The Wiener index of unicyclic graphs given number of pendant vertices or cut vertices

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Abstract The Wiener index is the sum of distances between all pairs of distinct vertices in a connected graph, which is the oldest topological index related to molecular branching. In this article, we give a condition to determine the graphs having the smallest Wiener index among all unicyclic graphs given number of pendant vertices, and we also determine the graphs having the smallest Wiener index among all unicyclic graphs given number of cut vertices.

Keywords Wiener index · Unicyclic graph · Pendant vertex · Cut vertex

Mathematics Subject Classification 05C05 · 05C12 · 94C15

1 Introduction

All graphs considered in this paper will be finite, simple and undirected. Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance $d_G(u, v)$ between distinct vertices $u$ and $v$ is the number of edges on a shortest path connecting these vertices in $G$. The distance $W(G, v)$ of a vertex $v \in V(G)$ is the sum of distances between $v$ and all other vertices of $G$. Let $\deg_G(v)$ be the degree of vertex $v$ and let $N_G(v)$ be the set of all vertices adjacent to $v$ in $G$. 

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The Wiener index $W(G)$ of a connected graph $G$ is a graph invariant based on distances [1,2]. It is defined as the sum of distances between all pairs of vertices in $G$:

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

The Wiener index is the oldest topological index related to molecular branching [3]. A quantity closely related to $W(G)$ is the average distance $\mu(G)$ of a graph defined by $\mu(G) = \frac{2W(G)}{n(n-1)}$, where $n = |V(G)|$ is the number of vertices of $G$. When $G$ represents a network (e.g., an interconnection network connecting many processors), $\mu(G)$ is the average distance between the nodes (or processors) of the network. Hence it is a measure of the average delay of messages for traversing from one node to another. It is obvious that studying $\mu(G)$ is equivalent to studying $W(G)$.

Many chemical applications of the Wiener index deal with acyclic organic molecules, whose molecular graphs are trees. Therefore, for trees, the greatest progress was made (see a recent survey [4]). It is worth indicating that many scholars investigated the relation of Wiener index and some isomorphic invariants of graphs, such as order, maximum degree, diameter, degree sequence, matching number, et al. (see, for example, [5–11]). In particular, Zhang et al. [9] identified the trees having the minimum Wiener index among all trees given number of pendant vertices. Since, for a tree, each non-pendant vertex is a cut vertex, Zhang et al. [9] also determined the trees with the minimum Wiener index among all trees given number of cut vertices.

Except trees, some results of Wiener index on the other graphs were also obtained. For example, Wiener [1] gave the largest and smallest Wiener index of unicyclic graphs. Tang and Deng [12] characterized the graphs with the first three smaller and larger Wiener index among all unicyclic graphs. Nasiri et al. [13] corrected some mistakes of [12] and completed the classifications of unicyclic graphs with the first minimal and maximal Wiener index. Du and Zhou [14] characterized the graphs with the minimum Wiener index among all unicyclic graphs given matching number. Yu and Feng [15] determined the graphs with the largest and smallest Wiener index among all unicyclic graphs given girth. Tan and Lin [16] determined the graphs having the second largest Wiener index among all unicyclic graphs given girth and determined the graphs with the largest Wiener index among all unicyclic graphs given maximum degree. Feng et al. [17] identified the graphs having the largest and smallest Wiener index among all bicyclic graphs. Tan and Wang [18] determined the graphs having the second to seventh largest Wiener index among all bicyclic graphs. Tan and Wang [19] identified the graphs with the minimum Wiener index among all cacti given matching number. Dankelmann [20,21] determined the graphs with the maximum Wiener index among all graphs given order and independence number or domination number, respectively. Tomescu and Melter [22] identified the minimum and maximum Wiener index of graphs given order and chromatic number. Šparl and Žerovnik [23] gave a graphic transformation and determined the graphs with the minimum Wiener index among all graphs given number of cut edges.

Let $\Phi(n, s)$ be the set of all unicyclic graphs with $n$ vertices and $s$ pendant vertices and let $\Psi(n, c)$ be the other set of all unicyclic graphs with $n$ vertices and $c$ cut vertices.

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For the graphs in $\Phi(n, s)$, some indices, such as the spectral radius of adjacency matrix, Laplacian matrix and signless Laplacian matrix et al., have been extensively investigated (see, for example, [24–26]). It is easy to see that there is no close relationship between the numbers of pendant vertices and cut vertices in a unicyclic graph.

Motivated by the results above, in particular, [9,12–16,24–26], in the work we give a condition to determine the graphs in $\Phi(n, s)$ having the smallest Wiener index, and we also determine the graphs in $\Psi(n, c)$ having the smallest Wiener index.

2 Preliminaries

Let $G$ be a connected graph. A pendant vertex of $G$ is a vertex of degree one and a pendant edge is an edge incident to a pendant vertex. A path $u_0u_1u_2\ldots u_k$ of $G$ with distinct vertices $u_0, u_1, \ldots, u_k$ is called a pendant path of length $k$ at $u_0$ if

$$\text{deg}_G(u_0) \geq 3, \text{deg}_G(u_1) = \cdots = \text{deg}_G(u_{k-1}) = 2, \text{deg}_G(u_k) = 1.$$ 

**Lemma 2.1** [4,27] Let $G$ be a connected graph with a cut vertex $u$ such that $G_1$ and $G_2$ are two connected subgraphs of $G$, $V(G_1) \cap V(G_2) = \{u\}$ and $G_1 \cup G_2 = G$. Then

$$W(G) = W(G_1) + W(G_2) + (|G_1| - 1)W(G_2, u) + (|G_2| - 1)W(G_1, u).$$

**Lemma 2.2** [11] Let $G$ be a connected graph and let $u$ and $v$ be two distinct vertices of $G$ in which $u$ is a cut vertex of $G$. Assume that $G_1$ and $G_2$ are two non-trivial connected subgraphs of $G$ such that $V(G_1) \cap V(G_2) = \{u\}$, $G_1 \cup G_2 = G$ and $v \in V(G_2)$. Write

$$n_1 = |V(G_1)|, \quad N_{G_1}(u) = \{u_1, u_2, \ldots, u_s\},$$

$$G' = G - uu_1 - uu_2 - \cdots - uu_s + vu_1 + vu_2 + \cdots + vu_s.$$ 

Then

$$W(G) - W(G') = (n_1 - 1)[[W(G, u) - W(G, v)] + (n_1 - 1)d_G(u, v)].$$

In particular, if $W(G, u) \geq W(G, v)$, then $W(G) > W(G').$

**Lemma 2.3** [28] Let $u$ be a vertex of a nontrivial connected graph $Q$. Let $Q(s, t)$ be the graph obtained from $Q$ by adding two pendant paths $uu_1 \ldots u_s$ and $uv_1 \ldots v_t$ at $u$. If $s \geq t \geq 1$, then $W(Q(s+1, t-1)) > W(Q(s, t)).$

**Lemma 2.4** [11] Let $G$ be a connected graph and $uv$ be an edge of $G$ with $\text{deg}_G(u) \geq 2$ and $\text{deg}_G(v) \geq 2$. Let $G_{s,t}$ be the graph obtained from $G$ by adding two pendant paths $uu_1u_2\ldots u_s$ and $vu_1v_2\ldots v_t$ at $u$ and $v$, respectively. If $s \geq t + 2$, then

$$W(G_{s,t}) > W(G_{s-1,t+1}).$$
Lemma 2.5 Let $Q$ and $N$ be two connected graphs with $|Q| \geq 2$. Let $NQ(l, i)$ be the graph obtained from $Q$, $N$ and a path $v_1v_2 \ldots v_l$ ($l \geq 2$) by identifying a vertex $v$ of $Q$ and $v_l$, and identifying a vertex $x$ of $N$ and $v_l$ (still denote the two new vertices by $v_i$ and $v_l$, respectively) (see Fig. 1). Then

\[
W(NQ(l, i)) - W(NQ(l, l)) = (|V(Q)| - 1)(l - i)(|V(N)| - i).
\] (2.1)

In particular, if $l > i$ and $|V(N)| > i$, then $W(NQ(l, i)) > W(NQ(l, l))$.

