On the extremal Wiener polarity index of unicyclic graphs with a given diameter*

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In memory of Professor Ante Graovac

Abstract

The Wiener polarity index $W_p(G)$ of a graph $G = (V, E)$ is defined to be the number of the unordered pairs of vertices $\{u, v\}$ such that the distance between u and v is three, which was proposed by Harold Wiener in 1947. In this paper, we characterize the extremal graphs among all the unicyclic graphs with order n and diameter d.

1 Introduction

Let $G = (V, E)$ be a connected simple graph. The distance in G of two different vertices u, v is the length of a shortest u-v path in G, denoted by $d_G(u, v)$ or $d(u, v)$; if no such path exists, we set $d(u, v) = \infty$. The greatest distance between any two vertices in G is the diameter of G, denoted by $diam(G)$. Let $N_G(v)$ be the neighborhood of v, and $d_G(v) = |N_G(v)|$ denote the degree of vertex v. For $i \in \{1, 2, \ldots, \text{diam}(G)\}$, we call

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$N_G^i(v) = \{u \in V(G) | d(u,v) = i\}$ the ith neighborhood of v. A vertex of degree one is called a pendant vertex. The length of a cycle C is the number of edges contained in C. The girth of G, denoted by $g(G)$, is the minimum length of the cycles in G. A unicyclic graph of order n is a connected graph with n vertices and n edges. In other words, every unicyclic graph has exactly one cycle. For all other notations and terminology, not given here, see e.g. [1].

The Wiener polarity index of G, denoted by $W_p(G)$, is defined by

$$W_p(G) = |\{\{u,v\} | d(u,v) = 3, u, v \in V(G)\}|,$$

which is the number of unordered pairs of vertices $\{u,v\}$ such that $d(u,v) = 3$. The name "Wiener polarity index" was introduced by Harold Wiener [21] in 1947. Wiener himself conceived the index only for acyclic molecules and defined it in a slightly different – yet equivalent – manner. In the same paper, Wiener also introduced another index for acyclic molecules, called *Wiener index* or *Wiener distance index* and defined by $W(G) := \sum_{\{u,v\} \subseteq V} d_G(u,v)$. Wiener [21] used a liner formula of W and W_P to calculate the boiling points t_B of the paraffins, *i.e.*, $t_B = aW + bW_p + c$, where a, b and c are constants for a given isomeric group. The Wiener index $W(G)$ is now very popular in chemical and mathematical literature, such as the contributions of Ante Graovac [2, 10, 13, 14, 19, 20]. For more results on Wiener index, we refer to the survey paper [8] written by Dobrynin, Entringer and Gutman.

Recently, the extremal Wiener polarity index of trees, unicyclic graphs and bicyclic graphs were studied, respectively, such as [4, 12, 15]; and the extremal Wiener polarity index of trees with given different parameters (e.g. order, diameter, maximum degree, the number of pendants, etc.) were studied (see [5, 6, 7, 16]). More results can refer to [3, 8, 9, 11, 17, 18].

In this paper, we will characterize the extremal graphs with respect to the Wiener polarity index among all unicyclic graphs with order n and diameter d.

2 The minimum Wiener polarity index of unicyclic graphs with order n and diameter d

In this section, we will characterize the minimum unicyclic graphs with respect to the Wiener polarity index among all unicyclic graphs with order n and diameter d. Since $W_p(G) = 0$ for any graph G with diameter $d \le 2$, we can assume that $d \ge 3$ in the following.

Firstly, we give a result about the Wiener polarity index of unicyclic graphs, which was established in [12].

Lemma 2.1. *[12] Let $U = (V, E)$ be a unicyclic graph and C denote the unique cycle of U. If $g(U) = 3$, with $V(C) = \{v_1, v_2, v_3\}$, then*

$$W_p(U) = \sum_{uv\in E}(d_U(u) - 1)(d_U(v) - 1) + 9 - 2d_U(v_1) - 2d_U(v_2) - 2d_U(v_3).$$

If $g(U) = 4$, with $V(C) = \{v_1, v_2, v_3, v_4\}$, then

$$W_p(U) = \sum_{uv\in E}(d_U(u) - 1)(d_U(v) - 1) + 4 - d_U(v_1) - d_U(v_2) - d_U(v_3) - d_U(v_4).$$

Moreover, if $g(U) \ge 5$, then we have

$$W_p(U) = \begin{cases} \sum\limits_{uv\in E}(d_U(u) - 1)(d_U(v) - 1) - 5, & \text{if } g(U) = 5; \\ \sum\limits_{uv\in E}(d_U(u) - 1)(d_U(v) - 1) - 3, & \text{if } g(U) = 6; \\ \sum\limits_{uv\in E}(d_U(u) - 1)(d_U(v) - 1), & \text{if } g(U) \ge 7. \end{cases}$$

□

Let $\mathcal{U}(n, d)$ be the set of unicyclic graphs with order n and diameter d, and $\mathcal{P}(U, d)$ denote the set of paths of length d in $U \in \mathcal{U}(n, d)$. Each path $P \in \mathcal{P}(U, d)$ can be taken as a spindle of $U \in \mathcal{U}(n, d)$. Let C be the unique cycle and $P = v_0v_1 \cdots v_d$ be a spindle in U. If $E(P)\cap E(C) = \emptyset$, then there is a path P_c connecting P and C. If $E(P)\cap E(C) \ne \emptyset$, then P and C have at least two common vertices. A hanging tree on vertex v in U, denoted by $T_U[v]$, is a rooted tree whose root is v. Specially, if $v \in V(P) \cup V(C) \cup V(P_c)$, then $T_U[v]$ is a rooted tree which contains no vertex on P or P_c.

In the following, we will show some operations on unicyclic graphs which can reduce the Wiener polarity index.

