Maximum Wiener Index of Unicyclic Graphs with Fixed Maximum Degree

Hui Dong and Bo Zhou*
Department of Mathematics, South China Normal University, Guangzhou 510631, China
e-mail: zhoubo@scnu.edu.cn

Abstract

We determine the maximum Wiener index of n-vertex unicyclic graphs with fixed maximum degree and characterize the unique extremal graph.

1 Introduction

Topological indices are numerical graph invariants that quantitatively characterize molecular structure. The Wiener index is one of the oldest and the most thoroughly studied topological indices [15, 16].

Let G be a simple connected graph with vertex set $V(G)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between u and v in G. The Wiener index of G is defined as [8]

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

The Wiener index found various applications including those in the structure-property-activity modelling [1, 3, 9, 13, 14] and has also been studied extensively in mathematics [2, 4, 5, 7, 10–12].

Stevanović [12] determined the unique n-vertex tree with fixed maximum degree having maximum Wiener index. In this paper, we determine the maximum Wiener index of n-vertex unicyclic graphs with fixed maximum degree Δ, and characterize the unique extremal graph, where $2 \leq \Delta \leq n-1$.

*Corresponding author.

2 Preliminaries

For $u \in V(G)$, and let $D_G(u)$ be the sum of distances between u and all vertices of G. Then $W(G) = \frac{1}{2}\sum_{u\in V(G)} D_G(u)$.

For an edge uv of the graph G, $G - uv$ denotes the graph obtained from G by deleting uv, and for an edge uv of the complement of G, $G + uv$ denotes the graph obtained from G by adding uv.

For a graph G with a vertex v of degree at least three, a pendant path at v of G is a path in G connecting v and a pendant vertex such that all internal vertices (if exist) in this path have degree two.

Let P_n be the path on $n \geq 1$ vertices, and C_n the cycle on $n \geq 3$ vertices.

Lemma 1. *Let Q_1 and Q_2 be vertex-disjoint connected graphs with at least two vertices. For $u \in V(Q_1)$ and $v \in V(Q_2)$, let G_1 be the graph obtained from Q_1 and Q_2 by joining u and v by a path of length $r \geq 1$, and G_2 the graph obtained from Q_1 and Q_2 by identifying u and v, which is denoted by w, and attaching a path P_r to w. Then $W(G_1) > W(G_2)$.*

Proof. It is easily seen that

$$\begin{aligned} W(G_1) - W(G_2) &= \sum_{\substack{x\in V(Q_1)\setminus\{u\}\\ y\in V(Q_2)\setminus\{v\}}} d_{G_1}(x,y) - \sum_{\substack{x\in V(Q_1)\setminus\{w\}\\ y\in V(Q_2)\setminus\{w\}}} d_{G_2}(x,y) \\ &= \sum_{\substack{x\in V(Q_1)\setminus\{u\}\\ y\in V(Q_2)\setminus\{v\}}} (d_{Q_1}(x,u) + r + d_{Q_2}(y,v)) \\ &\quad - \sum_{\substack{x\in V(Q_1)\setminus\{w\}\\ y\in V(Q_2)\setminus\{w\}}} (d_{Q_1}(x,w) + d_{Q_2}(y,w)) \\ &= (|V(Q_1)|-1)(|V(Q_2)|-1)r > 0, \end{aligned}$$

and then $W(G_1) > W(G_2)$. □

Let $C_r(T_1, T_2, \ldots, T_r)$ be the unicyclic graph with cycle $C_r = v_1v_2\ldots v_rv_1$ such that the deletion of all edges on C_r results in r vertex-disjoint trees $T_1, T_2, \ldots, T_r$ with $v_i \in V(T_i)$, and we say T_i is a branch at v_i for $i = 1, 2, \ldots, r$. If T_i is trivial for some i with $1 \leq i \leq r$, then we use $-$ to denote T_i in $C_r(T_1, T_2, \ldots, T_r)$.

We use computational techniques from [6] for the difference of the Wiener indices of two graphs in the following lemmas.