Proof Let $Z$ be the graph obtained from $N$ and the path $v_1v_2 \ldots v_l$ by identifying $v_l$ and the vertex $x$ of $N$. By taking the vertex $v_i$ of $NQ(l, i)$ as $u$ in Lemma 2.1 we get

\[
\] (2.2)

On the other hand, it is easy to see that

\[
W(Z, v_i) = \frac{1}{2} i(i - 1) + \frac{1}{2} (l - i)(l - i + 1) + W(N, x) + (|N| - 1)(l - i).
\] (2.3)

So by Eqs. (2.2) and (2.3) it follows that

\[
W(NQ(l, i)) - W(NQ(l, l)) = (|V(Q)| - 1)(l - i)(|V(N)| - i).
\]

We arrive at Eq. (2.1). It is obvious that the additional claim holds by Eq. (2.1). □

Definition 2.6 Let $G$, $H$ be two connected graphs and let $uv$ be a non-pendant edge of $G$ such that it is not contained in triangles. Let $A$ be the graph obtained from $G$ and $H$ by identifying $u$ and a vertex $\tilde{u}$ of $H$ (still denote the new vertex by $u$). Let $A^{uv}$ be the graph obtained from $G$ and $H$ in the following way: delete $uv$, identify $u$ and $v$, and denote the new vertex by $w$; add an edge $wz$ and identifying $z$ and $\tilde{u}$ (still denote the new vertex by $z$). Write

\[
V_u = \{x : x \in V(G) \text{ and each shortest path from } u \text{ to } x \text{ does not contain } uv\},
\]

\[
V_v = \{x : x \in V(G) \text{ and some shortest path from } u \text{ to } x \text{ contains } uv\},
\]

\[
\Omega(u, v) = \{(x, y) : x \in V_u - \{u\}, y \in V_v - \{v\} \text{ and some shortest path from } x \text{ to } y \text{ contains } uv\},
\]

\[
\Theta(u, v) = \{x : x \in V(G), \ d_G(x, u) = d_G(x, v)\}.
\]

Lemma 2.7 [19] Let $A$ and $A^{uv}$ be the two graphs presented in Definition 2.6. Then

\[
W(A) - W(A^{uv}) = |
\Omega(u, v)| - |
\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1).\]
3 The graphs in $\Phi(n, s)$ with the smallest Wiener index

**Lemma 3.1** Let $x$ be a vertex of a connected graph $H$. Let $H_s$ be the graph formed from $H$ and a cycle $C_s = u_1u_2 \cdots u_su_1$ by joining $x$ to the vertex $u_1$ of $C_s$ with an edge $xu_1$, while let $H'_s$ be the other graph formed from $H_s$ by deleting the edge $u_1u_s$ and adding a new edge $xu_s$ (see Fig. 2). Then

$$W(H_s) - W(H'_s) = \begin{cases} \frac{1}{2} s(|V(H)| - \frac{s-2}{4}), & \text{if } s \text{ is an even number;} \\ \frac{1}{2} (s - 1)(|V(H)| - \frac{s+1}{4}), & \text{if } s \text{ is an odd number.} \end{cases}$$

**Proof** In Lemma 2.7 taking $A = H'_s, A^{uv} = H_s$, where $G = C_{s+1}, u = x$ and $v = u_s$. If $s = 2l$ is an even number, then

$$V_u = \{x, u_1, u_2, \ldots, u_l\}, \quad V_v = \{u_{l+1}, u_{l+2}, \ldots, u_{2l}\}, \quad \Theta(u, v) = \{u_l\},$$

$$\Omega(u, v) = \{(u_i, u_j) : i = 1, 2, \ldots, l - 2; j = l + i + 1, l + i + 2, \ldots, 2l - 1\}.$$ 

So by Lemma 2.7 it follows that

$$W(H_s) - W(H'_s) = W(A^{uv}) - W(A) = l \left(|V(H)| - \frac{l - 1}{2}\right)$$

$$= \frac{1}{2} s \left(|V(H)| - \frac{s - 2}{4}\right).$$

If $s = 2l - 1$ is an odd number, then

$$V_u = \{x, u_1, u_2, \ldots, u_{l-1}\}, \quad V_v = \{u_l, u_{l+1}, \ldots, u_{2l-1}\}, \quad \Theta(u, v) = \emptyset,$$

$$\Omega(u, v) = \{(u_i, u_j) : i = 1, 2, \ldots, l - 2; j = l + i, l + i + 1, \ldots, 2l - 2\}.$$ 

So by Lemma 2.7 it follows that

$$W(H_s) - W(H'_s) = W(A^{uv}) - W(A) = (l - 1) \left(|V(H)| - \frac{l}{2}\right)$$

$$= \frac{s - 1}{2} \left(|V(H)| - \frac{s + 1}{4}\right).$$

Fig. 2 Graph $H_s$ and transformed graph $H'_s$
In the following of this section we always denote the unique cycle in a unicyclic graph by $C_m = v_1v_2\ldots v_mv_1$. It is obvious that a unicyclic graph $G$ with the cycle $C_m$ can be obtained from $C_m$ by adding $m$ proper trees to vertices $v_1$, $v_2$, \ldots, $v_m$, respectively. Note that $\Phi(n, 0) = \{C_n\}$, so now assume that $s \geq 1$.

Let $T(z, k_1, k_2, \ldots, k_s)$ be the starlike tree obtained by adding $s$ pendant paths of length $k_1$, $k_2$, \ldots, $k_s$, respectively, to a fixed vertex $z$. Let $G(n, m, t; k_1, k_2, \ldots, k_s)$ be the $n$-vertex unicyclic graph obtained from $C_m$ and $T(z, k_1, k_2, \ldots, k_s)$ by connecting the vertices $v_1$ and $z$ with a path of length $t$. Set $n-m = ps+q$, where $0 \leq q \leq s-1$.

Let $U(n, m, s)$ be the graph formed from $C_m$ by adding $q$ pendant paths of length $p+1$ and $s-q$ pendant paths of length $p$ to the vertex $v_1$ of $C_m$, namely $U(n, m, s)$ is the unicyclic graph with $n$ vertices, $s$ pendant vertices and girth $m$ obtained from $C_m$ by adding $s$ pendant paths of almost equal length to the vertex $v_1$ of $C_m$, where two examples for $n = 19$, $m = 6$ and $s = 4$ are shown in Fig. 3. It is obvious that $U(n, m, s)$ can be uniquely determined by $(m, n, s)$ for given $n$ and $s$. Let $U_M$ be a graph having the smallest Wiener index in $\Phi(n, s)$. For convenience, in the following always denote the component containing the vertex $v_i$ in $U_M - E(C_m)$ by $C_m(i = 1, 2, \ldots, m)$.

**Lemma 3.2** There exists an integer $m$ with $3 \leq m \leq n-s$ such that $U_M \cong U(n, m, s)$.

**Proof** Let $C_m$ be the unique cycle of $U_M$. The result obviously holds for $s = 1$. Thus in the following assume that $s \geq 2$. In order to complete the proof, we only need to prove the four following claims.

**Claim 1** $U_M$ contains at most one vertex of degree of at least 3 not in $C_m$.

Suppose, for a contradiction, that $U_M$ contains two vertices, say $x$ and $y$, not being in $C_m$ such that $deg_{U_M}(x) \geq 3$ and $deg_{U_M}(y) \geq 3$. Assume, without loss of generality, that $W(U_M, x) \geq W(U_M, y)$. Write $N_{U_M}(x) = \{x_1, x_2, \ldots, x_r, x'\}$, where $r = deg_{U_M}(x) - 1$ and $x'$ is the vertex on the unique path from $x$ to $C_m$. Set

$$U = U_M - xx_2 - xx_3 - \cdots - xx_r + yy_2 + yy_3 + \cdots + yx_r.$$ 

Then $U \in \Phi(n, s)$ and $W(U_M) > W(U)$ by Lemma 2.2, a contradiction to the choice of $U_M$. Therefore, the claim holds.

**Claim 2** $U_M$ contains at most one vertex of degree of at least 3 in $C_m$.

Suppose, for a contradiction, that $U_M$ contains two vertices, say $x$ and $y$, in $C_m$ such that $deg_{U_M}(x) \geq 3$ and $deg_{U_M}(y) \geq 3$. Assume, without loss of generality,
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that $W(U_M, x) \geq W(U_M, y)$. Write $N_{U_M}(x) = \{x_1, \ldots, x_r, x', x''\}$, where $r = \deg_{U_M}(x) - 2$, while $x'$ and $x''$ are the two vertices in $C_m$. Set

$$U = U_M - xx_1 - xx_2 - \cdots - xx_r + yx_1 + yx_2 + \cdots + yx_r.$$ 

Then $U \in \Phi(n, s)$ and $W(U_M) > W(U)$ by Lemma 2.2, a contradiction to the choice of $U_M$. Therefore, the claim holds.

Since $U_M$ has pendant vertices, $U_M$ contains at least one vertex of degree not less than 3 in $C_m$. Therefore, from Claim 2 we see that $U_M$ only contains one vertex of $C_m$, say $v_1$, with degree not less than 3.

**Claim 3** If $U_M$ contains one vertex $z$ not being in $C_m$ such that $\deg_{U_M}(z) \geq 3$, then $z \in V(C_m^1)$ and $\deg_{U_M}(v_1) = 3$.

