned}$$

and the difference is

$$W(C_n) - W(C^n_{m_1,m_2}) = \frac{1}{8}((m_1-1)m_2^2 + (m_2-1)m_1^2 - 6m_1m_2 + 5m_1 + 5m_2 - 4).$$

An easy calculation gives

$$\begin{aligned}
W(C_n) - W(C^n_{m_1,m_2}) &> \frac{1}{8}(3(m_1-m_2)^2+5m_1+5m_2-4) > 0 && \text{if } m_1, m_2 \geqslant 5,\\
W(C_n) - W(C^n_{m_1,m_2}) &= \frac{1}{8}(2m_2^2-4m_2+2) > 0 && \text{if } m_1 = 3,\\
W(C_n) - W(C^n_{m_1,m_2}) &= \frac{1}{8}(2m_1^2-4m_1+2) > 0 && \text{if } m_2 = 3,
\end{aligned}$$

and this completes the proof. □

Lemma 3.6. *Let u be the pendant vertex and v be a nonpendant vertex of the unicyclic graph $U'_{n,g}$. Then $D_{U'_{n,g}}(u) > D_{U'_{n,g}}(v)$.*

P r o o f. Let v_g be the vertex of degree 3 in $U'_{n,g}$. Then

$$D_{U'_{n,g}}(u) = D_{P_{n-g+1}}(u) + (g-1)(n-g) + D_{C_g}(v_g). \tag{3.2}$$

If v is a vertex on the cycle C_g of $U'_{n,g}$, then

$$D_{U'_{n,g}}(v) = D_{C_g}(v) + d(v, v_g)(n-g) + D_{P_{n-g+1}}(v_g).$$

Since $D_{P_{n-g+1}}(u) = D_{P_{n-g+1}}(v_g)$,

$$D_{U'_{n,g}}(u) - D_{U'_{n,g}}(v) = (n-g)(g-1-d(v,v_g)) > 0.$$

If v is not on the cycle C_g of $U'_{n,g}$, then

$$D_{U'_{n,g}}(v) = D_{P_{n-g+1}}(v) + d(v,v_g)(g-1) + D_{C_g}(v_g).$$

Since $D_{P_{n-g+1}}(u) > D_{P_{n-g+1}}(v)$ and $D_{C_g}(v_g) = D_{C_g}(v)$,

$$D_{U'_{n,g}}(u) - D_{U'_{n,g}}(v) > (g-1)(n-g-d(v,v_g)) > 0.$$

This completes the proof. □

The next corollary follows from Lemma 3.6 and Corollary 2.3.

Corollary 3.7. *Let G be a connected graph with at least two vertices and $u \in V(G)$. Suppose v is the pendant vertex of $U'_{n,g}$ and w is a nonpendant vertex of $U'_{n,g}$. Let G_1 and G_2 be the graphs obtained from G and $U'_{n,g}$ by identifying u of G with the vertices v and w of $U'_{n,g}$, respectively. Then $W(G_1) > W(G_2)$.*

Lemma 3.8. *Let u be a vertex of a connected graph G. For $m \geqslant 4$, let G_1 be the graph obtained by identifying the vertex u of G with the pendant vertex of $U'_{m+1,m}$ and G_2 be the graph obtained by identifying the vertex u with the pendant vertex of $U'_{m+1,3}$. Then $W(G_2) > W(G_1)$.*

P r o o f. By Lemma 2.2, we have

$$W(G_1) = W(G) + W(U'_{m+1,m}) + (|V(G)| - 1)D_{U'_{m+1,m}}(u) + mD_G(u)$$

and

$$W(G_2) = W(G) + W(U'_{m+1,3}) + (|V(G)| - 1)D_{U'_{m+1,3}}(u) + mD_G(u).$$

By Theorem 3.2, $W(U'_{m+1,3}) > W(U'_{m+1,m})$. So, the difference is

$$W(G_2) - W(G_1) > (|V(G)| - 1)(D_{U'_{m+1,3}}(u) - D_{U'_{m+1,m}}(u)).$$

By (3.2), we have $D_{U'_{m+1,3}}(u) = \frac{1}{2}(m-1)(m+2)$ and

$$D_{U'_{m+1,m}}(u) = \begin{cases} m + \dfrac{m^2}{4} & \text{if } n \text{ is even,} \\ m + \dfrac{m^2-1}{4} & \text{if } n \text{ is odd.} \end{cases}$$