Lemma 2. *For fixed integers i and j with $2 \leq i < j \leq r$, let $G_{a_i,a_j} = C_r(T_1, T_2, \ldots, T_r)$, where $T_s = P_{a_s+1}$ with an end vertex v_s and $a_s \geq 0$ for $s = 2, \ldots, r$, and all branches not at v_i and v_j are fixed. If $a_i, a_j \geq 1$, then*

$$W(G_{a_i,a_j}) < \max\{W(G_{a_i+a_j,0}), W(G_{0,a_i+a_j})\}.$$

Proof. Let $G = G_{a_i,a_j}$ and $G_1 = G_{a_i+a_j,0}$. Let v be the neighbor of v_j in T_j. Let v_i^* be the pendant vertex of G in T_i. Obviously, $G_1 = G - vv_j + vv_i^*$. Let $Z = V(T_j)\setminus\{v_j\}$, $W = V(T_i)$ and $n = |V(G)|$. Let $G_2 = G - vv_j + vv_i$ and $a_1 = |V(T_1)| - 1$. Note that $\sum_{\substack{x\in Z\\ y\in W}} d_{G_1}(x,y) = \sum_{\substack{x\in Z\\ y\in W}} d_{G_2}(x,y)$ and $\sum_{\substack{x\in Z\\ y\in V(C_r)}} d_{G_2}(x,y) = \sum_{\substack{x\in Z\\ y\in V(C_r)}} d_G(x,y)$. Then

$$\begin{aligned}
W(G_1) - W(G_2) &= \sum_{\substack{x\in Z\\ y\in V(G)\setminus(Z\cup W)}} (d_{G_1}(x,y) - d_{G_2}(x,y))\\
&= \sum_{\substack{x\in Z\\ y\in V(G)\setminus(Z\cup W)}} a_i = a_i a_j (n - a_i - a_j - 1),\\
W(G_2) - W(G) &= \sum_{\substack{x\in Z\\ y\in V(G)\setminus(Z\cup V(C_r))}} (d_{G_2}(x,y) - d_G(x,y))\\
&= \sum_{x\in Z}\sum_{\substack{1\le k\le r\\ k\ne j}} a_k\left(d_G(v_k,v_i) - d_G(v_k,v_j)\right)\\
&= a_j \sum_{\substack{1\le k\le r\\ k\ne j}} a_k\left(d_G(v_k,v_i) - d_G(v_k,v_j)\right),
\end{aligned}$$

and thus

$$\begin{aligned}
& W(G_{a_i+a_j,0}) - W(G_{a_i,a_j})\\
= \;& a_i a_j (n - a_i - a_j - 1) - a_j \sum_{\substack{1\le k\le r\\ k\ne j}} a_k\left(d_G(v_k,v_j) - d_G(v_k,v_i)\right).
\end{aligned}$$

If $\sum_{\substack{1\le k\le r\\ k\ne j}} a_k\left(d_G(v_k,v_j) - d_G(v_k,v_i)\right) < a_i(n - a_i - a_j - 1)$, then $W(G_{a_i,a_j}) < W(G_{a_i+a_j,0})$. Otherwise,

$$\begin{aligned}
& W(G_{0,a_i+a_j}) - W(G_{a_i,a_j})\\
= \;& a_i a_j (n - a_i - a_j - 1) + a_i \sum_{\substack{1\le k\le r\\ k\ne i}} a_k\left(d_G(v_k,v_j) - d_G(v_k,v_i)\right)\\
= \;& a_i a_j (n - a_i - a_j - 1) - a_i(a_i + a_j) d_G(v_i,v_j)\\
& + a_i \sum_{\substack{1\le k\le r\\ k\ne j}} a_k\left(d_G(v_k,v_j) - d_G(v_k,v_i)\right)\\
\ge \;& a_i a_j (n - a_i - a_j - 1) - a_i(a_i + a_j) d_G(v_i,v_j)\\
& + a_i^2 (n - a_i - a_j - 1)\\
= \;& a_i(a_i + a_j)(n - a_i - a_j - 1 - d_G(v_i,v_j))\\
\ge \;& a_i(a_i + a_j)\left(r - 1 - \frac{r}{2}\right) > 0,
\end{aligned}$$

implying that $W(G_{a_i,a_j}) < W(G_{0,a_i+a_j})$. □

For $n \geq r \geq 3$, let $U_{n,r} = C_r(P_{n-r+1}, -, \ldots, -)$, where v_1 is an end vertex of the path P_{n-r+1}. In particular, $U_{n,n} = C_n$. We have [6]