By Claim 2, it is easy to see that $z \in V(C_m^1)$. Assume that $\deg_{U_M}(v_1) \geq 4$. Write

$$N_{U_M}(v_1) = \{\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_r, v_2, v_m\},$$

$$N_{U_M}(z) = \{\bar{z}_1, \bar{z}_2, \ldots, \bar{z}_q, z'\},$$

where $r = \deg_{U_M}(v_1) - 2$, $q = \deg_{U_M}(z) - 1$, $v_2$ and $v_m$ are the vertices in $C_m$, $z'$ and $\bar{v}_1$ are two vertices on the unique path from $z$ to $v_1$. If $W(U_M, z) \geq W(U_M, v_1)$, then set

$$U = U_M - z\bar{z}_2 - z\bar{z}_3 - \cdots - z\bar{z}_q + v_1\bar{z}_2 + v_1\bar{z}_3 + \cdots + v_1\bar{z}_q.$$ 

If $W(U_M, z) < W(U_M, v_1)$, then set

$$U = U_M - v_1\bar{v}_2 - v_1\bar{v}_3 - \cdots - v_1\bar{v}_r + z\bar{v}_2 + z\bar{v}_3 + \cdots + z\bar{v}_r.$$ 

It is obvious that $U \in \Phi(n, s)$ and from Lemma 2.2 we have that $W(U_M) > W(U)$, a contradiction to the choice of $U_M$. Therefore, the claim holds.

By Claims 1–3 it is easy to see that there exist integers $m, t, k_1, k_2, \ldots, k_s$ with $t \geq 0$, $3 \leq m \leq n - 3$ and $k_1 \geq k_2 \geq \ldots \geq k_s \geq 1$ such that

$$U_M \cong G(n, m, t; k_1, k_2, \ldots, k_s). \quad (3.1)$$

**Claim 4** In $U_M \cong G(n, m, t; k_1, k_2, \ldots, k_s)$, hold $k_1 - k_s \leq 1$ and $t = 0$.

Assume that $k_1 - k_s \geq 2$. Let $za_1a_2 \ldots a_{k_s}$ and $zb_1b_2 \ldots b_{k_1}$, respectively, be the shortest and longest pendant paths at $z$ in $G(n, m, t; k_1, k_2, \ldots, k_s)$. Put

$$U = U_M - b_{k_1} + a_{k_s}b_{k_1}.$$ 

It is obvious $U \in \Phi(n, s)$ and $W(U_M) > W(U)$ by Lemma 2.3, a contradiction to the choice of $U_M$. Therefore, $k_1 - k_s \leq 1$.

Assume that $t \geq 1$ and $z_0z_1 \ldots z_{t-1}z_t$ is the unique path connecting $z$ and $v_1$ in $U_M$ in which $z_0 = v_1$ and $z_t = z$. We distinguish the two following cases.
**Case 1** Assume that \( m + t - 1 > k_s + 1 \).

Write \( N_{U_M}(z) = \{\tilde{z}_1, \tilde{z}_2, \ldots, \tilde{z}_s, z_{t-1}\} \), where \( \tilde{z}_i \) is on the pendant path of length \( k_i \) at \( z \) in \( U_M(i = 1, 2, \ldots, s) \). Set

\[
U = U_M - z\tilde{z}_1 - z\tilde{z}_2 - \cdots - z\tilde{z}_{s-1} - z_{t-1}\tilde{z}_1 - z_{t-1}\tilde{z}_2 - \cdots - z_{t-1}\tilde{z}_{s-1} \\
\cong G(n, m, t - 1; k_1, k_2, \ldots, k_{s-1}, k_s + 1).
\]

It is obvious \( U \in \Phi(n, s) \) and \( W(U_M) > W(U) \) by Lemma 2.5, a contradiction to the choice of \( U_M \).

**Case 2** Assume that \( m + t - 1 \leq k_s + 1 \).

Let \( H \) denote the subgraph containing the vertex \( z_1 \) in \( U_M - z_0z_1 \) and let

\[
U = U_M - v_Mv_1 + v_Mz_1 \cong G(n, m + 1, t - 1; k_1, k_2, \ldots, k_s).
\]

Then \( U \in \Phi(n, s) \). In Lemma 2.7 we take

\[
G = z_1v_1v_2 \cdots v_Mz_1 \cong C_{m+1}, \ u = z_1, \ v = v_1, \ A = U, \ A^{uv} = U_M.
\]

Then it is easy to see that \( |V_u| = \left\lceil \frac{m+1}{2} \right\rceil, \ |V_v| = \left\lceil \frac{m+1}{2} \right\rceil, \ |\Theta(u, v)| \geq 0 \) and

\[
|\Omega(u, v)| \leq (|V_u| - 1)(|V_v| - 1) \leq \frac{1}{4}m(m - 1).
\]

Note that \( k_1 \geq k_2 \geq \cdots \geq k_s \geq 1, \ s \geq 2, \ k_s + 1 \geq m + t - 1 \) and \( m \geq 3 \), so we have

\[
|V(H)| = t + \sum_{i=1}^{s} k_i \geq 1 + sk_s \geq 1 + 2k_s \geq 1 + 2(m + t - 2) \geq m + 2.
\]

Thus by Lemma 2.7 we have that

\[
W(U) - W(U_M) \leq \frac{1}{4}m(m - 1) - 0 - \frac{1}{2}(m - 1)(m + 1) = -\frac{1}{4}(m - 1)(m + 2) < 0,
\]

namely \( W(U_M) > W(U) \), a contradiction to the choice of \( U_M \).

By Eq. (3.1) and Claim 4, we see that there exists an integer \( m \) with \( 3 \leq m \leq n - s \) and \( s \) integers \( k_1, k_2, \ldots, k_s \) with \( k_1 \geq k_2 \geq \cdots \geq k_s \geq 1 \) and \( k_1 - k_s \leq 1 \) such that

\[
U_M \cong G(n, m, 0; k_1, k_2, \ldots, k_s) \cong U(n, m, s).
\]

This proof is complete. \( \Box \)
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From the definition of $U(n, m, s)$ we know that it is uniquely determined by $m$ for given $n$ and $s$. On the other hand, Lemma 3.2 indicates that each graph in $\Phi(n, s)$ having the minimum Wiener index must be isomorphic with $U(n, m, s)$ for some integer $m$. Hence in order to determine the graphs in $\Phi(n, s)$ having the minimum Wiener index, we only need to determine $m$ when $U(n, m, s)$ has the minimum Wiener index.

**Theorem 3.3** Assume that $s \geq 2$ and assume that $U(n, m, s)$ is a graph in $\Phi(n, s)$ with the smallest Wiener index.

1. If $m$ is an even number, then
   \[
   \max\{3, \alpha\} \leq m \leq \min\{n - s, \tilde{\alpha}\},
   \] (3.2)
   where
   \[
   \alpha = \frac{(2n-1)s^2+4n(s-2)-s\sqrt{4(n^2-4n+1)s^2-8n(n+1)s+8n(n+2)}}{3s^2-8},
   \]
   \[
   \tilde{\alpha} = \frac{(2n+1)s^2+4n(s-2)-8s-s\sqrt{4(n^2-20n+25)s^2-8(n^2-3n+2)s+8n(n-2)}}{3s^2-8}.
   \] (3.3)

2. If $m$ is an odd number, then
   \[
   \max\{3, \beta\} \leq m \leq \min\{n - s, \tilde{\beta}\}
   \] (3.4)
   where
   \[
   \beta = \frac{2[(n-1)s^2+2n(s-2)]-s\sqrt{4(n^2+4n+1)s^2-8n(n+2)s+8(n^2+1)}}{3s^2-8},
   \]
   \[
   \tilde{\beta} = \frac{2[(n+1)s^2+2n(s-2)-4s]-s\sqrt{4(n^2-28n+25)s^2-8(n^2-4n+4)s+8n(n+1)}}{3s^2-8}.
   \] (3.5)

**Proof** Assume that $4 \leq m \leq n - s - 1$. Let $l, k$ be the lengths of the longest and shortest pendant paths of $U(n, m, s)$, respectively. Then $l = k$ if $s$ is a divisor of $n - m$ and $l = k + 1$ otherwise. Set

\[
p = n - m - l, \quad q = n - m - k, \quad N_{U(n,m,s)}(v_1) = \{v_2, v_m, u_1, u_2, \ldots, u_s\},
\]

where $u_1$ and $u_s$ are the vertices in two pendant paths of lengths $l$ and $k$, respectively. Let $Q_1$ and $Q_2$ denote the graphs containing the vertex $v_1$ in $U(n, m, s) - v_2 - v_m - u_1$ and $U(n, m, s) - v_2 - v_m - u_s$, respectively. Then

\[
|V(Q_1)| = p + 1, \quad |V(Q_2)| = q + 1.
\]

Using the notations of Lemma 2.5, we have that

\[
U(n, m, s) = C_m Q_1(l + 1, l + 1) = C_m Q_2(k + 1, k + 1).
\]

By Lemma 2.5 we have that

\[
W(C_m Q_1(l + 1, l)) - W(C_m Q_1(l + 1, l + 1)) = p(m - l).
\] (3.6)
Regarding the graph containing the vertex \( u_1 \) in \( C_m Q_1(l + 1, l) - v_1 u_1 \) as \( H \) in Lemma 3.1, then by Lemma 3.1 we have that

\[
W(C_m Q_1(l + 1, l)) - W(C_{m+1} Q_1(l, l)) = \begin{cases} 
\frac{m}{2}(p + l - \frac{m-2}{4}), & \text{if } m \text{ is even;} \\
\frac{m-1}{2}(p + l - \frac{m+1}{4}), & \text{if } m \text{ is odd.}
\end{cases} \tag{3.7}
\]