So,

$$D_{U'_{m+1,3}}(u) - D_{U'_{m+1,m}}(u) = \begin{cases} \dfrac{m^2-2m-4}{4} & \text{if } m \text{ is even,} \\ \dfrac{m^2-2m-3}{4} & \text{if } m \text{ is odd,} \end{cases}$$

which is greater than 0 and this completes the proof. □

Corollary 3.9. *Let $m_1, m_2 \geqslant 3$ be two integers and let $m_1 + m_2 \leqslant n$. Then $W(C^n_{3,3}) \geqslant W(C^n_{m_1,m_2})$ and equality happens if and only if $m_1 = m_2 = 3$.*

P r o o f of Theorem 1.1. (i) Let $G \in \mathfrak{H}_{n,k}$. Suppose G is not isomorphic to $T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)$. If G is a tree, then by Theorem 3.1, $W(G) < W(T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k))$.

Suppose G is not a tree. Then construct a spanning tree G' from G by deleting some edges. Then by Lemma 2.1, $W(G') > W(G)$. The number of pendant vertices of G' is greater than or equal to k. Suppose G' has more than k pendant vertices. Since $k \geqslant 2$, G' has at least one vertex of degree greater than 2 and at least two paths attached to it. Consider a vertex v of G' with $d(v) \geqslant 3$ and two paths P_{l_1}, P_{l_2}, $l_1 \geqslant l_2$ attached at v. Using grafting of edge operation on G', we get a new tree $\widetilde{G}$ with number of pendant vertices one less than the number of pendant vertices of G'

and by Corollary 2.4, $W(\widetilde{G}) > W(G')$. We continue this process untill we get a tree with k pendant vertices from $\widetilde{G}$. By Lemma 2.4, every step in this process increases the Wiener index. So, we will reach at a tree T of order n with k pendant vertices. By Theorem 3.1, we have $W(T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)) \geqslant W(T) > W(G)$. Hence, $T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,k}$.

Now by replacing d, l and k with $n-k$, $\lfloor\frac{k}{2}\rfloor$ and $\lceil\frac{k}{2}\rceil$, respectively, in (2.6), we get the value of $W(T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k))$ as in the statement. This completes the proof.

(ii) Let $G \in \mathfrak{H}_{n,1}$. Suppose G is not isomorphic to $U'_{n,3}$. Since G is connected and has exactly one pendant vertex, it must contain a cycle. Let C_g be a cycle in G. If G is a unicyclic graph, then by Theorem 3.2, $W(U'_{n,3}) > W(G)$. If G has more than one cycle, then construct a new graph G' from G by deleting edges from all cycles other than C_g so that the graph remains connected. Then by Lemma 2.1, $W(G') > W(G)$ and G' is a unicyclic graph on n vertices with girth g. By Theorem 3.2, $W(U'_{n,3}) \geqslant W(G') > W(G)$. Hence, $U'_{n,3}$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,1}$. We get the value of $W(U'_{n,3})$ from (2.4) and this completes the proof.

(iii) Let $n \geqslant 7$ and let $G \in \mathfrak{H}_{n,0}$. Suppose G is not isomorphic to $C^n_{3,3}$. Then we have two cases:

Case 1: For some integers $m_1, m_2 \geqslant 3$ with $n = m_1 + m_2 - 1$, $C^n_{m_1,m_2}$ is a subgraph of G.