$$\begin{aligned} W(U_{n,r}) &= \frac{n^3}{6} + \left(\left\lfloor \frac{r^2}{4} \right\rfloor - \frac{r^2}{2} + \frac{r}{2} - \frac{1}{6}\right) n \\ &\quad -\frac{r}{2}\left\lfloor \frac{r^2}{4} \right\rfloor + \frac{r^3}{3} - \frac{r^2}{2} + \frac{r}{6}, \qquad (1) \\ D_{U_{n,r}}\left(v_{\lfloor \frac{r}{2} \rfloor + 1}\right) &= \left\lfloor \frac{r^2}{4} \right\rfloor + \frac{1}{2}(n-r)\left(n - r + 1 + 2\left\lfloor \frac{r}{2} \right\rfloor\right). \qquad (2) \end{aligned}$$

Lemma 3. *For fixed integers i and r with $2 \leq i \leq \lfloor \frac{r}{2} \rfloor + 1$ and $r \geq 3$, let $G_i(a,r) = C_r(T_1, T_2, \ldots, T_r)$, where T_1 is fixed, $T_i = P_{a+1}$ with an end vertex v_i, and all branches not at v_1 and v_i are trivial. Let $G(a,r) = G_{\lfloor \frac{r}{2} \rfloor + 1}(a,r)$ and $k = a + r$. For fixed $k \geq 4$, $W(G_i(a,r)) < \max\{W(G(k-3,3)), W(G(k-4,4))\}$ if $r = 4$ and $i = 2$, or if $r \geq 5$.*

Proof. We first show the following claim.
Claim. $W(G_i(a,r)) \leq W(G(a,r))$ with equality if and only if $G_i(a,r) = G(a,r)$.

If $|V(T_1)| = 1$ or $a = 0$, then $G_i(a,r)$ is (isomorphic to) $G(a,r)$. Suppose that $|V(T_1)| \geq 2$ and $a \geq 1$. Suppose that $G_i(a,r) \neq G(a,r)$, i.e., $i < \lfloor \frac{r}{2} \rfloor + 1$. Let $G = G_i(a,r)$. Let v be the neighbor of v_i in T_i. Then $G(a,r) = G - v_i v + v_{\lfloor \frac{r}{2} \rfloor + 1} v$. Let $X = V(T_i) \setminus \{v_i\}$. Note that $\sum_{\substack{x \in X \\ y \in V(G) \setminus (V(T_1) \setminus \{v_1\})}} d_{G(a,r)}(x,y) = \sum_{\substack{x \in X \\ y \in V(G) \setminus (V(T_1) \setminus \{v_1\})}} d_G(x,y)$. Then

$$\begin{aligned} W(G(a,r)) - W(G) &= \sum_{\substack{x \in X \\ y \in V(T_1) \setminus \{v_1\}}} \left(d_{G(a,r)}(x,y) - d_G(x,y)\right) \\ &= \sum_{\substack{x \in X \\ y \in V(T_1) \setminus \{v_1\}}} d_G(v_i, v_{\lfloor \frac{r}{2} \rfloor + 1}) \\ &= a(|V(T_1)| - 1)\left(\left\lfloor \frac{r}{2} \right\rfloor + 1 - i\right) > 0, \end{aligned}$$

and thus $W(G_i(a,r)) < W(G(a,r))$. This proves the claim.

If $r = 4$ and $i = 2$, then $k = a + 4$, $G_2(a,4) \neq G_3(a,4) = G(a,4)$, and thus by Claim, $W(G_2(a,4)) < W(G(k-4,4)) \leq \max\{W(G(k-3,3)), W(G(k-4,4))\}$.