We define **Operation** I (see Figure 1) as follows. We construct two graphs A and B from U, where $A = U \setminus (T_U[v] \setminus v)$, and $B = B(V(T_U[v] \setminus v), \emptyset)$. Then join every vertex in B to a vertex $v' \in A$, and we obtain a new graph, denoted by U'. We call this operation *transport* $T_U[v]$ to v'.

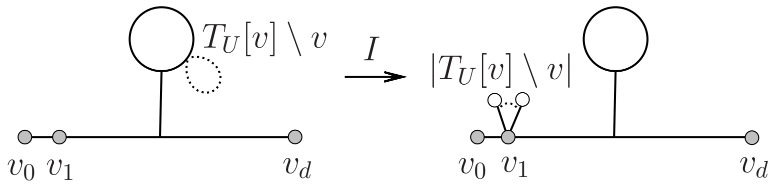

Figure 1: Operation I on U.

We define **Operation** II as follows. Let U be a unicyclic graph. If $d_U(v) = 2$, then let $U' = B - vv' - vv'' + v'v'' + vx$, where v', $v'' \in N_U(v)$, $x \in V(U)$. We call such an operation *smooth* v to x.

By considering whether there exists some $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$ or not, we will give different operations on unicyclic graphs as follows.

(1) If there exists some $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$, then we pick $P = v_0 v_1 \cdots v_d$ as the spindle. Let $C = w_1 w_2 \dots w_p$ be its unique cycle, and $P_c = v_c u_1 \dots u_t w_1$ be the path connecting path P and cycle C, where $v_c \in P \cap P_c$ $(1 \le c \le d-1)$ is the common vertex of P and P_c. Specially, if $|P_c| = 1$, then $w_1 = v_s$.

Let $U_3(s, t)$ $(s + t = n - d - 3)$ be a unicyclic graph, which is obtained from a path $P = v_0 v_1 \cdots v_d$ of length d by adding s pendant vertices to v_1, t pendant vertices to v_{d-1}, respectively, and identifying a vertex of a triangle with v_1 or v_{d-1} (see Figure 2).

In the following we will show the steps to obtain $U_3(s, t)$ from a unicyclic graph U.

Step 1. By transporting $T_U[v_2] \setminus v_2$ and $T_U[v_{d-2}] \setminus v_{d-2}$ to v_1 or v_{d-1} , we get a new graph, denoted by U_1. Observe that $d_{U_1}(v_2) = d_{U_1}(v_{d-2}) = 2$.

Step 2. Transport all $T_{U_1}[v_i] \setminus v_i$ $(i \in \{3, \dots, d-3\})$, $T_{U_1}[u_j]$ $(1 \le j \le t)$, $T_{U_1}[w_k] \setminus w_k$

Figure 2: The unicyclic graph $U_3(s,t)$.

$(1 \leq k \leq p)$ to v_1 or v_{d-1}. We obtain a new graph U_2. Observe that $d_{U_2}(v_c) = d_{U_2}(w_1) = 3$, $d_{U_2}(v_i) = d_{U_2}(u_j) = d_{U_2}(w_k) = 2$ $(i \in \{2,\dots,c-1,c+1,\dots,d-2\},\ 1 \leq j \leq t,\ 2 \leq k \leq p)$, $T_{U_2}[v_1]$ and $T_{U_2}[v_{d-1}]$ are stars. Note that $d_{U_2}(v_c) = d_{U_2}(w_1) = 4$ whenever $v_c = w_1$.

Step 3. By smoothing w_i $(3 \leq i \leq p-1)$ to v_1 or v_{d-1}, we obtain a new graph, denoted by U_3.

Step 4. Firstly, we construct two graphs $A = U_3[w_1, w_2, w_p]$ and $B = U_3 \backslash w_2 \backslash w_p$; secondly, identify $w_1 \in A$ with v_1 (or v_{d-1}) $\in B$ and transport $T_B[v_c]$ to v_1 (or v_{d-1}); finally, we reach the desired unicyclic graph $U_4 = U_3(s,t)$.

Lemma 2.2. *Let U be a unicyclic graph in $\mathcal{U}(n,d)$ $(d \geq 5)$ and $P = v_0v_1\cdots v_d$ be the spindle of U. Let U' denote the corresponding unicyclic graph obtained from U by the Step 1, Step 2 and Step 4 above. Then $W_p(U') \leq W_p(U)$.*

Proof. We show the proof by the following three cases corresponding to the operation in the three steps, respectively.

Firstly, we consider the change on Wiener polarity index brought by the operation in Step 1. For arbitrary vertex $x \in N_U(v_2) \cap V(T_U[v_2])$, there exist at least two vertices v_0, v_4 such that $d_U(v_0,x) = d_U(v_4,x) = 3$. But after transporting x to v_1, there is only one vertex v_3 such that $d_{U'}(v_3,x) = 3$, which implies that $W_p(U') + 1 \leq W_p(U)$. If we transport corresponding vertices to v_{d-1}, the case is similar to the above.

Secondly, we consider the change on Wiener polarity index brought by the operation in Step 2. It can be checked that for arbitrary vertex $u \in T_U[v] \setminus v$, there exists at least one vertex y such that $d_U(y,u) = 3$. But after transporting u to v_1 (or v_{d-1}) there exists only one vertex v_3 (or v_{d-3}) such that $d_{U'}(v_3,u) = 3$ (or $d_{U'}(v_{d-3},u) = 3$), since

$d(v_2) = d(v_{d-2}) = 2$. Thus $W_p(U) \geq W_p(U')$, as stated.