Since $C^n_{m_1,m_2}$ is a subgraph of G, by deleting some edges (if required) from G we get $C^n_{m_1,m_2} \in \mathfrak{H}_{n,0}$ and by Lemma 2.1, $W(G) \leqslant W(C^n_{m_1,m_2})$. Again by Lemma 3.4 and Lemma 3.5, we have

$$W(G) \leqslant W(C^n_{m_1,m_2}) < W(C_n) < W(C^n_{3,3}).$$

Case 2: There are no integers $m_1, m_2 \geqslant 3$ with $n = m_1 + m_2 - 1$ such that $C^n_{m_1,m_2}$ is a subgraph of G.

If G is a two connected graph, then by Theorem 3.3 and Lemma 3.4, $W(G) \leqslant W(C_n) < W(C^n_{3,3})$. So let G have at least one cut-vertex.

Since G has a cut-vertex and no pendant vertices, so G contains two cycles with at most one common vertex. Let C_{g_1} and C_{g_2} be two cycles of G with at most one common vertex. Since $C^n_{m_1,m_2}$ with $m_1 + m_2 - 1 = n$ is not a subgraph of G, $g_1 + g_2 \leqslant n$. Clearly G has at least $n+1$ edges.

If G has exactly $n+1$ edges, then there is no common vertex between C_{g_1} and C_{g_2} and $G = C^n_{g_1,g_2}$. As G is not isomorphic to $C^n_{3,3}$, by Corollary 3.9, $W(G) < W(C^n_{3,3})$.

Now let $|E(G)| \geqslant n+2$. Suppose $|E(G)| = n+k$, where $k \geqslant 2$. Choose $k-1$ edges $\{e_1, \ldots, e_{k-1}\} \subset E(G)$ such that $e_i \notin E(C_{g_1}) \cup E(C_{g_2})$, $i = 1, \ldots, k-1$ and $G \setminus \{e_1, \ldots, e_{k-1}\}$ is connected. Let $G_1 = G \setminus \{e_1, \ldots, e_{k-1}\}$ (G_1 may have some pendant vertices). Then by Lemma 2.1, $W(G_1) > W(G)$. If G_1 has no pendant vertices, then $G_1 = C^n_{g_1,g_2}$ for some $g_1, g_2 \geqslant 3$. By Corollary 3.9, $W(G) < W(G_1) \leqslant W(C^n_{3,3})$.

Suppose G_1 has some pendant vertices. Then for some $p < n$, $C^p_{g_1,g_2}$ is a subgraph of G_1. By grafting of edges operation (if required), we can form a new graph G_2 from G_1, where G_2 is a connected graph on n vertices obtained by attaching some paths to some vertices of $C^p_{g_1,g_2}$. Then by Corollary 2.4, $W(G_2) \geqslant W(G_1)$. If more than one path are attached to different vertices of $C^p_{g_1,g_2}$ in G_2, then using the graph operation as mentioned in Lemma 2.7, form a new graph G_3 from G_2, where G_3 has exactly one path attached to $C^p_{g_1,g_2}$. Then by Lemma 2.7, $W(G_3) \geqslant W(G_2)$.

Let u be the vertex on $C^p_{g_1,g_2}$ of G_3 at which the path is attached. Then again, we have two cases:

Case 1: $u \in V(C_{g_1}) \cup V(C_{g_2})$. Without loss of generality, assume that $u \in V(C_{g_1})$. Then the induced subgraph of G_3 containing the vertices of C_{g_1} and the vertices of the path attached to it, is the graph U'_{k,g_1} for some $k > g_1$. Let v be the pendant vertex of U'_{k,g_1}. Since the two cycles C_{g_1} and C_{g_2} have at most one vertex in common, we have two subcases:

Subcase 1.1: $V(C_{g_1}) \cap V(C_{g_2}) = \{w\}$. Let H_1 be the induced subgraph of G_3 containing the vertices $\{V(G_3) \setminus V(U'_{k,g_1})\} \cup \{w\}$. Clearly H_1 is the cycle C_{g_2}. Then identify the vertex v of U'_{k,g_1} with the vertex w of H_1 to form a new graph G_4. By Corollary 3.7, $W(G_4) > W(G_3)$ and G_4 is the graph $C^n_{g_1,g_2}$. By Corollary 3.9, $W(G) < W(G_4) \leqslant W(C^n_{3,3})$.