Write

\[
\Delta_1(m) = W(C_m Q_1(l + 1, l + 1)) - W(C_{m+1} Q_1(l, l)).
\]

Then by Eqs. (3.6) and (3.7) it follows that

\[
\Delta_1(m) = \begin{cases} 
-p(m - l) + \frac{m}{2}(p + l - \frac{m-2}{4}), & \text{if } m \text{ is even;} \\
-p(m - l) + \frac{m-1}{2}(p + l - \frac{m+1}{4}), & \text{if } m \text{ is odd.}
\end{cases} \tag{3.8}
\]

Again regarding the graph containing the vertex \( u_s \) in \( C_{m-1} Q_2(k + 2, k + 1) - v_1 u_s \) as \( H \) in Lemma 3.1, then by Lemma 3.1 we have that

\[
W(C_{m-1} Q_2(k + 2, k + 1)) - W(C_m Q_2(k + 1, k + 1)) = \begin{cases} 
\frac{m-2}{2}(q + k - \frac{m-4}{4}), & \text{if } m \text{ is even;} \\
\frac{m-1}{2}(q + k - \frac{m-7}{4}), & \text{if } m \text{ is odd.}
\end{cases} \tag{3.9}
\]

Again by Lemma 2.5 we have that

\[
W(C_{m-1} Q_2(k + 2, k + 1)) - W(C_{m-1} Q_2(k + 2, k + 2)) = q(m - k - 2).
\tag{3.10}
\]

Write

\[
\Delta_2(m) = W(C_m Q_2(k + 1, k + 1)) - W(C_{m-1} Q_2(k + 2, k + 2)).
\]

Then by Eqs. (3.9) and (3.10) it follows that

\[
\Delta_2(m) = \begin{cases} 
q(m - k - 2) - \frac{m-2}{2}(q + k - \frac{m-4}{4}), & \text{if } m \text{ is even;} \\
q(m - k - 2) - \frac{m-1}{2}(q + k - \frac{m-7}{4}), & \text{if } m \text{ is odd.}
\end{cases} \tag{3.11}
\]

By the assumption of \( U(n, m, s) \) we know that

\[
\Delta_1(m) \leq 0, \quad \Delta_2(m) \leq 0. \tag{3.12}
\]

(1) Assume that \( m \) is an even number.
If \( s \) is a divisor of \( n - m \), then \( l = k = \frac{n-m}{s} \). By Eqs. (3.8), (3.11) and (3.12) we get
\[
\begin{align*}
- (n - m - \frac{n-m}{s}) (m - \frac{n-m}{s}) + m \left( n - m - \frac{m-2}{4} \right) & \leq 0 \\
(n - m - \frac{n-m}{s}) (m - \frac{n-m}{s} - 2) - \frac{m}{2} \left( n - m - \frac{m-4}{4} \right) & \leq 0
\end{align*}
\]
By solving the system of inequalities on \( m \) we can easily get that
\[
\alpha \leq m \leq \tilde{\alpha},
\] where \( \alpha \) and \( \tilde{\alpha} \) see Eq. (3.3).

If \( s \) is not a divisor of \( n - m \), then there exists an integer \( r(1 \leq r \leq s - 1) \) such that \( k = \frac{n-m-r}{s} \) and \( l = k + 1 \). By Eqs. (3.8), (3.11) and (3.12) we have that
\[
\begin{align*}
- (n - m - \frac{n-m-r}{s} - 1) (m - \frac{n-m-r}{s} - 1) + m \left( n - m - \frac{m-2}{4} \right) & \leq 0 \\
(n - m - \frac{n-m-r}{s}) (m - \frac{n-m-r}{s} - 2) - \frac{m}{2} \left( n - m - \frac{m-4}{4} \right) & \leq 0
\end{align*}
\]
and thus from \( 1 \leq r \leq s - 1 \) we have that
\[
\begin{align*}
- (n - m - \frac{n-m-(s-1)}{s} - 1) (m - \frac{n-m-(s-1)}{s} - 1) + m \left( n - m - \frac{m-2}{4} \right) & \leq 0 \\
(n - m - \frac{n-m-1}{s}) (m - \frac{n-m-1}{s} - 2) - \frac{m}{2} \left( n - m - \frac{m-4}{4} \right) & \leq 0
\end{align*}
\]
By solving the system of inequalities on \( m \) we can easily get that
\[
\eta \leq m \leq \hat{\eta},
\] where
\[
\begin{align*}
\eta = \frac{(2n-1)s^2 + 4n(s-2) - 8 - s \sqrt{(4n^2 - 4n + 1)s^2 - 8n(n+4)s + 8(n^2 + 4n + 5)}}{3s^2 - 8}, \\
\hat{\eta} = \frac{(2n+1)s^2 + 4n(s-2) - 8(s-1) - s \sqrt{(4n^2 - 20n+25)s^2 - 8(n^2 - 6n+8)s + 8(n^2 - 4n+5)}}{3s^2 - 8},
\end{align*}
\]
It is easy to prove that \( \eta > \alpha \) and \( \tilde{\alpha} > \hat{\eta} \). Therefore, by Eqs. (3.13) and (3.14) it follows that \( \alpha \leq m \leq \tilde{\alpha} \). So by \( 3 \leq m \leq n - s \) the Eq. (3.2) holds.

(2) Assume that \( m \) is an odd number.

If \( s \) is a divisor of \( n - m \), then \( l = k = \frac{n-m}{s} \). By Eqs. (3.8), (3.11) and (3.12) we get
\[
\begin{align*}
- (n - m - \frac{n-m}{s}) (m - \frac{n-m}{s}) + m \left( n - m - \frac{m+1}{4} \right) & \leq 0 \\
(n - m - \frac{n-m}{s}) (m - \frac{n-m}{s} - 2) - \frac{m}{2} \left( n - m - \frac{m+7}{4} \right) & \leq 0
\end{align*}
\]
By solving the system of inequalities on \( m \) we can easily get that
\[
\beta \leq m \leq \hat{\beta},
\] where \( \beta \) and \( \hat{\beta} \) see Eq. (3.5).
If $s$ is not a divisor of $n - m$, then there exists an integer $r (1 \leq r \leq s - 1)$ such that 
\[ k = \frac{n - m - r}{s} \] and $l = k + 1$. By Eqs. (3.8), (3.11) and (3.12) we have that
\[
\begin{cases}
-(n - m - \frac{n - m - r}{s} - 1)(m - \frac{n - m - r}{s} - 1) + \frac{m - 1}{2} (n - m - \frac{m + 1}{4}) \leq 0 \\
(n - m - \frac{n - m - r}{s})(m - \frac{n - m - r}{s} - 2) - \frac{m - 1}{2} (n - m - \frac{m - 7}{4}) \leq 0
\end{cases}
\]
and thus from $1 \leq r \leq s - 1$ we have that
\[
\begin{cases}
-(n - m - \frac{n - m - (s - 1)}{s} - 1)(m - \frac{n - m - (s - 1)}{s} - 1) + \frac{m - 1}{2} (n - m - \frac{m + 1}{4}) \leq 0 \\
(n - m - \frac{n - m - 1}{s})(m - \frac{n - m - 1}{s} - 2) - \frac{s - 1}{2} (n - m - \frac{m - 7}{4}) \leq 0
\end{cases}
\]
By solving the system of inequalities on $m$ we can easily get that
\[
\theta \leq m \leq \tilde{\theta}, 
\]
where
\[
\begin{cases}
\theta = \frac{2 [(n - 1)s^2 + 2n(s - 2) - 4] - s\sqrt{(4n^2 + 4n + 1)s^2 - 8n(n + 5)s + 8(n^2 + 2n + 8)}}{3s^2 - 8}, \\
\tilde{\theta} = \frac{2 [(n + 1)s^2 + 2n(s - 2) - 4(s - 1)] - s\sqrt{(4n^2 - 28n + 25)s^2 - 8(n^2 - 7n + 10)s + 8(n^2 + 2n + 8)}}{3s^2 - 8}.
\end{cases}
\]

It is easy to prove that $\theta > \beta$ and $\tilde{\theta} > \tilde{\theta}$. Therefore, by Eqs. (3.15) and (3.16) it follows that $\beta \leq m \leq \tilde{\theta}$. So by $3 \leq m \leq n - s$ the Eq. (3.4) holds. \hfill \Box