Finally, for the case in step 4, similar to the proof above, $W_p(U) \geq W_p(U')$ follows directly. $\square$

Lemma 2.3. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ $(d \geq 5)$, C be its unique cycle and U' denote the unicyclic graph obtained by smoothing $w \in V(C)$ to v_1 or v_{d-1} in the Step 3. Then $W_p(U') \leq W_p(U)$.*

Proof. By a similar discussion as Lemma 2.2, the conclusion follows. $\square$

Now we can give the following theorem:

Theorem 2.1. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ $(d \geq 5)$ and there exists some $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$ to be the spindle of U. Let U^* be the unicyclic graph obtained from U by the above four steps. Then $W_p(U^*) \leq W_p(U)$, with the equality holds if and only if $U^* \cong U_3(s, t)$ $(s + t = n - d - 3)$.*

Proof. Let $C = w_1 w_2 \ldots w_p w_1$ be the cycle of U, and $P_c = v_c u_1 \ldots u_t w_1$ be the path connecting path P and cycle C. By Lemmas 2.2 and 2.3, we have $W_p(U^*) \leq W_p(U)$. It suffices to show that the equality holds if and only if $U^* \cong U_3(s, t)$ $(s + t = n - d - 3)$. To prove the conclusion we first give the following claims.

Claim 1. $d_{U^*}(v_2) = 2$ and $d_{U^*}(v_{d-2}) = 2$.

Suppose that $d_{U^*}(v_2) \neq 2$, then for arbitrary vertex $v \in N_{U^*}(v_2) \cap V(T_{U^*}[v_2])$, there are at least two vertices v_0, v_4 such that $d(v_0, v) = d(v_4, v) = 3$. But after transporting v to v_1, there is exactly one vertex $v_3 \in V(P)$ such that $d(v_3, v) = 3$. Thus, $d_{U^*}(v_2) = 2$. Similarly, we have $d_{U^*}(v_{d-2}) = 2$.

Claim 2. $V(T_{U^*}[v] \backslash v) = \emptyset$, where $v \in \{v_2, \ldots, v_{d-2}, u_1, \ldots, u_t, w_1, \ldots, w_p\}$.

Suppose that there is some vertex $x \in V(T_{U^*}[v] \backslash v)$ adjacent to v, then there are at least two vertices v', $v'' \in V(P) \cup V(P_c) \cup V(C)$ such that $d(v', v) = d(v'', v) = 3$. But after transporting v to v_1 or v_{d-1}, there is exactly one vertex v_3 (or v_{d-3}) $\in V(P)$ such that $d(v_3, x) = 3$ (or $d(v_{d-3}, x) = 3$), since $d_{U^*}(v_2) = d_{U^*}(v_{d-2}) = 2$. Thus, all the pendant vertices of U^* are adjacent to v_1 or v_{d-1}.

Claim 3. $|P_c| = 0$.

Suppose that $|P_c| \geq 1$, then for vertex u_1, there are at least two vertices v_{c-2}, v_{c+2} $(c-2, c+2 \in \{0, 1, \ldots, d\})$ such that $d(v_{c-2}, u_1) = d(v_{c+2}, u_1) = 3$. But after after applying the operation in **Step 4**, there is exactly one vertex v_3 (or v_{d-3}) $\in V(P)$ such that $d(v_3, u_1) = 3$ (or $d(v_{d-3}, u_1) = 3$), since $d_{U^*}(v_2) = d_{U^*}(v_{d-2}) = 2$. Thus, $|P_c| = 0$.

Claim 4. $|C| = 3$.

Suppose that $|C| \geq 4$, then for vertex w_2, there are at least two vertices v_{c-1}, w_5 (or v_{c+1}) $(c-1, c+1 \in \{0, 1, \ldots, d\})$ such that $d(v_{c-1}, w_2) = d(w_5, w_2) = 3$ (or $d(v_{c-1}, w_2) = d(v_{c+1}, w_2) = 2$), since $|P_c| = 0$. But after smoothing w_2 to v_1 or v_{d-1}, there is exactly one vertex v_3 (or v_{d-3}) $\in V(P)$ such that $d(v_3, w_2) = 3$ (or $d(v_{d-3}, w_2) = 3$). Thus, $|C| = 3$.

Claim 5. $v_c = v_1$ or v_{d-1}.

Suppose that $v_c \neq v_1$ or v_{d-1}, then for vertex w_1, there are at least two vertices v_{c-2}, v_{c+2} $(c-2, c+2 \in \{0, 1, \ldots, d\})$ such that $d(v_{c-2}, w_1) = d(v_{c+2}, w_1) = 3$, since $|P_c| = 0$ and $|C| = 3$. But after identifying w_1 with v_1 (or v_{d-1}), there is exactly one vertex v_3 (or v_{d-3}) $\in V(P)$ such that $d(v_3, w_1) = 3$ (or $d(v_{d-3}, w_1) = 3$). Thus, $v_c = v_1$ or v_{d-1}.

Combining all the claims above, we complete the proof. □

(2) There is no path $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$. We pick $P = v_0 v_1 \cdots v_d$ as the spindle and let $C = v_f v_{f+1} \cdots v_g w_q \cdots w_1 v_f$ $(1 \leq f < g \leq d)$ be the unique cycle of U.

We define **Operation** III (see Figure 3) as follows. Let U be a unicyclic graph with $E(P) \cap E(C) \neq \emptyset$. Let $P = v_0 v_1 \cdots v_d$ be the spindle and $C = v_f v_{f+1} \cdots v_g w_q \cdots w_1 v_f$ $(1 \leq f < g \leq d)$ be the unique cycle of U. If $d_U(w_1) = 2$, then let $U' = U - v_f w_1 - w_1 w_2 + v_{f+1} w_2 + w_1 v_1$, where $v_1 \in V(P)$. We call such an operation *shrink* w_1 to v_1.

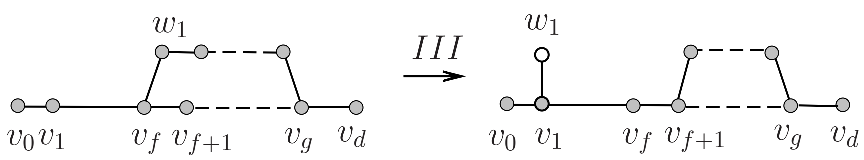

Figure 3: Operation III on U.