Subcase 1.2: $V(C_{g_1}) \cap V(C_{g_2}) = \emptyset$. Let H_2 be the induced subgraph of G_3 containing the vertices $V(G_3) \setminus V(U'_{k,g_1})$. In G_3 there is exactly one vertex $w_1 \in U'_{k,g_1}$ adjacent to exactly one vertex w_2 of H_2. Form a new graph G_5 from G_3 by deleting the edge $\{w_1, w_2\}$ and adding the edge $\{v, w_2\}$. By Corollary 3.7, $W(G_5) > W(G_3)$ and G_5 is the graph $C^n_{g_1,g_2}$. Again, by Corollary 3.9, we have $W(G) < W(G_5) \leqslant W(C^n_{3,3})$.

Case 2: $u \notin V(C_{g_1}) \cup V(C_{g_2})$. Let w be the pendant vertex of G_3 and let w_3 be a vertex on $C^p_{g_1,g_2}$ of G_3 adjacent to u. Form a new graph G_6 from G_3 by deleting the edge $\{u, w_3\}$ and adding the edge $\{w, w_3\}$. By Corollary 3.7, $W(G_6) > W(G_3)$ and G_6 is the graph $C^n_{g_1,g_2}$. Again, by Corollary 3.9, we have $W(G) < W(G_6) \leqslant W(C^n_{3,3})$. Hence, $C^n_{3,3}$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,0}$ for $n \geqslant 7$.

We have $W(C^n_{3,3}) = \frac{1}{6}(n^3 - 13n + 24)$ by (3.1) and this completes the proof. □

It can be checked easily that for $3 \leqslant n \leqslant 5$, the cycle C_n has the maximum Wiener index over $\mathfrak{H}_{n,0}$ and for $n = 6$, the Wiener index is maximized by both the graphs C_6 and $C^6_{3,3}$.

P r o o f of Theorem 1.2. (i) Let $G \in \mathfrak{H}_{n,k}$, $0 \leqslant k \leqslant n-3$ and let $v_1, v_2, \ldots, v_{n-k}$ be the nonpendant vertices of G. Suppose G is not isomorphic to K^k_n. If the induced subgraph $G[v_1, v_2, \ldots, v_{n-k}]$ is not complete, then form a new graph G' from G by joining all the nonadjacent nonpedant vertices of G with new edges. Then $G' \in \mathfrak{H}_{n,k}$ and by Lemma 2.1, $W(G') < W(G)$. If $G' = K^k_n$, then $W(K^k_n) < W(G)$.

Otherwise, G' has at least two vertices of degree greater than or equal to $n-k$. (If the induced subgraph $G[v_1, v_2, \ldots, v_{n-k}]$ is complete, then $G[v_1, v_2, \ldots, v_{n-k}]$ has at least two vertices of degree greater than or equal to $n-k$.) Form a new graph G'' from G' by moving all the pendant vertices to one of the vertex $v_1, v_2, \ldots, v_{n-k}$. Then $G'' = K_n^k$ and by Corollary 2.6, $W(K_n^k) = W(G'') < W(G') \leqslant W(G)$. Hence, for $0 \leqslant k \leqslant n-3$, K_n^k uniquely minimizes the Wiener index over $\mathfrak{H}_{n,k}$.

Let $u \in V(K_n^k)$ be a vertex of degree $n-1$. Then by Lemma 2.2, we have

$$\begin{aligned} W(K_n^k) &= W(K_{n-k}) + W(K_{1,k}) + (|V(K_{n-k})| - 1)k + kD_{K_{n-k}}(u) \\ &= \binom{n-k}{2} + k^2 + 2k(n-k-1). \end{aligned}$$

(ii) Let $G \in \mathfrak{H}_{n,n-2}$. Suppose G is not isomorphic to $T(1, n-3, 2)$. Then G is isomorphic to a tree $T(k, l, 2)$ for some $k, l \geqslant 2$. Now form a tree $T(1, n-3, 2)$ from G by moving pendant vertices from one end to another. Then by Corollary 2.6, $W(T(1, n-3, 2)) < W(G)$ and by taking $d = 2$, $l = 1$ and $k = n-3$ in (2.6), we have $W(T(1, n-3, 2)) = n^2 - n - 2$. □