Let $k$ denote the length of the shortest pendant paths of $U(n, m, s)$ and let $r$ denote the number of pendant paths of length $k + 1$ in which $n - m = sk + r$ and $0 \leq r \leq s - 1$. By Lemma 2.1 we can get that
\[
W(U(n, m, s)) = \frac{m + 2(sk + r)}{m} W(C_m) + \frac{1}{2} (m - 1)(k + 1)(sk + 2r)
+ \left[ r^2 + \frac{1}{2} k(3k - 2)r + \frac{1}{6} sk(3sk - 2k + 2) \right] (k + 1),
\]
(3.17)
where
\[
W(C_m) = \begin{cases}
\frac{1}{8} m^3, & \text{if } m \text{ is an even number;} \\
\frac{1}{8} m(m^2 - 1), & \text{if } m \text{ is an odd number.}
\end{cases}
\]

It is obvious that $\Phi(n, 1) = \{U(n, m, 1) : 3 \leq m \leq n - 1\}$ and we have that
\[
W(U(n, m, 1)) = \frac{(2n - m)W(C_m)}{m} + \frac{(n + 2m - 1)(n - m + 1)(n - m)}{6}.
\]
So it is easy to get that
\[
W(U(n, m + 1, 1)) - W(U(n, m, 1)) = \begin{cases} 
\frac{1}{8}m(5m - 4n - 2), & \text{if } m \text{ is even}; \\
\frac{1}{8}(m - 1)(5m - 4n + 1), & \text{if } m \text{ is odd}. 
\end{cases}
\]
It follows that \(W(U(n, m + 1, 1)) > W(U(n, m, 1))\) if \(m\) is even and \(m > \frac{4n+2}{5}\) or if \(m\) is odd and \(m > \frac{4n-1}{5}\). Therefore, we can easily obtain the following results.

**Theorem 3.4** \(U(n, m, 1)\) is the graph in \(\Phi(n, 1)\) having the smallest Wiener index if and only if
\[
m = \begin{cases} 
4t + 1, & \text{if } n = 5t, 5t + 1; \\
4t + 2, 4t + 3, & \text{if } n = 5t + 2; \\
4t + 3, & \text{if } n = 5t + 3; \\
4t + 3, 4t + 4, & \text{if } n = 5t + 4.
\end{cases}
\]

**Remark 3.5** By Theorem 3.4, for \(s \geq 2\), we see that it seems to be difficult to completely determine the graphs in \(\Phi(n, s)\) with the smallest Wiener index. Write \(\xi_{x, y, z} = 2x - 2y - z\). Assume that \(s\) is a divisor of \(n - m\), i.e., \(k = \frac{n-m}{s} = l\) and \(p = n - m - k = q > 1\).

If \(m\) is an even number, then by Eqs. (3.8), (3.11) and (3.12) we have that
\[
-\xi_{p,k,1} + \sqrt{\xi_{p,k,1}^2 + 8pk} \leq m \leq -\xi_{p,k,1} + 2 + \sqrt{\xi_{p,k,1}^2 + 8pk}. \tag{3.18}
\]
It is obvious that there are at most three consecutive integers \(m\) satisfying Eq. (3.18).

If \(m\) is an odd number, then by Eqs. (3.8), (3.11) and (3.12) we have that
\[
-\xi_{p,k,0} + \sqrt{\mu - 4k + 1} \leq m \leq -\xi_{p,k,0} + 4 + \sqrt{\mu + 12k + 9}, \tag{3.19}
\]
where \(\mu = 4(p^2 + k^2 - p) > 4k^2\). Note that
\[
\sqrt{\mu + 12k + 9} - \sqrt{\mu - 4k + 1} = \frac{16k + 8}{\sqrt{\mu + 12k + 9} + \sqrt{\mu - 4k + 1}} < \frac{8(2k + 1)}{(2k + 3) + (2k - 1)} = 4,
\]
so there are at most seven consecutive integers \(m\) satisfying Eq. (3.19).

Although the upper and lower bounds on \(m\) in Eqs. (3.18) and (3.19) still contain \(m\), the two inequalities give the bounds of numbers of \(m\) satisfying inequalities. Since \(\alpha \leq m \leq \tilde{\alpha}\) and Eq. (3.18) (resp. \(\beta \leq m \leq \tilde{\beta}\) and Eq. (3.19)) result from the same condition, they have the same solutions on \(m\). Hence by the discussions above we see that there are at most two consecutive even integers \(m\) satisfying Eqs. (3.2) and there are at most four consecutive odd integers \(m\) satisfying (3.4). These indicate that Theorem 3.3 almost determine the graphs in \(\Phi(n, s)\) having the minimum Wiener index. In fact, a large number of examples indicate that the number of \(m\) satisfying Eqs.
(3.2) or (3.4) is much less than six. For example, for \( n = 1400 \) and \( s = 27, m = 100 \) satisfies Eq. (3.2) and \( m = 99, 101 \) satisfy Eq. (3.4). By Eq. (3.17) we see that

\[
W(U(1400, 100, 27)) = 47362300, \quad W(U(1400, 99, 27)) = 47436312, \\
W(U(1400, 101, 27)) = 47288238.
\]

Thus \( U(1400, 101, 27) \) is the unique graph in \( \Phi(1400, 27) \) with the smallest Wiener index. Of course, there are a large number of examples such that \( m \) with the conditions Eq. (3.2) or Eq. (3.4) is unique, and thus the graph in \( \Phi(n, s) \) with the smallest Wiener index is uniquely determined. For example, for \( n = 400, s = 11, \) there are not even numbers \( m \) satisfying Eq. (3.2) and there is a unique odd number \( m = 65 \) satisfying Eq. (3.4). So \( U(400, 65, 11) \) is the unique graph in \( \Phi(400, 11) \) with the smallest Wiener index.

Note that \( m \) of \( U(n, m, s) \) satisfies Eq. (3.2) or Eq. (3.4), and

\[
\min\{\max\{3, \alpha\}, \max\{3, \beta\}\} = \max\{3, \min\{\alpha, \beta\}\}, \\
\max\{\min\{n - s, \tilde{\alpha}\}, \min\{n - s, \tilde{\beta}\}\} = \min\{n - s, \max\{\tilde{\alpha}, \tilde{\beta}\}\},
\]

so by Eqs. (3.2) and (3.4) we immediately obtain the following result.

**Corollary 3.6** If \( s \geq 2 \) and \( U(n, m, s) \) is a graph in \( \Phi(n, s) \) having the smallest Wiener index, then \( \max\{3, \min\{\alpha, \beta\}\} \leq m \leq \min\{n - s, \max\{\tilde{\alpha}, \tilde{\beta}\}\} \).

### 4 The graphs in \( \Psi(n, c) \) with the smallest Wiener index

A vertex of a unicyclic graph is called a branching vertex if it is not on the cycle and has degree at least 3 or it is on the cycle and has degree at least 4. Let \( \tilde{U}_M \) be a unicyclic graph with the smallest Wiener index in \( \Psi(n, c) \). Note that \( \Psi(n, 0) = \{C_n\} \), so in the following we always assume that \( c \geq 1 \). For convenience, from now we always denote the unique cycle of \( \tilde{U}_M \) by \( C = v_1v_2\ldots v_kv_1 \) and denote the component containing the vertex \( v_i \) in \( \tilde{U}_M - E(C) \) by \( C_i \), in particular, write \( |V(C_i)| = c_i(i = 1, 2, \ldots, k) \). Now we investigate the properties and structure of \( \tilde{U}_M \).

**Lemma 4.1** \( \tilde{U}_M \) has at most one branching vertex.

**Proof** Suppose, for a contradiction, that \( \tilde{U}_M \) has two branching vertices, say \( u \) and \( v \). We distinguish the three following cases.

**Case 1.** Assume that both \( u \) and \( v \) are not on the cycle \( C \) of \( \tilde{U}_M \).

Assume, without loss of generality, that \( W(\tilde{U}_M, u) \geq W(\tilde{U}_M, v) \). Write

\[
N_{\tilde{U}_M}(u) = \{u', u_1, u_2, \ldots, u_p\},
\]

where \( u' \) is the vertex on the unique path from \( u \) to \( C \). Note that \( p \geq 2 \) from the definition of branching vertex, so put

\[
U' = \tilde{U}_M - uu_2 - uu_3 - \cdots - uu_p + vu_2 + vu_3 + \cdots + vu_p.
\]

\( \square \) Springer
It is obvious that $u$ and $v$ still are cut vertices of $U'$. This indicates that $U' \in \mathcal{U}(n, c)$. But from Lemma 2.2 we have $W(\tilde{U}_M) > W(U')$, a contradiction to the choice of $\tilde{U}_M$.

**Case 2.** Assume that both $u$ and $v$ are on the cycle $C$ of $\tilde{U}_M$.

Assume, without loss of generality, that $W(\tilde{U}_M, u) \geq W(\tilde{U}_M, v)$. Write

$$N_{\tilde{U}_M}(u) = \{u', u'', u_1, u_2, \ldots, u_p\},$$

where $u'$ and $u''$ are the vertices on $C$. Note that $p \geq 2$ from the definition of branching vertex, so put

$$U' = \tilde{U}_M - uu_2 - uu_3 - \cdots - uu_p + vu_2 + vu_3 + \cdots + vu_p.$$

It is obvious that $u$ and $v$ still are cut vertices of $U'$. This indicates that $U' \in \Psi_{1}(n, c)$. But from Lemma 2.2 we have $W(\tilde{U}_M) > W(U')$, a contradiction to the choice of $\tilde{U}_M$.