Suppose that $r \geq 5$. By Claim, we need only to show that $W(G(a,r)) < \max\{W(G(k-3,3)), W(G(k-4,4))\}$ for $a \geq 0$. Note that $U_{r+a,r}$ is a subgraph of $G(a,r)$. Let $A_1 = V(U_{r+a,r-2}) \setminus \{v_1\}$, $A_2 = V(U_{r+a,r}) \setminus \{v_1\}$ and $A_3 = V(T_1) \setminus \{v_1\}$. Using Eqs. (1) and (2), we have

$$W(G(a+2, r-2)) - W(G(a,r))$$

$$
\begin{aligned}
&= (W(U_{r+a,r-2}) - W(U_{r+a,r})) \\
&\quad + \left(\sum_{\substack{x\in A_1\\ y\in A_3}} d_{G(a+2,r-2)}(x,y) - \sum_{\substack{x\in A_2\\ y\in A_3}} d_{G(a,r)}(x,y) \right) \\
&= (W(U_{r+a,r-2}) - W(U_{r+a,r})) \\
&\quad +(|V(T_1)|-1)(D_{U_{r+a,r-2}}(v_1) - D_{U_{r+a,r}}(v_1)) \\
&= \frac{r^2}{2} + \left(a - 2\left\lfloor\frac{r}{2}\right\rfloor - n + \frac{1}{2}\right) r + \left\lfloor\frac{r^2}{4}\right\rfloor \\
&\quad +2\left\lfloor\frac{r}{2}\right\rfloor (n-a) + (a+2)(n-a-2) \\
&= \begin{cases} -\frac{1}{4}r^2 + \frac{1}{2}r - a^2 + (n-4)a + 2n - 4 & \text{if } r \text{ is even,} \\ -\frac{1}{4}r^2 + \frac{3}{2}r - a^2 + (n-3)a + n - \frac{17}{4} & \text{if } r \text{ is odd.} \end{cases}
\end{aligned}
$$

Suppose that r is even. Let $f(r) = -\frac{r^2}{4}+\frac{1}{2}r-a^2+(n-4)a+2n-4$. Then $f(6) = (a+2)n - a^2 - 4a - 10 \geq (a+2)(a+6) - a^2 - 4a - 10 = 4a+2 > 0$. Let r_1 and r_2 be the two roots of $f(r) = 0$, where $r_1 \leq r_2$. Note that $r_1 < 6 < r_2$. Thus $f(r) \geq 0$ for $6 \leq r \leq r_2$, and $f(r) < 0$ for $r > r_2$. Suppose that k is even. Then $r \leq k$. Thus $W(G(a,r))$ is maximum only if $(a,r) = (k-4,4)$ for $r_2 \geq k$, and $(a,r) = (k-4,4)$ or $(0,k)$ for $r_2 < k$. It is easily seen that

$$
\begin{aligned}
& W(G(k-4,4)) - W(G(0,k)) \\
&= -\frac{5}{24}k^3 + \left(\frac{n}{4} + \frac{3}{2}\right)k^2 - \left(\frac{3}{2}n + \frac{25}{6}\right)k + 2n + 6 \\
&= \left(\frac{k^2}{4} - \frac{3}{2}k + 2\right)n - \frac{5}{24}k^3 + \frac{3}{2}k^2 - \frac{25}{6}k + 6 \\
&\geq \left(\frac{k^2}{4} - \frac{3}{2}k + 2\right)k - \frac{5}{24}k^3 + \frac{3}{2}k^2 - \frac{25}{6}k + 6 \\
&= \frac{k^3}{24} - \frac{13}{6}k + 6 > 0,
\end{aligned}
$$

and thus $W(G(k-4,4)) > W(G(0,k))$. Similarly, if k is odd, then $r \leq k-1$, $W(G(a,r))$ is maximum only if $(a,r) = (k-4,4)$ or $(1,k-1)$, and we have by direct calculation that $W(G(k-4,4)) > W(G(1,k-1))$. Therefore $W(G(a,r)) < W(G(k-4,4))$.

If r is odd, then by similar arguments as above, $W(G(a,r)) < W(G(k-3,3))$. □

Lemma 4. *For any unicyclic graph H with $u \in V(H)$, let $H(a_1, a_2, \ldots, a_t)$ be the graph obtained from H by attaching $t \geq 2$ paths P_{a_1}, P_{a_2}, $\ldots$, P_{a_t} to u, where $a_1 \geq a_2 \geq \cdots \geq a_t \geq 1$. For fixed $k = a_1 + a_2 + \cdots + a_t$,*

$W(H(a_1, a_2, \ldots, a_t)) \leq W(H(k-t+1, 1, \ldots, 1))$ *with equality if and only if* $a_1 = k - t + 1$ *and* $a_i = 1$ *for* $i = 2, 3, \ldots, t$.