P r o o f of Theorem 1.3. We first prove that for $k \geqslant 3$, if $T \in \mathfrak{T}_{n,k}$ has minimum Wiener index, then there is a unique vertex $v \in V(T)$ with $d(v) \geqslant 3$. Let there be two vertices $u, v \in V(T)$ with $d(u) = n_1 \geqslant 3$, $d(v) = n_2 \geqslant 3$. Let $N_T(u) = \{u_1, u_2, \ldots, u_{n_1}\}$ and $N_T(v) = \{v_1, v_2, \ldots, v_{n_2}\}$, where u_1 and v_1 lie on the path joining u and v (u_1 may be v and v_1 may be u). Let T_1 be the largest subtree of T containing $u, u_2, u_3, \ldots, u_{n_1-1}$ but not u_1, u_{n_1} and T_2 be the largest subtree of T containing $v, v_2, v_3, \ldots, v_{n_2-1}$ but not v_1, v_{n_2}. We rename the vertices $u \in V(T_1)$ and $v \in V(T_2)$ by u' and v', respectively. Let $H = T \setminus \{u_2, u_3, \ldots, u_{n_1-1}, v_2, v_3, \ldots, v_{n_2-1}\}$. Construct two trees T' and T'' from H, T_1 and T_2 by identifying the vertices u, u', v' and v, u', v', respectively. Clearly, both $T', T'' \in \mathfrak{T}_{n,k}$ and by Lemma 2.5, either $W(T') < W(T)$ or $W(T'') < W(T)$, which is a contradiction.

Let T be the tree which minimizes the Wiener index in $\mathfrak{T}_{n,k}$. For $k = 2$, the only possible tree is the path P_n, which is isomorphic to $T_{n,2}$. So assume $3 \leqslant k \leqslant n-2$. Then there exists a unique vertex $v \in V(T)$ with $d(v) \geqslant 3$ and $d(v)$ number of paths are attached to v. Suppose P and P' are two paths attached at v in T of length l and l', respectively, with $l - l' \geqslant 2$. By grafting of edge, form a tree $\widetilde{T}$ from T such that the lengths of paths corresponding to P and P' in $\widetilde{T}$ are $l-1$ and $l'+1$, respectively. Then by Corollary 2.4, $W(\widetilde{T}) < W(T)$, which is a contradiction. Hence, the difference of the lengths of any two paths attached at v in T is at most one. Therefore, T uniquely minimizes the Wiener index over $\mathfrak{T}_{n,k}$ and T is isomorphic to $T_{n,k}$. □

For $r = 0$, the tree $T_{n,k}$ is isomorphic to the tree T_k^q and hence by (2.8),

$$W(T_{n,k}) = k\binom{q+2}{3} + \frac{q^2(q+1)k(k-1)}{2}.$$

For $1 \leqslant r < k$, by Lemma 2.2, we have

$$W(T_{n,k}) = W(T_r^{q+1}) + W(T_{k-r}^q) + r(q+1)D_{T_{k-r}^q}(v) + (k-r)qD_{T_r^{q+1}}(v),$$

where v is the vertex of $T_{n,k}$ with $T_{n,k} \setminus v = rP_{q+1} \cup (k-r)P_q$. Thus, by using (2.7) and (2.8), the value of $W(T_{n,k})$ can be obtained.

4. Proof of Theorem 1.4

Any graph on n vertices has at most $n-2$ cut-vertices. The path P_n is the only graph on n vertices with $n-2$ cut-vertices. Hence, for $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ we consider $0 \leqslant s \leqslant n-3$. Let $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}^{\mathfrak{t}}$ be the set of all trees on n vertices with s cut-vertices. In a tree, every vertex is either a pendant vertex or a cut-vertex. So $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}^{\mathfrak{t}} = \mathfrak{T}_{n,n-s}$. Hence, the next result follows from Theorems 1.3 and 3.1.