**Case 3.** Assume that only one of $u$ and $v$ is on the cycle $C$ of $\tilde{U}_M$.

Assume, without loss of generality, that $u$ is on $C$. Write

$$N_{\tilde{U}_M}(u) = \{u', u'', u_1, u_2, \ldots, u_p\}, \quad N_{\tilde{U}_M}(v) = \{v', v_1, v_2, \ldots, v_q\},$$

where $u'$ and $u''$ are the vertices on $C$ and $v'$ is the vertex on the unique path from $v$ to $C$. By the definition of branching vertex we have $p \geq 2$ and $q \geq 2$. If $W(\tilde{U}_M, u) \geq W(\tilde{U}_M, v)$, then set

$$U' = \tilde{U}_M - uu_2 - uu_3 - \cdots - uu_p + vu_2 + vu_3 + \cdots + vu_p.$$

Otherwise, set

$$U' = \tilde{U}_M - vv_2 - vv_3 - \cdots - vv_q + uv_2 + uv_3 + \cdots + uv_q.$$

Obviously $u$ and $v$ still are cut vertices of $U'$. It follows that $U' \in \Psi(n, c)$. But by Lemma 2.2 we always have that $W(\tilde{U}_M) > W(U')$, a contradiction to the choice of $\tilde{U}_M$.

By Lemma 4.1 and the definition of branching vertex of unicyclic graphs we see that $\tilde{U}_M$ with the unique cycle $C$ has one of following properties:

(i) $\tilde{U}_M$ has not branching vertices. In this case $\tilde{U}_M$ is the unicyclic graph obtained from $C$ by adding a pendant path of proper length to each vertex of $C$.

(ii) $\tilde{U}_M$ has a unique branching vertex contained in some $C^i$. In this case except $v_i$ each other vertex of $C$ has a pendant path with a proper length.

**Lemma 4.2** Two arbitrary pendant paths at a vertex or two adjacent vertices in $\tilde{U}_M$ have almost equal lengths.

\[ \square \]
Assume the contrary. We distinguish the two following cases.

**Case 1** Assume that there exist two pendant paths \(wa_1a_2\ldots a_s\) and \(wb_1b_2\ldots b_t\) at \(w\) in \(\tilde{U}_M\) with \(|s - t| \geq 2\).

Assume, without loss of generality, that \(s - t \geq 2\). Put \(w = b_0, U' = \tilde{U}_M - a_s + b_t a_s\).

It is easy to see that \(U' \in \Psi(n, c)\). But by Lemma 2.3 we have that \(W(\tilde{U}_M) > W(U')\), a contradiction to the choice of \(\tilde{U}_M\).

**Case 2** Assume that there exist two pendant paths \(wa_1a_2\ldots a_s\) and \(\tilde{w}b_1b_2\ldots b_t\) at two adjacent vertices \(w\) and \(\tilde{w}\) of \(\tilde{U}_M\) with \(|s - t| \geq 2\).

Assume, without loss of generality, that \(s - t \geq 2\). Put \(\tilde{w} = b_0, U' = \tilde{U}_M - a_s + b_t a_s\).

It is easy to see that \(U' \in \Psi(n, c)\). But by Lemma 2.4 we have that \(W(\tilde{U}_M) > W(U')\), a contradiction to the choice of \(\tilde{U}_M\). \(\Box\)

**Lemma 4.3** The length \(k\) of the cycle \(C\) of \(\tilde{U}_M\) is not greater than 5.

**Proof** Suppose, for a contradiction, that \(k \geq 6\). We distinguish the two following cases depending on the odevity of \(k\).

**Case 1** Assume that \(k\) is an even number.

Write \(k = 2s\) in which \(s \geq 3\). Assume, without loss of generality, that

\[
c_k \geq \max\{c_1, c_2, \ldots, c_{k-1}\}.
\]

Then by the assumption of \(c \geq 1\) we see that \(v_k\) is a cut vertex of \(\tilde{U}_M\). Taking \(u = v_1\) and \(v = v_k\) in Lemma 2.7, then \(\tilde{U}_{uv}^M \in \Psi(n, c)\) and \(H = C^1\). It is easy to see that

\[
\Theta(u, v) = \emptyset, \quad V_u = \{v_1\} \bigcup \left( \bigcup_{i=2}^{s} V(C^i) \right).
\]

From \(s \geq 3\) we get that

\[
\Omega(u, v) \supseteq \left\{ (x, y) : x \in V_u - \{v_1\}, y \in V(C^k) - \{v_k\} \right\} \bigcup \left\{ (x, y) : x \in V(C^2), y \in V(C^{k-1}) \right\}.
\]

So by \(c_k \geq c_1 = |V(H)|\) it follows that

\[
|\Omega(u, v)| \geq (|V_u| - 1)(c_k - 1) + c_2 c_{k-1} \geq (|V_u| - 1)(|V(H) - 1) + 1.
\]

Therefore, by Lemma 2.7 we have that

\[
W(\tilde{U}_M) - W(\tilde{U}_{uv}^M) = |\Omega(u, v)| - |\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1) \geq 1.
\]

It implies that \(W(\tilde{U}_M) > W(\tilde{U}_{uv}^M)\), a contradiction to the choice of \(\tilde{U}_M\).
Case 2  Assume \( k \) is an odd number.

Write \( k = 2s + 1 \) in which \( s \geq 3 \). Assume, without loss of generality, that

\[
c_k \geq \max\{c_1, c_2, \ldots, c_{k-1}\}, \quad c_{k-1} \geq c_1.
\]

(4.1)

It is obvious that \( v_k \) is a cut vertex of \( \tilde{U}_M \). Taking \( u = v_1 \) and \( v = v_k \) in Lemma 2.7, then \( Q = \tilde{U}_M^{uv} \in \Psi(n, c) \) and \( H = C^1 \). It is easy to see that

\[
\Theta(u, v) = V(C^{s+1}), \quad V_u = \{v_1\} \bigcup \left( \bigcup_{i=2}^{s+1} V(C_i) \right).
\]

(4.2)

From \( s \geq 3 \) we get that

\[
\Omega(u, v) \supseteq \left\{ (x, y) : x \in V_u - \{v_1\} \bigcup V(C^{s+1}) \right\}, \quad y \in V(C^k) - \{v_k\}
\]

\[
\bigcup \left\{ (x, y) : x \in V(C^2), \quad y \in V(C^{k-1}) \right\}.
\]

So

\[
|\Omega(u, v)| \geq (c_k - 1) \sum_{i=2}^{s} c_i + c_2 c_{k-1}.
\]

(4.3)

From Eqs. (4.2) and (4.3), by Lemma 2.7 we get that

\[
W(\tilde{U}_M) - W(Q) = |\Omega(u, v)| - |\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1)
\]

\[
\geq \left[ (c_k - 1) \sum_{i=2}^{s} c_i + c_2 c_{k-1} \right] - c_{s+1} - (c_1 - 1) \sum_{i=2}^{s+1} c_i.
\]

(4.4)

It is obvious that \( v_k \) is a cut vertex of \( Q \). Taking \( u = v_2 \) and \( v = v_k \) in Lemma 2.7, then \( Q^{u_2v_k} \in \Psi(n, c) \) and \( H = C^2 \). It is easy to see that

\[
\Theta(v_2, v_k) = \emptyset, \quad V_{v_2} = \{v_2\} \bigcup \left( \bigcup_{i=3}^{s+1} V(C_i) \right).
\]

(4.5)

Since

\[
\Omega(v_2, v_k) \supseteq \left\{ (x, y) : x \in V_{v_2} - \{v_2\}, \quad y \in \left( V(C^k) \bigcup V(C^1) \right) - \{v_k\} \right\}
\]

\[
\bigcup \left\{ (x, y) : x \in V(C^3), \quad y \in V(C^{k-1}) \right\},
\]

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we have that
\[ |\Omega(v_2, v_k)| \geq (c_1 + c_k - 1) \sum_{i=3}^{s+1} c_i + c_3 c_{k-1}. \] (4.6)

From Eqs. (4.5) and (4.6), by Lemma 2.7 we have that
\[
W(Q) - W(Q^{v_2v_k}) = |\Omega(v_2, v_k)| - |\Theta(v_2, v_k)| - (|V(H)| - 1)(|V_{v_2}| - 1)
\geq \left[(c_1 + c_k - 1) \sum_{i=3}^{s+1} c_i + c_3 c_{k-1}\right] - 0 - (c_2 - 1) \sum_{i=3}^{s+1} c_i.
\] (4.7)