Proof. Let $G = H(a_1, a_2, \ldots, a_t)$. Suppose that there is some i such that $a_i \geq 2$ for $2 \leq i \leq t$. Let $G_1 = H(b_1, b_2, \ldots, b_t)$ with $b_1 = a_i + 1$, $b_i = a_i - 1$ and $b_j = a_j$ for $j \neq 1, i$. Let u_1 and u_2 be the pendant vertices of G in the paths P_{a_1} and P_{a_i}, respectively, and u_3 the neighbor of u_2 in G. Then $G_1 = G - u_2u_3 + u_1u_2$. Let $G_2 = G - u_2u_3 + uu_2$. Then

$$\begin{aligned} W(G_1) - W(G) &= (D_{G_1}(u_2) - D_{G_2}(u_2)) + (D_{G_2}(u_2) - D_G(u_2)) \\ &= a_1(n - a_1 - 2) - (a_i - 1)(|V(G)| - a_i - 1) \\ &= (a_1 - a_i + 1)(|V(G)| - a_1 - a_i - 1) > 0, \end{aligned}$$

and thus $W(G_1) > W(G)$. Repeating the above transformation from G to G_1, we may finally have the desired result. □

For $a \geq 1$, $b \geq 0$ and $r = 3, 4$, let $U_{n,r}(a, b)$ be the graph obtained from a graph H which is $C_3(-, -, P_{b+1})$ for $r = 3$ and $C_4(-, -, P_{b+1}, -)$ for $r = 4$ by attaching $n - a - b - r$ pendant vertices and a path P_a to v_1 of H. In either case, v_3 is an end vertex of P_{b+1}. Let $k = n - a - b - r$. Recall that [7]

$$\begin{aligned} & W\left(U_{n,r}(a, b)\right) \\ = \ & \left(a + b + \frac{r}{2}\right)\left\lfloor\frac{r^2}{4}\right\rfloor + \binom{a+1}{3} + \binom{b+1}{3} \\ & + r\left(\binom{a+1}{2} + \binom{b+1}{2}\right) + \frac{1}{2}ab\left(2\left\lfloor\frac{r}{2}\right\rfloor + a + b + 2\right) \\ & + k\left(\left\lfloor\frac{r^2}{4}\right\rfloor + r + \frac{1}{2}a(a+3) + \frac{1}{2}b\left(2\left\lfloor\frac{r}{2}\right\rfloor + b + 3\right)\right) + k(k-1). \end{aligned} \quad (3)$$

Lemma 5. *For* $a \geq 1$, $b \geq 0$ *and* $r = 3, 4$, *let* $s = a + b \geq 2$ *and* $k = n - s - r$.

(*i*) *If* $r = 3$, *or* $r = 4$ *and* $k = 0$, *then* $W(U_{n,r}(a, b)) \leq W(U_{n,r}(s, 0))$ *with equality if and only if* $U_{n,r}(a, b) = U_{n,r}(s, 0)$;

(*ii*) *If* $r = 4$, $k = 1$, *then* $W(U_{n,r}(a, b)) \leq W(U_{n,r}(s, 0)) = W(U_{n,r}(1, s-1))$ *with equality if and only if* $U_{n,r}(a, b) = U_{n,r}(s, 0)$ *or* $U_{n,r}(1, s-1)$;

(*iii*) *If* $r = 4$ *and* $k \geq 2$, *then* $W(U_{n,r}(a, b)) \leq W(U_{n,r}(1, s-1))$ *with equality if and only if* $U_{n,r}(a, b) = U_{n,r}(1, s-1)$.