Theorem 4.1. *For $0 \leqslant s \leqslant n-3$, the tree $T(\lfloor\frac{n-s}{2}\rfloor, \lceil\frac{n-s}{2}\rceil, s)$ maximizes the Wiener index and the tree $T_{n,n-s}$ minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}^{\mathfrak{t}}$.*

A block in a graph G is a maximal connected component without any cut-vertices in it. Let B_G be the graph corresponding to G with $V(B_G)$ as the set of blocks of G and two vertices u and v of B_G are adjacent whenever the corresponding blocks contain a common cut-vertex of G. A vertex of G with minimum eccentricity is called a *central vertex*. We call a block B in G a *pendant block* if there is exactly one cut-vertex of G in B. The block corresponding to a central vertex in B_G is called a *central block* of G. Two blocks in G are said to be *adjacent blocks* if they share a common cut-vertex.

Lemma 4.2. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Then every block of G is a complete graph.*

P r o o f. Let B be a block of G which is not complete. Then there are at least two nonadjacent vertices in B. Let u and v be two nonadjacent vertices in B. Form a new graph G' from G by joining the edge $\{u,v\}$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ and by Lemma 2.1, $W(G') < W(G)$, which is a contradiction. □

Lemma 4.3. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Then every cut-vertex of G is shared by exactly two blocks.*

P r o o f. Let c be a cut-vertex in G shared by more than two blocks, say $B_1, B_2, \ldots, B_k$, $k \geqslant 3$. Construct a new graph G' from G by joining all the non-adjacent vertices of $\bigcup_{i=2}^{k} B_i$. Then $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ and by Lemma 2.1, $W(G') < W(G)$, which is a contradiction. □

Lemma 4.4. *Let $m \geqslant 3$. For $i, j \in \{1, 2, \ldots, m\}$, if $l_i \leqslant l_j - 2$, then*

$$W(K_m^n(l_1, \ldots, l_i + 1, \ldots, l_j - 1, \ldots, l_m)) < W(K_m^n(l_1, \ldots, l_i, \ldots, l_j, \ldots, l_m)).$$

P r o o f. Let u be the pendant vertex of $K_m^n(l_1, \ldots, l_i + 1, \ldots, l_j - 1, \ldots, l_m)$ on the path P_{l_i+1} and v be the pendant vertex of $K_m^n(l_1, \ldots, l_i, \ldots, l_j, \ldots, l_m)$ on the path P_{l_j}. Let w_1 and w_2 be the vertices adjacent to u and v, respectively. Then using Lemma 2.2 we have

$$\begin{aligned} W(K_m^n(l_1, \ldots, l_i + 1, \ldots, l_j - 1, \ldots, l_m)) - W(K_m^n(l_1, \ldots, l_i, \ldots, l_j, \ldots, l_m)) \\ = D_{K_m^{n-1}(l_1,\ldots,l_i,\ldots,l_j-1,\ldots,l_m)}(w_1) - D_{K_m^{n-1}(l_1,\ldots,l_i,\ldots,l_j-1,\ldots,l_m)}(w_2) < 0, \end{aligned}$$

since $l_i < l_j - 1$ and $m \geqslant 3$. □

Let G be a graph in which every cut-vertex is shared by exactly two blocks. Then B_G is a tree. So, B_G has either one central vertex or two adjacent central vertices and hence G has either one central block or two central blocks with a common cut-vertex.