Let $U_4(n-d-2, 0)$ be a unicyclic graph, which is obtained from a path $P = v_0 v_1 \cdots v_d$

of length d by adding $n-d-2$ pendant vertices to v_1, and identifying three vertices of a quadrangle to v_{d-2}, v_{d-1}, and v_d respectively; $U_5(n-d-3,0)$ be a unicyclic graph, which is obtained from a path $P=v_0v_1\cdots v_d$ of length d by adding $n-d-3$ pendant vertices to v_1, and identifying three vertices of a pentagons to v_{d-2}, v_{d-1}, and v_d, respectively (see Figure 4).

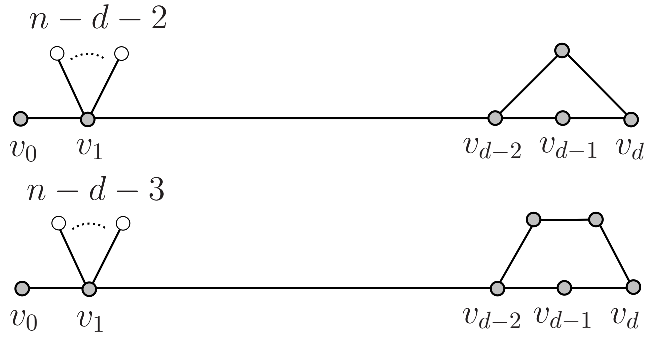

Figure 4: $U_4(n-d-2,0)$ and $U_5(n-d-3,0)$.

We say that a pair of vertices (v_i, v_{i+1}) $(0 \le i \le d-1)$ is on cycle C, if there is at least one vertex of v_i and v_{i+1} on cycle C. By considering whether (v_1, v_2) and (v_{d-2}, v_{d-1}) are on cycle C or not, there are two cases.

Case 1. There is at most one pair of (v_1, v_2) and (v_d, v_{d-1}) on the cycle C.

We get the desired graph by the following four steps.

Step 1. Without loss of generality, assume that (v_1, v_2) is not on cycle C. Then we transport $T_U[v_2]$ to v_1, and denote the new graph by U_1. Observe that $d_{U_1}(v_2)=2$.

Step 2. Transport all $T_{U_1}[v_i]$ $(i \in \{3,\ldots,d-1\})$ and $T_{U_1}[w_j]$ $(j \in \{1,\ldots,q\})$ to v_1, and we get a unicyclic graph U_2, where the vertices on U_2 other than v_1 have no hanging trees.

Step 3. Firstly, smooth w_1, w_2, $\ldots$, w_t to v_1 such that $0 \le (q-t)-(g-f-1) \le 1$. Secondly, shrink $w_{t+1}, w_{t+2}, \ldots, w_{q-1}$ to v_1, respectively. If $(q-t)-(g-f-1)=0$, then we get a new graph U_3 with a unique cycle $C=w_sv_{g-2}v_{g-1}v_gw_q$. If $(q-t)-(g-f-1)=1$, then we get a new graph U_3' with a unique cycle $C'=w_qv_{g-1}v_gw_q$.

Step 4. If $(q-t)-(g-f-1)=0$, then $U_4=U_3-w_qv_{g-2}-w_qv_g+w_qv_{d-2}+w_qv_d$; if $(q-t)-(g-f+1)=1$, then $U_4'=U_3'-w_qv_{g-1}-w_qv_g+w_qv_{d-1}+w_qv_d$.

Observe that $U_4 = U_4(n-d-2, 0)$ and $U_4' = U_3(s, 0)$ $(s = n-d-3)$.

Remark 1. For the situation that $v_g = v_d$ is on the cycle of U and $(q-t)-(g-f-1) = 1$, if we shrink vertices $w_{t+1}, w_{t+2}, \ldots, w_{q-2}$ to v_1, then we get a new graph U_3' with a unique cycle $C' = w_{q-1}v_{g-2}v_{g-1}v_g w_q w_{q-1}$; if we shrink vertices $w_{t+1}, w_{t+2}, \ldots, w_{q-1}$ to v_1, then we get a new graph U_3' with a unique cycle $C' = w_q v_{g-1} v_g w_q$. Thus, $U_4' = U_5(n-d-3, 0)$ or $U_3(s, 0)$ $(s = n-d-3)$.

Remark 2. It is easy to check that $W_p(U_3(n-d-3, 0)) = W_p(U_3(s, t))$ $(s+t = n-d-3)$.

Case 2. Both (v_1, v_2) and (v_{d-2}, v_{d-1}) are on the cycle C. By considering whether v_1 or v_d is on cycle C or not, we have the following two subcases.

Subcase 1. v_1 or v_{d-1} is not on cycle C. Without loss of generality, assume that v_1 is not on cycle C (i.e., $C = v_2v_3 \ldots v_g w_q \ldots w_1 v_2$).

Firstly, by transporting all $T_U[v_2]$, $T_U[v_3]$, $T_U[w_1]$, $T_U[w_2]$ to v_1, shrinking w_1 to v_1, we obtain a graph U_1 with a cycle $C_1 = v_3 \ldots v_g w_q \ldots w_2 v_3$. Observe that $d_{U_1}(v_2) = 2$. Then we can return to the situation in Case 1.

Subcase 2. v_1 and v_{d-1} are both on cycle C.

If v_0 or v_d is not on cycle C, without loss of generality, assume that v_0 is not on cycle C, then by transporting all $T_U[v_2]$, $T_U[v_3]$, $T_U[w_1]$, $T_U[w_2]$, $T_U[w_3]$ to v_1, shrinking w_1 and w_2 to v_1, we obtain a graph U_1 with a cycle $C_1 = v_3 \ldots v_g w_q \ldots w_3 v_3$. Observe that $d_{U_1}(v_2) = 2$; If v_0 and v_d are both on cycle C (it is obvious that $U = C = v_0 \ldots v_d w_q \ldots w_1 v_0$ and $0 \leq q-(d-1) \leq 1$), then by shrinking w_1, w_2 and w_3 to v_1, we obtain a graph U_1' with a cycle $C_1' = v_3 \ldots v_d w_q \ldots w_4 v_3$. Observe that $d_{U_1'}(v_2) = 2$. Now we can return to the situation in Case 1.