Proof. Let u_1 and u_2 be respectively the pendant vertices of $U_{n,r}(a, b)$ in the pendant paths at v_1 and v_3 if $b \geq 1$, and u be a pendant neighbor of v_1 if $k \geq 1$. Let $G_1 = U_{n,r}(a, b)$. Let w be the neighbor of u_1 in G_1. For $a \geq 2$, let $G_2 = G_1 - u_1w + u_1u_2$, $G_3 = G_1 - u_1w + u_1v_1$ and $G_4 = G_1 - u_1w + u_1v_3$. Obviously, $G_2 = U_{n,r}(a-1, b+1)$. Then

$$\begin{aligned} & W(U_{n,r}(a-1,b+1)) - W(U_{n,r}(a,b)) \\ = & (D_{G_2}(u_1) - D_{G_4}(u_1)) + (D_{G_4}(u_1) - D_{G_3}(u_1)) \\ & +(D_{G_3}(u_1) - D_{G_1}(u_1)) \\ = & b(a+k+r-2) + \left\lfloor \frac{r}{2} \right\rfloor (k+a-1-b) - (a-1)(k+r-1+b) \\ = & (1-a+b)\left(k + \left\lfloor \frac{r-1}{2} \right\rfloor\right) + k\left\lfloor \frac{r}{2} \right\rfloor. \end{aligned}$$

If $r = 3$, then $W(U_{n,3}(a-1, b+1)) \geq W(U_{n,3}(a,b))$ if and only if $a - b \leq \frac{2k+1}{k+1}$, implying that $W(U_{n,3}(a,b))$ is maximum only if $(a,b) = (1, s-1)$ or $(s, 0)$. Similarly, if $r = 4$, then $W(U_{n,4}(a,b))$ is maximum only if $(a,b) = (1, s-1)$ or $(s,0)$. Using Eq. (3), we have

$$W(U_{n,r}(1,s-1)) - W(U_{n,r}(s,0)) = \begin{cases} -(s-1) & \text{if } r = 3, \\ (s-1)(k-1) & \text{if } r = 4. \end{cases}$$

Then the result follows. □

3 Results

Let $U^{n,\Delta} = U_{n,3}(n-\Delta, 0)$ if $3 \leq \Delta \leq n-1$. Let $\mathbb{U}(n,\Delta)$ be the set of n-vertex unicyclic graphs with maximum degree Δ, where $2 \leq \Delta \leq n-1$. Obviously, $\mathbb{U}(n,2) = \{C_n\}$ and $\mathbb{U}(n,n-1) = \{U^{n,n-1}\}$. Recall that $W(C_n) = \frac{n}{2}\left\lfloor \frac{n^2}{4} \right\rfloor$.

Theorem 1. *Let $G \in \mathbb{U}(n,\Delta)$ with $3 \leq \Delta \leq n-1$. Then*

$$W(G) \leq \frac{1}{6}n^3 - \frac{7}{6}n + \frac{1}{3}\Delta^3 - \frac{1}{2}(n+1)\Delta^2 + \frac{1}{6}(9n-5)\Delta$$

with equality if and only if $G = U^{n,\Delta}$.

Proof. The case $\Delta = n-1$ is trivial.

Suppose that $\Delta \leq n-2$. Let G be a graph with maximum Wiener index in $\mathbb{U}(n,\Delta)$. Let C be the unique cycle in G with length r. Obviously, $3 \leq r \leq n-1$.

Let $U'_{n,\Delta} = U_{n,4}(1, n-\Delta-2)$ for $3 \leq \Delta \leq n-2$, and let $U''_{n,\Delta}$ be the unicyclic graph obtained by joining a triangle and the center of the star on Δ vertices by a path of length $n-\Delta-2$ if $3 \leq \Delta \leq n-3$. Using Eq. (3), we have

$$W(U^{n,\Delta}) = \frac{1}{6}n^3 - \frac{7}{6}n + \frac{1}{3}\Delta^3 - \frac{1}{2}(n+1)\Delta^2 + \frac{1}{6}(9n-5)\Delta,$$

$$\begin{aligned} W(U'_{n,\Delta}) &= \frac{1}{6}n^3 - \frac{19}{6}n + \frac{1}{3}\Delta^3 - \frac{1}{2}(n+1)\Delta^2 + \frac{1}{6}(9n+7)\Delta + 3, \\ W(U''_{n,\Delta}) &= W(U^{n,\Delta+1}) + (\Delta - 2)(n - \Delta - 2). \end{aligned}$$

Case 1. There is a vertex, say v_1 on C of degree Δ.