From \(c_3 \geq 1\) and Eqs. (4.1), (4.4) and (4.7) it follows that
\[
W(\tilde{U}_M) - W(Q^{v_2v_k}) = [W(\tilde{U}_M) - W(Q)] + [W(Q) - W(Q^{v_2v_k})]
\geq \left[(c_k - 1) \sum_{i=2}^{s} c_i + c_2 c_{k-1}\right] - c_{s+1} - (c_1 - 1) \sum_{i=2}^{s+1} c_i
\]
\[+ \left[(c_1 + c_k - 1) \sum_{i=3}^{s+1} c_i + c_3 c_{k-1}\right] - (c_2 - 1) \sum_{i=3}^{s+1} c_i
\]
\[= c_2[(c_{k-1} - c_1) + (c_k - c_{s+1})] + (c_k c_3 - c_{s+1})
\]
\[+ (c_k - c_2) \sum_{i=3}^{s} c_i + c_3 c_{k-1} + c_{s+1} + c_k \sum_{i=4}^{s+1} c_i
\]
\[\geq c_3 c_{k-1} + c_{s+1} > 0.
\]

It implies that \(W(\tilde{U}_M) > W(Q^{v_2v_k})\), a contradiction to the choice of \(\tilde{U}_M\). \(\square\)

From Lemma 4.3 we see that the length \(k\) of the cycle \(C\) of \(\tilde{U}_M\) satisfies \(3 \leq k \leq 5\). Let \(C_{m,l}\) denote the unicyclic graph obtained from a cycle \(C\) of length \(m\) by adding a pendant path of length \(l - 1\) at each vertex of \(C\). It is obvious that \(C_{m,l}\) has \(ml\) vertices and \(m(l - 1)\) cut vertices.

**Lemma 4.4** If the length \(k\) of the cycle \(C\) of \(\tilde{U}_M\) is equal to 4, then \(\tilde{U}_M \cong C_{4,l}\).

**Proof** Suppose, for a contradiction, that \(\tilde{U}_M \not\cong C_{4,l}\). We distinguish the two cases.

**Case 1** Assume that not all of \(c_1, c_2, c_3\) and \(c_4\) are equal.

Now there must exist a \(i(1 \leq i \leq 4)\) such that \(c_i \neq c_{i+1}\), where \(i + 1\) is regarded as 1 when \(i = 4\). Assume, without loss of generality, that \(c_4 > c_1\). Then by the assumption of \(c \geq 1\) we see that \(v_4\) is a cut vertex of \(\tilde{U}_M\). Taking \(u = v_1\) and \(v = v_4\)
in Lemma 2.7, then $\tilde{U}^u_M \in \Psi(n, c)$ and $H = C^1$. It is easy to see that
\[
\Theta(u, v) = \emptyset, \quad V_u = \{v_1\} \bigcup V(C^2).
\]
\[
\Omega(u, v) = \left\{(x, y) : x \in V(C^2), y \in V(C^4) - \{v_4\}\right\}.
\]
So by Lemma 2.7 we have that
\[
W(\tilde{U}_M) - W(\tilde{U}^u_M) = |\Omega(u, v)| - |\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1)
= c_2(c_4 - 1) - 0 - c_2(c_1 - 1)
= c_2(c_4 - c_1) > 0.
\]
This indicates that $W(\tilde{U}_M) > W(\tilde{U}^u_M)$, a contradiction to the choice of $\tilde{U}_M$.

Case 2 Assume that $c_1 = c_2 = c_3 = c_4 = l$.

From $\tilde{U}_M \not\cong C_{4,l}$ we see that at least one of $C^1, C^2, C^3$ and $C^4$ is not a pendant path. Assume, without loss of generality, that $C^1$ is not a pendant path. Then $C^1$ contains the unique branching vertex of $\tilde{U}_M$. So all of $C^2, C^3$ and $C^4$ are pendant paths.

Case 2.1 Assume that $v_1$ is the unique branching vertex of $\tilde{U}_M$.

By Lemma 4.2 we know that $C^1$ is the starlike tree obtained by adding $r(r \geq 2)$ pendant paths with almost equal lengths at $v_1$. Let $a_1a_2 \ldots a_s$ be a shortest pendant path at $v_1$ and let $b_1b_2 \ldots b_l$ be the pendant path at $v_2$, where $a_1 = v_1$ and $b_1 = v_2$. It is easy to see that $s \geq 2$ and $l \geq 2(s - 1) + 1 \geq 3$. Write $U' = \tilde{U}_M - b_2 + a_s b_l$. Then $U' \in \Psi(n, c)$. From Lemma 4.2 we know that $l - s \leq 1$. So by combining $s \geq 2$ and $l \geq 2(s - 1) + 1$ we get that $s = 2, r = 2$ and $l = 3$. Write $Q = \tilde{U}_M - b_3$. By Lemma 2.1 it is easy to see that
\[
W(\tilde{U}_M) - W(U') = W(Q, b_2) - W(Q, a_2) = 1.
\]
This indicates that $W(\tilde{U}_M) > W(U')$, a contradiction to the choice of $\tilde{U}_M$.

Case 2.2 Assume that $v_1$ is not the unique branching vertex of $\tilde{U}_M$.

Let $a_i$ be the unique branching vertex of $\tilde{U}_M$. Then $a_i$ is not in $C$ and $deg_{\tilde{U}_M}(a_i) \geq 3$. Let $b_0b_1b_2 \ldots b_s$ be the unique path from $a_i$ to $v_1$ in which $b_0 = a_i$ and $b_s = v_1$ and let $a_1a_2 \ldots a_i$ be a pendant path at $a_i$. Write $\tilde{N}_{\tilde{U}_M}(a_i) = \{a_i-1, b_1, u_1, u_2, \ldots, u_l\}$. Let $Q$ be the graph containing $v_1$ in $\tilde{U}_M - b_{s-1} b_s$. Then $|V(Q)| = 3l + 1 > c_1 > i$. Set
\[
U' = \tilde{U}_M - a_i u_1 - a_i u_2 - \cdots - a_i u_l + v_1 u_1 + v_1 u_2 + \cdots + v_1 u_l.
\]
Then $U' \in \Psi(n, c)$ and by Lemma 2.5 we have that $W(\tilde{U}_M) > W(U')$, a contradiction to the choice of $\tilde{U}_M$. \square

Lemma 4.5 If the length $k$ of the cycle $C$ of $\tilde{U}_M$ is equal to 5, then $\tilde{U}_M \cong C_{5,l}$.\hfill \& Springer
Proof Suppose, for a contradiction, that $\tilde{U}_M \not\cong C_{5,1}$. We distinguish the two cases.

**Case 1** Assume that not all of $c_1, c_2, c_3, c_4$ and $c_5$ are equal.

Assume, without loss of generality, that

$$c_5 \geq \max\{c_1, c_2, c_3, c_4\}, \quad c_4 \geq c_1. \quad (4.8)$$

**Case 1.1** Assume that $c_5 > c_1$ or $c_5 > c_2$.

It is obvious that $v_5$ is a cut vertex of $\tilde{U}_M$. Taking $u = v_1$ and $v = v_5$ in Lemma 2.7, then $Q = \tilde{U}^{uv}_M \in \Psi(n, c)$ and $H = C^1$. It is easy to see that

$$\Theta(u, v) = V(C^3), \quad V_u = \{v_1\} \cup V(C^2) \cup V(C^3),$$

$$\Omega(u, v) = \{(x, y) : x \in V(C^2), y \in V(C^5) - \{v_5\}\}.$$ 

So by Lemma 2.7 we have that

$$W(\tilde{U}_M) - W(Q) = |\Omega(u, v)| - |\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1)$$

$$= c_2(c_5 - 1) - c_3 - (c_1 - 1)(c_2 + c_3). \quad (4.9)$$

It is obvious that $v_5$ is a cut vertex of $Q$. Taking $u = v_2$ and $v = v_5$ in Lemma 2.7, then $Q^{v_2v_5} \in \Psi(n, c)$ and $H = C^2$. It is easy to see that

$$\Theta(v_2, v_5) = \emptyset, \quad V_{v_2} = \{v_2\} \cup V(C^3),$$

$$\Omega(v_2, v_5) = \{(x, y) : x \in V(C^3), y \in (V(C^5) \cup V(C^4)) - \{v_5\}\}.$$ 

So by Lemma 2.7 we have that

$$W(Q) - W(Q^{v_2v_5}) = |\Omega(v_2, v_5)| - |\Theta(v_2, v_5)| - (|V(H)| - 1)(|V_{v_2}| - 1)$$

$$= c_3(c_1 + c_5 - 1) - (c_2 - 1). \quad (4.10)$$

By Eqs. (4.9) and (4.10) we get that

$$W(\tilde{U}_M) - W(Q^{v_2v_5}) = [W(\tilde{U}_M) - W(Q)] + [W(Q) - W(Q^{v_2v_5})]$$

$$= c_2(c_5 - 1) - c_3 - (c_1 - 1)(c_2 + c_3)$$

$$+ c_3(c_1 + c_5 - 1) - c_3(c_2 - 1)$$

$$= c_2(c_5 - c_1) + c_3(c_5 - c_2) > 0,$$

namely $W(\tilde{U}_M) > W(Q^{v_2v_5})$, a contradiction to the choice of $\tilde{U}_M$.