Lemma 2.4. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ $(d \geq 5)$, $P = v_0 v_1 \cdots v_d$ be its spindle, and $C = v_f v_{f+1} \cdots v_g w_q \cdots w_1 v_f$ $(1 \leq f < g \leq d)$ denote its unique cycle. If $d_U(v_2) = 2$ and $d_U(w_1) = 2$, then $W_p(U') \leq W_p(U)$, where U' is the unicyclic graph obtained from U by shrinking w_1 to v_1.*

Proof. We just consider the change on the Wiener polarity index brought by Operation III: shrink $w_1 \in V(C)$ to v_1.

It is easy to check that there is at least one vertex $v \in V(P)$ such that $d_U(v, w_1) = 3$.

But after shrinking $w_1 \in V(C)$ to v_1 there exists only one vertex $v_3 \in V(U')$ such that $d_{U'}(v_3, w_1) = 3$. Thus, $W_p(U') \le W_p(U)$ follows. $\square$

Combining Lemmas 2.2, 2.3 and 2.4, we can easily get the following theorem:

Theorem 2.2. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ $(d \ge 5)$, and there exists no path $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$. Then $W_p(U^*) \le W_p(U)$, where $U^* \in \{U_3(s, t)\ (s+t = n-d-3), U_4(n-d-2, 0), U_5(n-d-3, 0)\}$.*

Proof. Let $P = v_0v_1 \cdots v_d$ be the spindle and let $C = v_f v_{f+1} \cdots v_g w_q \cdots w_1 v_f$ $(1 \le f < g \le d)$ be the unique cycle of U. By Lemmas 2.2, 2.3 and 2.4, we have $W_p(U^*) \le W_p(U)$. It suffices to show that equality holds if and only if $U^* \in \{U_3(s, t)\ (s + t = n - d - 3), U_4(n - d - 2, 0), U_5(n - d - 3, 0)\}$.

Suppose that $d_{U^*}(v_2) \ne 2$, then for arbitrary vertex $v \in N_{U^*}(v_2) \cap V(T_{U^*}[v_2])$, there are at least two vertices v_0, v_4 such that $d(v_0, v) = d(v_4, v) = 3$. But after transporting v to v_1, there is exactly one vertex $v_3 \in V(P)$ such that $d(v_3, v) = 3$. Thus, $d_{U^*}(v_2) = 2$.

Suppose that there is some vertex $x \in V(T_{U'}[v] \backslash v)$ adjacent to v, where $v \in \{v_2, \ldots, v_{d-1}, w_1, \ldots, w_q\}$, then there are at least two vertices v', $v'' \in V(P) \cup V(C)$ such that $d(v', v) = d(v'', v) = 3$. But after transporting v to v_1, there is exactly one vertex $v_3 \in V(P)$ such that $d(v_3, x) = 3$, since $d_{U^*}(v_2) = 2$. Thus, all the pendant vertices of U^* are adjacent to v_1.

Suppose that $|C| \ge 6$, then for vertex w_1, there are at least two vertices v_{f-2} (or w_4) and v_{f+2} such that $d(v_{f-2}, w_1) = d(v_{f+2}, w_1) = 3$ (or $d(w_4, w_1) = d(v_{f+2}, w_1) = 3$). But after smoothing or shrinking w_1 to v_1, there is exactly one vertex $v_3 \in V(P)$ such that $d(v_3, w_1) = 3$. Thus, $|C| \le 5$.

For the case that $|C| = 3$, suppose that $v_f \ne v_{d-1}$, then for vertex w_1, there are at least two vertices v_{f-2}, v_{f+2} $(f-2, f+2 \in \{0, 1, \ldots, d\})$ such that $d(v_{f-2}, w_1) = d(v_{f+2}, w_1) = 3$. But after identifying v_f with v_{d-1}, v_g with v_d, there is exactly one vertex $v_{d-3} \in V(P)$ such that $d(v_{d-3}, w_1) = 3$. Thus, $v_f = v_{d-1}$ and $v_g = v_d$. Therefore, $U^* \cong U_3(s, t)$ $(s + t = n - d - 3)$ as stated.

For the case that $|C| = 4$, suppose that $v_f \ne v_{d-2}$, then for vertex w_1, there are at least two vertices v_{f-2}, v_{f+2} $(f-2, f+2 \in \{0, 1, \ldots, d\})$ such that $d(v_{f-2}, w_1) = d(v_{f+2}, w_1) = 3$.

But after identifying v_f and v_{d-2}, v_g and v_d, there is exactly one vertex $v_{d-4} \in V(P)$ such that $d(v_{d-4}, w_1) = 3$. Thus, $v_f = v_{d-2}$ and $v_g = v_d$. Therefore, $U^* \cong U_4(n-d-2, 0)$ as stated.

Similar to the case $|C| = 4$, if $|C| = 5$, then $U^* \cong U_5(n-d-5, 0)$ follows.

Combining all the situations above, the proof is complete. $\square$

For any $U^* \in \{U_3(s,t), U_4(s+t, 0), U_5(s+t-1, 0)\}$, we can easily get the following by some calculations:

$$W_p(U^*) = n - 3.$$

Finally, by Theorems 2.1, 2.2 and some calculations, the minimum Wiener polarity index of unicyclic graphs with order n and diameter d is determined.