By Lemma 1, the degrees of vertices outside C are one or two, and the degrees of vertices on C different from v_1 are two or three. By Lemma 2, there is at most one vertex on C different from v_1 of degree three. Thus G is a graph obtainable from the cycle C by attaching $\Delta - 2$ paths to v_1 and at most one path to a vertex on C different from v_1. By Lemmas 3 and 4, We have $G = U_{n,r}(a,b)$ with $\Delta = n - a - b - r + 3$, where $r = 3, 4$. If $r = 3$, then by Lemma 5 (i), we have $G = U_{n,3}(n-\Delta, 0) = U^{n,\Delta}$. If $r = 4$, then by Lemma 5 (i)–(iii), we have $G = U_{n,4}(n - \Delta - 1, 0)$ for $\Delta = 3$, and $G = U_{n,4}(n - \Delta - 1, 0)$ or $U'_{n,\Delta}$ for $\Delta = 4$ (and $n \geq 6$), and $G = U'_{n,\Delta}$ for $\Delta \geq 5$. Note that

$$\begin{aligned} W(U^{n,\Delta}) - W(U_{n,4}(n-\Delta-1,0)) &= n - 4 > 0 \text{ if } \Delta = 3, \\ W(U^{n,\Delta}) - W(U_{n,4}(n-\Delta-1,0)) &= W(U^{n,\Delta}) - W(U'_{n,\Delta}) \\ &= 2n - 11 > 0 \text{ if } \Delta = 4, \\ W(U^{n,\Delta}) - W(U'_{n,\Delta}) &= 2(n-\Delta) - 3 > 0 \text{ if } \Delta \geq 5. \end{aligned}$$

Thus $G = U^{n,\Delta}$ with $\Delta \geq 3$.

Case 2. There is no vertex on C of degree Δ.

There is some vertex v outside C of degree Δ and $4 \leq \Delta \leq n - 3$. Suppose without loss of generality that v_1 is the vertex on C that is nearest to v. By Lemma 1, the degrees of vertices outside C different from v are one or two, and the degrees of vertices on C are two or three. By Lemma 2, there is at most one vertex on C different from v_1 of degree three. By Lemma 4, there is at most one pendant path at v in G with length at least two. Let $\widetilde{G}$ be the graph obtained from G by deleting the vertices of the branch at v_1 except v_1.

Suppose that $\widetilde{G} \neq C_3$. By Lemma 3, we have $G = G(k-3, 3)$ or $G(k-4, 4)$, where $k = |V(\widetilde{G})|$. Thus $\widetilde{G} = C_3(-, P_{k-2}, -)$ or $C_4(-,-,P_{k-3},-)$, where $4 \leq k \leq n - \Delta$. Let H be the graph obtained from $C_3(-, P_{k-2}, -)$ by adding the branch at v_1 such that $\widetilde{G} = C_3(-, P_{k-2}, -)$, i.e., $G = H$ if $\widetilde{G} = C_3(-, P_{k-2}, -)$. Let u the pendant vertex of $C_3(-, P_{k-2}, -)$ of H. Let w be the neighbor of v_1 outside the triangle in H. Let $G_1 = H - v_1w + uw$. Obviously, $G_1 \in \mathbb{U}(n, \Delta)$. If $\widetilde{G} = C_3(-, P_{k-2}, -)$, then by setting $G_2 = H - v_1w + v_2w$, we have

$$\begin{aligned} W(G_1) - W(G) &= (W(G_1) - W(G_2)) + (W(G_2) - W(G)) \\ &= 2(k-3)(n-k) - (k-3)(n-k) \end{aligned}$$

$$= \quad (k-3)(n-k) > 0,$$

and if $\widetilde{G} = C_4(-,-,P_{k-3},-)$, then using Eqs. (1) and (2), and by similar calculation of $W(G(a+2,r-2)) - W(G(a,r))$ as in the proof of Lemma 3, we have $W(H) - W(G) = k-4$, and thus

$$\begin{aligned} W(G_1) - W(G) &= (W(G_1) - W(H)) + (W(H) - W(G)) \\ &= (k-3)(n-k) + (k-4) > 0. \end{aligned}$$

In either case, we have $W(G_1) > W(G)$, a contradiction. Thus $\widetilde{G} = C_3$.