Lemma 4.5. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. If $s \geqslant 2$, then every pendant block of G is K_2.*

P r o o f. All the blocks in G are complete by Lemma 4.2. Suppose B is a pendant block of G which is not K_2. Let $V(B) = \{v_1, v_2, \ldots, v_m\}$ with $m > 2$. Assume v_1 is the cut-vertex of G in B which is shared by another block B' with $V(B') = \{v_1 = u_1, u_2, \ldots, u_r\}$ and $r \geqslant 2$. Construct a new graph G' from G as follows: Delete the edges $\{v_2, v_j\}$, $j = 3, 4, \ldots, m$ and add the edges $\{v_j, u_i\}$, $j = 3, 4, \ldots, m$ and $i = 2, 3, \ldots, r$. When G changes to G', the only type of distances which increase are $d(v_2, v_j)$, $j = 3, 4, \ldots, m$. Each such distance increases by one and hence the total increment in distances for v_j, $j = \{3, \ldots, m\}$ is exactly $m - 2$. The distance $d(v_j, u_i)$, $j = 3, 4, \ldots, m$, $i = 2, 3, \ldots, r$ decrease by one. Since $r \geqslant 2$, the total distance decreased by such pair of vertices is at least $m - 2$. Since $s \geqslant 2$, there exists a vertex w belonging to another block B'' such that $d(v_j, w)$, $j = 3, 4, \ldots, m$ decreases by one. So $W(G') < W(G)$, which is a contradiction. □

Lemma 4.6. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. If $s \geqslant 2$, then all noncentral blocks of G are K_2.*

P r o o f. Since G minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$, by Lemmas 4.2 and 4.5, all blocks of G are complete and all pendant blocks are K_2. Assume that G has a nonpendant and noncentral block. By Lemma 4.3, every cut-vertex of G is shared by exactly two blocks. Let B be a central block in G. Then there exist a noncentral, nonpendant block B_1 and a cut-vertex (of G) $c_1 \in V(B_1)$ such that a path P_l is attached to B_1 at c_1. Since B_1 is a nonpendant block, so there is a cut-vertex (of G) $c_2 \in V(B_1)$ different from c_1, shared by another block B_2 such that the vertices corresponding to the blocks B_1, B_2 and B (starting from B_1) in the tree B_G lie on a path.

Let $V(B_1) = \{c_1 = u_1, u_2, \ldots, u_{m_1} = c_2\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = c_2\}$. Construct a new graph G' from G as follows: Delete the edges $\{c_1, u_i\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and add the edges $\{u_i, v_j\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and $v_j \in V(B_2) \setminus \{c_2\}$.

For $i = 2, \ldots, m_1 - 1$, let H_i be the maximal connected component of G containing exactly one vertex u_i of B_1. Let $P_l\colon\ t_1 t_2 \ldots t_l$ be the path with t_1 identified with c_1. When G changes to G', the only type of distances which increase in G' are $d_{G'}(u, t_j)$, where $u \in \bigcup\limits_{i=2}^{m_1-1} V(H_i)$ and $j = 1, 2, \ldots, l$. Each such distance increases by one in G'. For any other pair of vertices, the distance between them either decreases or remains the same. Since B_1 is not a central block, for each t_j, $j = 1, 2, \ldots, l$ there exists a vertex $t'_j \in V(G) \setminus \Big(\bigcup\limits_{i=2}^{m_1-1} V(H_i) \cup \{t_1, t_2, \ldots, t_l, v_1, v_2, \ldots, v_{m_2}\}\Big)$ such that $d_{G'}(u, t'_j)$ decreases by one, where $u \in \bigcup\limits_{i=2}^{m_1-1} V(H_i)$. So, the increment in distance by the pairs u, t_j is neutralized by the pairs u, t'_j. Apart from this, at least the distances $d_{G'}(u_i, v_j)$ for $i = 2, 3, \ldots, m_1 - 1$ and $j = 1, 2, \ldots, m_2 - 1$ decrease by one. So $W(G') < W(G)$, which is a contradiction. Hence, for $s \geqslant 2$, all noncentral blocks of G are K_2. $\square$

P r o o f of Theorem 1.4. Let G be a graph, which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. We first claim that G is isomorphic to $K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$.

By Lemmas 4.2 and 4.3, every block of G is complete and every cut-vertex of G is shared by exactly two blocks. If $s = 0$, then G has exactly one block. So $G = K_n$ and K_n is isomorphic to $K^n_n(1, 1, \ldots, 1)$.