Theorem 2.3. *Let U be a unicyclic graph in $\mathcal{U}(n,d)$ $(d \geq 3)$, and U^* denote the unicyclic graph with minimum Wiener polarity index.*

(1) If $d = 3$, then $U^* \cong U_3(0,t)$ $(t = n-6)$, and $W_p(U^*) = n-3$;

(2) If $d = 4$, then $U^* \cong U_3(s,t)$ $(s+t = n-7)$, and $W_p(U^*) = n-3$;

(3) If $d \geq 5$, then $U^* \cong U_3(s,t)$ $(s+t = n-d-3)$, $U_4(n-d-2, 0)$, $U_5(n-d-3, 0)$, and $W_p(U^*) = n-3$. $\square$

3 The maximum Wiener polarity index of unicyclic graphs with order n and diameter d

In this section, we will determine the maximum Wiener polarity index among all unicyclic graphs with order n and diameter d, and characterize the extremal unicyclic graph. Note that the unicyclic graphs with maximum Wiener polarity index among all unicyclic graphs with order n and diameter $d = 3$ was characterized in [12], and that the extremal graph of unicyclic graphs with order n, diameter d $(n \leq d+7)$ can be characterized easily, we only consider the case that $d \geq 4$ and $n \geq d+8$ in the following paper.

Let P be the spindle of U and C be its unique cycle. In [12], a transformation is introduced on unicyclic graphs with $g(U) \geq 4$, named **Sigma**. In order to characterize the unicyclic graphs with diameter d and order n with respect to the maximum Wiener polarity index, we need to introduce a similar operation.

We define **Operation** IV (" sigma") (see Figure 5) as follows. Let U be a unicyclic graph with a unique cycle C, and $T_U[v]$ denote a hanging tree on vertex $v \in V(P) \cup V(C)$. Among all hanging trees, suppose $P_l = vt_1 \cdots t_l$ is one of the longest path from the root v to a leaf t_l of the hang tree $T_U[v]$. If $l \geq 2$, then after deleting the edge vt_1 from U, we obtain a unicyclic graph A and a tree B such that $v \in A$ and $t_1 \in B$. Let U' denote the unicyclic graph obtained from A and B by identifying t_1 and v' ($v' \in V(P) \cup V(C)$ is a neighbor of v), and adding a new pendant vertex x to v.

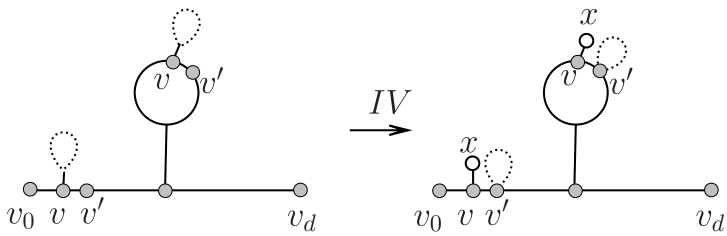

Figure 5: Operation IV on U.

Now we consider the maximum Wiener polarity index of unicyclic graphs with order n and diameter d ($d \geq 4$, $n \geq d+8$) by the following cases.

(1) If there exists some $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$, then we pick $P = v_0v_1 \cdots v_d$ as the spindle. Let $C = w_1w_2 \ldots w_p$ be its unique cycle, and $P_c = v_cu_1 \ldots u_tw_1$ be the path connecting path P and cycle C, where $v_c \in P \cap P_c$ ($1 \leq c \leq d-1$) is the common vertex of P and P_c. Specially, $w_1 = v_c$ whenever $|P_c| = 1$. We get the desired graph by the following steps.

Step 1. Firstly, apply Operation IV ("sigma") on vertices v_i ($2 \leq i \leq d-2$), w_k ($1 \leq k \leq p$) $\in V(U)$; secondly, if $w_1 = v_c$, then we do nothing; if $w_1 \neq v_c$, then by regarding the spindle as a pendant vertex adjacent to u_1, we can apply Operation IV on vertex $w_1 \in V(C)$. Finally we obtain graph U_1, where $P = v_0v_1 \cdots v_d$ remains to be the spindle, $P'_c = v_cw_1$ is a path connecting v_c and cycle C. Observe that $T_{U_1}[v_i]$ ($1 \leq i \leq d-1$) and $T_{U_1}[w_j]$ ($1 \leq j \leq p$) are stars.

Step 2. Let $V_i := T_{U_1}[v_i] \setminus v_i$ ($1 \leq i \leq d-1$), $W_j := T_{U_1}[w_j] \setminus w_j$ ($1 \leq j \leq p$). By considering whether $w_1 = v_c$ or not, we have the following two cases.

Case 1. $w_1 = v_c$.

Firstly, for V_i ($i \in \{1, \dots, c-1, c+1, \dots, d-1\}$), if $|i-c|$ is odd, then move V_i to w_2; if $|i-c|$ is even, then move V_i to w_1. Secondly, for W_j ($j \in \{3, \dots, p-1\}$), if j is odd, then move W_j to w_1 and smooth vertex w_j to w_2; if j is even, then move W_j to w_2 and smooth vertex w_j to w_1.

Case 2. $w_1 \neq v_c$.

Firstly, for V_i ($i \in \{1, \dots, d-1\}$), if $|i-c|$ is odd, then move V_i to w_1; if $|i-c|$ is even, then move V_i to w_2. Secondly, for W_j ($j \in \{3, \dots, p-1\}$), if j is odd, then move W_j to w_1 and smooth vertex w_j to w_2; if j is even, then move W_j to w_2 and smooth vertex w_j to w_1. Finally, identify w_1 with v_c, delete edge w_1v_c, and meanwhile add a pendant vertex to w_1.

At last, we get a new graph U_2, where the unique cycle of U_2 is a triangle. Observe that $T_{U_2}[w_i]$ ($i = 1,\ 2,\ p$) is a star and $V(T_{U_2}[v_k] \backslash v_k) = \emptyset$ ($k \in \{1, \dots, c-1, c+1, \dots, d-1\}$).

(2) There is no path $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$, where $C = v_f v_{f+1} \cdots v_g w_q \cdots w_1 v_f$ ($1 \leq f < g \leq d$) is the unique cycle of U. We pick $P = v_0 v_1 \cdots v_d$ as the spindle. We reach the desired graph by the following two steps.