Suppose that $G \neq U''_{n,\Delta}$. Let w be the pendant vertex of the longest pendant path at v, and w_1 the neighbor of w. Then $d_G(v,w) \geq 2$. Let $t = d_G(v,w_1) \geq 1$. Note that $n - \Delta - t \geq 3$. Let $x_1, x_2, \ldots, x_{\Delta-2}$ be the pendant neighbors of v. For $G_3 = G - vx_1 - \cdots - vx_{\Delta-2} + w_1x_1 + \cdots + w_1x_{\Delta-2} \in \mathbb{U}(n,\Delta)$, we have

$$\begin{aligned} W(G_3) - W(G) &= t(n-\Delta-t)(\Delta-2) - t(\Delta-2) \\ &= t(\Delta-2)(n-\Delta-t-1), \end{aligned}$$

and thus $W(G_3) > W(G)$, a contradiction. It follows that $G = U''_{n,\Delta}$.

Combining Cases 1 and 2, we have $G = U^{n,\Delta}$ or $U''_{n,\Delta}$ for $4 \leq \Delta \leq n-3$, and $G = U^{n,\Delta}$ for $\Delta = 3, n-2$. But $W(U^{n,\Delta}) > W(U''_{n,\Delta})$ for $4 \leq \Delta \leq n-3$ because $W(U^{n,\Delta}) - W(U''_{n,\Delta}) = n-3 > 0$. Then $G = U^{n,\Delta}$. □

Let $f(\Delta) = \frac{1}{6}n^3 - \frac{7}{6}n + \frac{1}{3}\Delta^3 - \frac{1}{2}(n+1)\Delta^2 + \frac{1}{6}(9n-5)\Delta$, where $3 \leq \Delta \leq n-1$. Obviously, the roots Δ_1 and Δ_2 of $f'(\Delta) = 0$ with $\Delta_1 < \Delta_2$ satisfy $\Delta_1 < 3$ and $\Delta_2 > n-1$. Then $f(\Delta)$ is decreasing in Δ, and thus $f(\Delta) \leq f(3) = \frac{1}{6}n^3 - \frac{7}{6}n + 2$ with equality if and only if $\Delta = 3$. Note that $W(C_n) < W(U^{n,3})$. It follows from Theorem 1 that among n-vertex unicyclic graphs with $n \geq 5$, $U^{n,3}$ is the unique graph with the maximum Wiener index, equal to $\frac{1}{6}n^3 - \frac{7}{6}n + 2$, see also [5]. Recall that connected graphs with maximum degree at most four are known as molecular graphs representing hydrocarbons [15]. Obviously, $U^{n,3}$ is a molecular graph.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (No. 11071089).

References

[1] D. Bonchev, O. Mekenyan, J.V. Knop, N. Trinajstić, On characterization of monocyclic structures, Croat. Chem. Acta 52 (1979) 361–367.

[2] D. Bonchev, N. Trinajstić, Information theory, distance matrix, and molecular Branching, J. Chem. Phys. 67 (1977) 4517–4533.

[3] J. Devillers, A.T. Balaban (Eds.), Topological indices and related descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, 1999.

[4] A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.

[5] Z. Du, B. Zhou, Minimum Wiener indices of trees and unicyclic graphs of given matching number, MATCH Commun. Math. Comput. Chem. 63 (2010) 101–112.

[6] Z. Du, B. Zhou, Degree distance of unicyclic graphs, Filomat 24 (no. 4) (2010) 95–120.

[7] Z. Du, B. Zhou, On the reverse Wiener indices of unicyclic graphs, Acta Appl. Math. 106 (2009) 293-306.

[8] H. Hosoya, Topological index: A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Japan 44 (1971) 2332–2339.

[9] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: Development and applications, Croat. Chem. Acta 68 (1995) 105–129.

[10] J. Plesník, On the sum of all distances in a graph or digraph, J. Graph Theory 8 (1984) 1–21.

[11] P. Sparl, J. Žerovnik, Graphs with given number of cut-edges and minimal value of Wiener number, Int. J. Chem. Model. 3 (2010) 131–138.

[12] D. Stevanović, Maximizing Wiener index of graphs with fixed maximum degree, MATCH Commun. Math. Comput. Chem. 60 (2008) 71–83.

[13] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinhein, 2000.

[14] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinhein, 2009.

[15] N. Trinajstić, Chemical Graph Theory, 2nd edn., CRC Press, Boca Raton, 1992.

[16] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.