**Case 1.2** Assume that $c_5 = c_1$ and $c_5 = c_2$.

By Eq. (4.8) it is easy to see that $c_1 = c_2 = c_4 = c_5$. Since not all of $c_1, c_2, c_3, c_4$ and $c_5$ are equal, we have that $c_3 < c_1 = c_2 = c_4 = c_5$. By replacing $c_5, c_1, c_2, c_4, c_3$
above with $c_5, c_4, c_3, c_1, c_2$, respectively, in a similar way we can also get a contradiction.

**Case 2** Assume that $c_1 = c_2 = c_3 = c_4 = c_5 = l$.

In a similar way to prove Case 2 in Lemma 4.4, we can get contradictions.  

For $c \geq 3$, let $\Delta_{n,c}$ be the unicyclic graph obtained from a triangle $v_1v_2v_3$ by adding $n - c - 2$ pendant paths of lengths $s_1, s_2, \ldots, s_{n-c-2}$, respectively, at $v_1$, a pendant path of length $s_{n-c-1}$ at $v_2$ and a pendant path of length $s_{n-c}$ at $v_3$, where $s_i = p + 1$ for $1 \leq i \leq q$, $s_i = p$ for $q + 1 \leq i \leq n - c$ and

$$n - 3 = p(n - c) + q, \quad 0 \leq q \leq n - c - 1.$$  

Three examples of $\Delta_{n,c}$ are shown in Fig. 4, where $(p, q) = (2, 1)$ in $\Delta_{14,9}$, $(p, q) = (2, 4)$ in $\Delta_{17,12}$ and $(p, q) = (3, 0)$ in $\Delta_{18,13}$.

**Lemma 4.6** If the length $k$ of the cycle $C$ of $\widetilde{U}_M$ is equal to $3$, then $\widetilde{U}_M \cong \Delta_{n,c}$.

**Proof** If $\widetilde{U}_M$ has no branching vertices, then $\widetilde{U}_M$ contains at most three pendant vertices. This indicates that $\widetilde{U}_M$ is the unicyclic graph formed from a triangle $v_1v_2v_3$ by adding a pendant path of proper length to $v_1$, $v_2$, $v_3$, respectively. So from Lemma 4.2 and the definition of $\Delta_{n,c}$ we easily see that $\widetilde{U}_M \cong \Delta_{n,c}$.

Next assume that $\widetilde{U}_M$ has at least a branching vertex. Suppose, for a contradiction, that $\widetilde{U}_M \not\cong \Delta_{n,c}$. By Lemmas 4.1 and 4.2 we see that there must exist only one of $C^1$, $C^2$ and $C^3$, say $C^1$, that contains the unique branching vertex of $\widetilde{U}_M$, while $C^i$ is a pendant path at $v_i (i = 2, 3)$. Assume, without loss of generality, that $c_2 \geq c_3$.

**Case 1** Assume that $v_1$ is the unique branching vertex of $\widetilde{U}_M$.

From Lemma 4.2 we know that $C^1$ is the starlike tree obtained by adding $r(r \geq 2)$ pendant paths with almost equal lengths to $v_1$. Let $a_1a_2 \ldots a_s$ be a shortest pendant path at $v_1$ and let $b_1b_2 \ldots b_l$ be the pendant path at $v_2$, where $a_1 = v_1$ and $b_1 = v_2$. By Lemma 4.2 and $\widetilde{U}_M \not\cong \Delta_{n,c}$ it is easy to see that $l - s = 1$. Put $U' = \widetilde{U}_M - b_l + a_s b_l$. Note that $s \geq 2$, so $U' \in \Psi(n, c)$. Write

$$B = \widetilde{U}_M - b_l, \quad D = C^1 - \{a_2, \ldots, a_s\}, \quad d = |V(D)| = c_1 - (s - 1).$$
By Lemma 2.1 we have that

\[
W(\tilde{U}_M) = W(B) + W(P_2) + (|V(B)| - 1) \times 1 + (2 - 1) \times W(B, b_{l-1}).
\]

\[
W(U') = W(B) + W(P_2) + (|V(B)| - 1) \times 1 + (2 - 1) \times W(B, a_s).
\]

\[
W(B, b_{l-1}) = W(C^3, v_3) + W(D, v_1) + (l - 1) \left(\frac{l - 2}{2} + c_3 + s - 1\right).
\]

\[
W(B, a_s) = W(C^3, v_3) + W(D, v_1) + (l - 1) \left(\frac{l - 2}{2} + s\right) + (s - 1) \left(\frac{s - 2}{2} + d\right) + c_3s.
\]

So it follows that \(W(\tilde{U}_M) - W(U') = c_1 - s \geq 1\), a contradiction to the choice of \(\tilde{U}_M\).

**Case 2** Assume that \(v_1\) is not the unique branching vertex of \(\tilde{U}_M\).

Let \(a_i\) be the unique branching vertex of \(\tilde{U}_M\). Then \(a_i\) is not in \(C\) and \(\deg_{\tilde{U}_M}(a_i) = \eta \geq 3\). Let \(b_0b_1b_2\ldots b_s\) be the path from \(a_i\) to \(v_1\), and \(a_1a_2\ldots a_i\) be a shortest pendant path at \(a_i\) and \(z_0z_1\ldots z_l\) be the pendant path at \(v_3\) in which \(b_0 = a_i, b_s = v_1\) and \(z_0 = v_3\). Write \(N_{\tilde{U}_M}(a_i) = \{a_{i-1}, b_1, u_1, u_2, \ldots, u_{\eta-2}\}\). Let \(Q\) be the graph containing \(v_1\) in \(\tilde{U}_M - b_0b_1\).

**Case 2.1** Assume that \(|V(Q)| > i\).

Put \(U' = \tilde{U}_M - a_iu_1 - a_iu_2 - \cdots - a_iu_{\eta-2} + b_1u_1 + b_1u_2 + \cdots + b_1u_{\eta-2}\). Then \(U' \in \Psi(n, c)\) and by Lemma 2.5 we have \(W(\tilde{U}_M) > W(U')\), a contradiction to the choice of \(\tilde{U}_M\).

**Case 2.2** Assume that \(|V(Q)| \leq i\). Let \(Z\) be the graph containing the vertex \(a_i\) in \(\tilde{U}_M - b_0b_1 - a_i\). Write

\[
U' = \tilde{U}_M - a_i + z_l, \quad Y = \tilde{U}_M - a_i, \quad \delta = \frac{s + t + 1}{j=1} j.
\]

Note that

\[
i \geq |V(Q)| \geq s + t + 1 + c_2 \geq s + t + 2,
\]

so \(U' \in \Psi(n, c)\). By Lemma 2.1 we have that

\[
W(\tilde{U}_M) = W(Y) + W(P_2) + (|V(Y)| - 1) \times 1 + (2 - 1) \times W(Y, a_2),
\]

\[
W(U') = W(Y) + W(P_2) + (|V(Y)| - 1) \times 1 + (2 - 1) \times W(Y, z_l),
\]

\[
W(Y, a_2) = \delta + (|V(Z)| - 1)(i - 1) + W(Z, a_i) + c_2(s + i - 1) + W(C^2, v_2),
\]

\[
W(Y, z_l) = \delta + (|V(Z)| - 1)(s + t + 1) + W(Z, a_i) + c_2(t + 1) + W(C^2, v_2).
\]
Therefore, by Eq. (4.11) we get that
\[ W(\tilde{U}_M) - W(U') = (|V(Z)| - 1)(i - s - t - 2) + c_2(i + s - t - 2) \geq 2sc_2 > 0, \]
namely \( W(\tilde{U}_M) > W(U') \), a contradiction to the choice of \( \tilde{U}_M \). \( \square \)

By a direct calculation we see that \( W(C_{4,l}) \neq W(C_{5,l}) \), where
\[
W(C_{4,l}) = \frac{2}{3}(2l + 1)(5l - 1)l = W(\Delta_{4l,4l-4}),
\]
\[
W(C_{5,l}) = \frac{5}{6}(13l^2 + 6l - 1)l = W(\Delta_{5l,5l-5}).
\]

Therefore, by Lemmas 4.1–4.6 we get the main results in this section as follows.

**Theorem 4.7** Assume that \( n \geq 5 \) and \( c \geq 1 \).

1. If \((n, c) = (4l, 4l - 4)\), then \( C_{4,l} \) and \( \Delta_{n,c} \) are all graphs having the smallest Wiener index in \( \Psi(n, c) \).
2. If \((n, c) = (5l, 5l - 5)\), then \( C_{5,l} \) and \( \Delta_{n,c} \) are all graphs having the smallest Wiener index in \( \Psi(n, c) \).
3. If \((n, c) \notin \{(4l, 4l - 4), (5l, 5l - 5)\}\), then \( \Delta_{n,c} \) is the unique graph having the smallest Wiener index in \( \Psi(n, c) \).

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**References**

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