Step 1. Apply Operation *IV* on v_i ($2 \leq i \leq d-2$) and w_j ($1 \leq j \leq q$). The new graph obtained is denoted by U_1, where $T_{U_1}[v_i]$ ($1 \leq i \leq d-1$) and $T_{U_1}[w_j]$ ($1 \leq j \leq q$) are stars.

Step 2. Let $V_i := T_{U_1}[v_i] \setminus v_i$ ($1 \leq i \leq d-1$), $W_j := T_{U_1}[w_j] \setminus w_j$ ($1 \leq j \leq q$).

Firstly, move W_l ($2 \leq l \leq q-1$) and V_k ($1 \leq k \leq f-1,\ f+2 \leq k \leq d-1$) to v_f and v_{f+1} alternately such that $T_{U_1}[a]$, $T_{U_1}[b]$ ($a,\ b \in \{v_1, \dots, v_{f-1}, v_{f+2}, \dots, v_{d-1}, w_2, \dots, w_s\}$) are moved to different vertices (i.e. v_f and v_{f+1}) whenever a is adjacent to b, move W_q to w_1. Secondly, shrink $w_2, \dots, w_q$ to v_{f+1} and v_f alternately. Thus, we get a new graph U_2 with a unique cycle $C' = w_1 v_f v_{f+1} w_1$. Observe that $T_{U_2}[v_f]$, $T_{U_2}[v_{f+1}]$ and $T_{U_2}[w_1]$ are stars.

Lemma 3.1. *Let U be a unicyclic graph with diameter $d \geq 4$ and $n \geq d+8$, C be its unique cycle. Let U^* be the unicyclic graph obtained by applying Operation IV on the corresponding vertices. Then $W_p(U) \leq W_p(U^*)$.*

Proof. Under the condition that $P = v_0v_1 \ldots v_d$ remains to be the spindle of the resultant unicyclic graph after the repeated operation, we get the conclusion directly by an analogous proof to that of Lemma 3.1. in [12]. $\square$

Lemma 3.2. *Let U be a unicyclic graph in $\mathcal{U}(n,d)$ ($d \geq 4,\ n \geq d+8$). By taking Step 2 in the two cases on the corresponding unicyclic graph we obtain a new graph U', satisfying $W_p(U) \leq W_p(U')$.*

Proof. During the procedure there are mainly three operations: "move", "smooth" and "shrink". We want to prove that each operation ensures that the value of the Wiener polarity index is not decreasing. Here we denote the final unicyclic graph by U'.

There are three kinds of unordered vertices pair $\{u,v\}$ such that $d_U(u,v) = 3$ on U: u and v are both pendant vertices; u and v are both on the cycle (or the spindle) of U; u is a pendant vertex and v is on the cycle (or the spindle) of U.

Since we move $V_i := T_{U_1}[v_i] \setminus v_i$ ($1 \leq i \leq d-1$), $W_j := T_{U_1}[w_j] \setminus w_j$ ($1 \leq j \leq p$ (or q)) to two adjacent vertices v_f and v_{f+1} alternately, we keep the unordered vertices pair $\{u,v\}$, where u and v are both pendant vertices. When we apply Operation II ("*smooth*"), in the same way, we smooth the vertices to two adjacent vertices v_f and v_{f+1} alternately which remains the unordered vertices pair $\{u,v\}$ of the second kind. At last, we only need to consider the unordered vertices pair $\{u,v\}$ of the third kind. Since there are at most three vertices w_1, w_2 and w_3 (or w_1, v_f and v_{f+1}) with pendant vertices, then if the unordered vertices pair $\{u,v\}$ in the original graph is composed by $u \in V_i$ ($i \in \{1,2,\ldots,d-1\}$) (or W_j ($j \in \{1,2,\ldots,p\ (q)\}$)) and $v \in V(C) \cup V(P)$, then after such an operation it will be replaced by u' (a vertex in the three hanging trees) and a vertex $v' \in N^2_{U'}(u')$.

Combining the three situations above, we complete the proof. $\square$

Let $U_3(a_1,a_2,a_3)$ ($a_1+a_2+a_3 = n-d-3$) be a unicyclic graph in $\mathcal{U}(n,d)$ ($d \geq 4$), which is obtained from a path $P = v_0v_1 \ldots v_d$ by identifying one vertex w_1 of a triangle $C = w_1w_2w_3$ with v_c ($2 \leq c \leq d-2$), and adding a_i ($i \in \{1,2,3\}$) pendant vertices to w_i. Let $U_3'(a_1',a_2',a_3')$ ($a_1'+a_2'+a_3' = n-d-2$) be a unicyclic graph in $\mathcal{U}(n,d)$ ($d \geq 4$), which is obtained from a path $P = v_0v_1 \ldots v_d$ by identifying two vertices w_2 and w_3 of a triangle $C = w_1w_2w_3$ with v_f and v_{f+1} (if $d \geq 5$, then $2 \leq f \leq d-3$; if $d = 4$, then

$f = 1$), and adding a'_i ($i \in \{1,2,3\}$) pendant vertices to w_i (see Figure 6). Denote the unicyclic graph $U_3(a_1, a_2, a_3)$ with $|a_i - a_j| \leq 1$ ($i, j \in \{1,2,3\}$) of order n and diameter d by U^*; the unicyclic graph $U'_3(a'_1, a'_2, a'_3)$ with $|a'_i - a'_j| \leq 1$ ($i, j \in \{1,2,3\}$) of order n and diameter d by U^{**}.

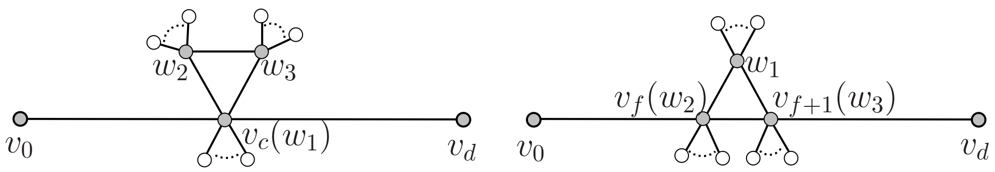

Figure 6: $U_3(a_1, a_2, a_3)$ and $U'_3(a'_1, a'_2, a'_3)$.