For $s = 1$, G has exactly two complete blocks with a common vertex w (say). Let B_1 and B_2 be the two blocks of G. If any of B_1 or B_2 is K_2, then G is isomorphic to $K^n_{n-1}(2, 1, \ldots, 1)$. Otherwise, let $V(B_1) = \{u_1, u_2, \ldots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = w\}$ with $m_1, m_2 > 2$. Construct a new graph G' from G as follows: Delete the edges $\{u_1, u_i\}$, $i = 2, 3, \ldots, m_1 - 1$ and add the edges $\{u_i, v_j\}$, $i = 2, 3, \ldots, m_1 - 1$, $j = 1, 2, \ldots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},1}$. Then the only type of distances which increase are $d(u_1, u_j)$, $j = 2, 3, \ldots u_{m_1-1}$ and each such distance increases by one. So, the total increment in distance is exactly $m_1 - 2$. Also each distance $d(u_i, v_j)$, $i = 2, 3, \ldots, m_1 - 1$, $j = 2, 3, \ldots m_2 - 1$ decreases by one. The total decrement is $(m_1 - 2)(m_2 - 1)$. Since $m_1, m_2 > 2$, $W(G') < W(G)$, which is a contradiction. Hence, G is isomorphic to $K^n_{n-1}(2, 1, \ldots, 1)$.

Now suppose $s \geqslant 2$. Then G has $s+1$ blocks and also G has either one central block or two adjacent central blocks. By Lemma 4.6, all noncentral blocks of G are K_2.

If G has exactly one central block, then G is isomorphic to $K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_s$. Suppose G has two central blocks and G is not isomorphic to $K^n_{n-s}(l_1, \ldots, l_{n-s})$ for any $l_1, l_2, \ldots, l_{n-s}$. Then each of the central blocks of G has at least 3 vertices. Let B_1 and B_2 be the two central blocks with a common vertex w. Let $V(B_1) = \{u_1, u_2, \ldots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = w\}$ with $m_1, m_2 > 2$. Let $H_1(H_2)$ be the maximal connected component of G containing exactly one vertex w of $B_2(B_1)$. Let $P_l\colon wu_1t_3 \ldots t_l$ be the longest path in H_1 starting at w containing u_1 such that none of the vertices $t_3, \ldots, t_l$ belongs to B_1. Take w as t_1 and u_1 as t_2 in P_l. Since B_1 and B_2 are central blocks, so there exists a path $P'_l\colon t'_1t'_2 \ldots t'_l$ on l vertices in H_2 starting at $w = t'_1$ and containing exactly two vertices of B_2. Construct a new graph G' from G as follows: Delete the edges $\{u_1, u_i\}$, $i = 2, 3, \ldots, m_1 - 1$ and add the edges $\{u_i, v_j\}$, $i = 2, 3, \ldots, m_1 - 1$, $j = 1, 2, \ldots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. The only type of distances which increase in G' are $d_{G'}(u, t_j)$, where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \ldots, l$ also each such distance increases by one. The distance $d_{G'}(u, t'_j)$ decreases by one, where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \ldots, l$. So, the increment in distance by the pairs $\{u, t_j\}$ is neutralized by the pairs $\{u, t'_j\}$. Since $m_2 \geqslant 3$, there exist at least one vertex w' in B_2 which is not in P'_l. For each $u \in V(H_1) \setminus V(P_l)$, the distance $d_{G'}(u, w')$ decreases by one. So, $W(G') < W(G)$, which is a contradiction. Hence, G is isomorphic to $K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$. Now the result follows from Lemma 4.4. □

5. Conclusion

In this article, we obtained the graphs which extremize the Wiener index over all connected graphs on n vertices with k pendant vertices. We also obtained the tree which minimizes the Wiener index over all trees on n vertices with k pendant vertices. In [13], the author has characterized the tree which maximizes the Wiener index over all trees on n vertices with fixed number of pendant vertices. We further obtained the graph which minimizes the Wiener index over all connected graphs on n vertices with s cut-vertices. It will be nice to obtain the graph which maximizes the Wiener index over all connected graphs on n vertices with fixed number of cut-vertices.

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