Theorem 3.1. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ ($d \geq 4$, $n \geq d+8$) and there exists some $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$ to be the spindle of U. Let U^* denote the unicyclic graph with maximum Wiener polarity index. Then $U^* \cong U_3^*$, and*

$$W_p(U^*) = \begin{cases} \frac{(n-d-3)(n-d+3)}{3} + d + 2, & if \ \ a_1 + a_2 + a_3 \equiv 0 \ (mod\ 3), \\ \frac{(n-d-4)(n-d+4)}{3} + d + 4, & if \ \ a_1 + a_2 + a_3 \equiv 1 \ (mod\ 3), \\ \frac{(n-d-5)(n-d+5)}{3} + d + 7, & if \ \ a_1 + a_2 + a_3 \equiv 2 \ (mod\ 3). \end{cases}$$

Proof. By Lemma 3.1 and Lemma 3.2, we know that the unicyclic graph with order n and diameter d ($d \geq 4$) attaining the maximum Wiener polarity index is $U_3(a_1, a_2, a_3)$ under the condition $E(P) \cap E(C) = \emptyset$. To complete the proof, it suffices to show that $U^* \cong U_3^*$.

By contradiction. Without loss of generality, assume that $a_1 - a_2 > 1$, then by moving a pendant edge of w_1 to w_2, we have a new graph denoted by U', and $W_p(U') - W_p(U) = (a_1 - 1 + 2 + a_3) - (a_2 + a_3 + 2) = a_1 - a_2 - 1 > 0$, a contradiction. Thus, $|a_i - a_j| \leq 1$ ($1 \leq i, j \leq 3$) is attained, which implies that $U^* \cong U_3^*$. We can calculate the value of $W_p(U^*)$ by Lemma 2.1.

Therefore, the proof is complete. □

Theorem 3.2. *Let U be a unicyclic graph in $\mathcal{U}(n, d)$ ($d \geq 4$, $n \geq d+8$), and there exists no path $P \in \mathcal{P}(U, d)$ such that $E(P) \cap E(C) = \emptyset$. Let U^* denote the unicyclic graph with maximum Wiener polarity index.*

(1) If $d = 4$*, then* $U^* \cong U_3'(a_1', a_2', a_3')$ *with* $|(a_1'+1) - a_i'| \le 1$ $(i \in \{2, 3\})$, $|a_2' - a_3'| \le 1$, *and*

$$W_p(U^*) = \begin{cases} \frac{(n-6)(n-1)}{3} + 3, & \textit{if } \ a_1' + a_2' + a_3' \equiv 0 \ (\textit{mod } 3), \\ \frac{n(n-7)}{3} + 5, & \textit{if } \ a_1' + a_2' + a_3' \equiv 1 \ (\textit{mod } 3), \\ \frac{(n-8)(n+1)}{3} + 8, & \textit{if } \ a_1' + a_2' + a_3' \equiv 2 \ (\textit{mod } 3); \end{cases}$$

(2) If $d \ge 5$*, then* $U^* \cong U_3^{**}$*, and*

$$W_p(U^*) = \begin{cases} \frac{(n-d-2)(n-d+4)}{3} + d, & \textit{if } \ a_1' + a_2' + a_3' \equiv 0 \ (\textit{mod } 3), \\ \frac{(n-d-3)(n-d+5)}{3} + d + 2, & \textit{if } \ a_1' + a_2' + a_3' \equiv 1 \ (\textit{mod } 3), \\ \frac{(n-d-4)(n-d+6)}{3} + d + 5, & \textit{if } \ a_1' + a_2' + a_3' \equiv 2 \ (\textit{mod } 3). \end{cases}$$

Proof. The proof is analogous to the proof of Theorem 3.1. □

Finally, by Theorems 3.1, 3.2 and some calculations, the maximum Wiener polarity index of unicyclic graphs with order n and diameter d $(d \ge 4,\ n \ge d+8)$ is determined.

Theorem 3.3. *Let* U *be a unicyclic graph in* $\mathcal{U}(n, d)$ $(d \ge 4,\ n \ge d+8)$*, and* U^* *denote the unicyclic graph with the maximum Wiener polarity index.*

(1) If $d = 4$*, then* $U^* \cong U_3'(a_1', a_2', a_3')$ *with* $|(a_1'+1) - a_i'| \le 1$ $(i \in \{2, 3\})$, $|a_2' - a_3'| \le 1$, *and*

$$W_p(U^*) = \begin{cases} \frac{(n-6)(n-1)}{3} + 3, & \textit{if } \ a_1' + a_2' + a_3' \equiv 0 \ (\textit{mod } 3), \\ \frac{n(n-7)}{3} + 5, & \textit{if } \ a_1' + a_2' + a_3' \equiv 1 \ (\textit{mod } 3), \\ \frac{(n-8)(n+1)}{3} + 8, & \textit{if } \ a_1' + a_2' + a_3' \equiv 2 \ (\textit{mod } 3); \end{cases}$$

(2) If $d \ge 5$*, then* $U^* \cong U_3^{**}$*, and*

$$W_p(U^*) = \begin{cases} \frac{(n-d-2)(n-d+4)}{3} + d, & \textit{if } \ a_1' + a_2' + a_3' \equiv 0 \ (\textit{mod } 3), \\ \frac{(n-d-3)(n-d+5)}{3} + d + 2, & \textit{if } \ a_1' + a_2' + a_3' \equiv 1 \ (\textit{mod } 3), \\ \frac{(n-d-4)(n-d+6)}{3} + d + 5, & \textit{if } \ a_1' + a_2' + a_3' \equiv 2 \ (\textit{mod } 3). \end{cases}$$

□

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