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On the Wiener Polarity Index*

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Abstract: The Wiener polarity index $W_P(G)$ of a graph G is the number of unordered pairs of vertices $\{u, v\}$ of G such that the distance of u and v is equal to 3. In this paper, we obtain the relation between Wiener polarity index and Zegreb indices, and the relation between Wiener polarity index and Wiener index (resp. hyper-Wiener index). Moreover, we determine the second smallest Wiener polarity index together with the corresponding graphs among all trees on n vertices, we also identify the smallest and the second smallest Wiener polarity indices together with the corresponding graphs, respectively, among all unicyclic graphs on n vertices.

1 Introduction

Let $G = (V, E)$ be a connected simple graph with $|V| = n$ and $|E| = m$. Sometimes we refer to G as an (n, m) graph. Let $N(u)$ be the first neighbor vertex set of u, then $d(u) = |N(u)|$ is called the degree of u. Specially, if $d(v) = 1$, then we call v a *pendant vertex* of G. $\Delta(G)$ is used to denote the *maximum degree* of vertices of G. As usual, let $K_{1,n-1}$, C_n and P_n be the star, cycle and path of order n, respectively.

The *distance* $d(u, v)$ between the vertices u and v of G is equal to the length of (number of edges in) the shortest path that connects u and v. Let $\gamma(G, k)$ denote the number of

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unordered vertex pairs of G, the distance of which is equal to k. The *Wiener polarity index*, denoted by $W_P(G)$, is equal to the number of unordered vertex pairs of distance 3, i.e., $W_P(G) = \gamma(G, 3)$.

There are two important graph-based structure-descriptors, called Wiener index and hyper-Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ is denoted by [1]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \sum_{k \geq 1} k\gamma(G,k), \tag{1}$$

and the *hyper-Wiener index* $WW(G)$ is defined as [2]

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\} \subseteq V(G)} d(u,v)^2 = \frac{1}{2}\sum_{k \geq 1} k(k+1)\gamma(G,k). \tag{2}$$

The name "Wiener polarity index" for the quantity defined in Eq. (1) is introduced by Harold Wiener [1] in 1947. In [1], Wiener used a linear formula of $W(G)$ and $W_P(G)$ to calculate the boiling points t_B of the paraffins, i.e.,

$$t_B = aW(G) + bW_P(G) + c,$$

where a, b, and c are constants for a given isomeric group.

As mentioned before, the Wiener index became popularity for a long time, numerous of its chemical applications and mathematical properties were reported [2-4]. Whereas the Wiener polarity index seems less well-known, the mathematical properties of Wiener polarity index and its applications in chemistry can be referred to [1,5-7] and the references cited therein.

In the present paper, we consider the Wiener polarity index for connected graphs. In Section 2, we discuss the relation between Wiener polarity index and Zagreb, Wiener, hyper-Wiener indices, respectively. In [7], the smallest and largest Wiener polarity indices together with the corresponding graphs among all trees on n vertices are obtained, respectively. In Section 3, we determine the second smallest Wiener polarity index together with the corresponding graphs among all trees on n vertices. Moreover, the smallest and the second smallest Wiener polarity indices together with the corresponding graphs among all unicyclic graphs on n vertices are identified, respectively, in Section 4.

2 The relation between Wiener polarity index and Zagreb, Wiener, hyper-Wiener indices

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as [8]:

$$M_1(G) = \sum_{v \in V} d(v)^2, \qquad M_2(G) = \sum_{uv \in E} d(u)d(v).$$

They are also two important topological indices and have been closely correlated with many chemical and mathematical properties [8-12].

The *girth* $g(G)$ of a connected graph G, is the length of a shortest cycle in G.

Theorem 2.1 *If G is a connected (n, m) graph, then*

$$W_P(G) \leq M_2(G) - M_1(G) + m, \tag{3}$$

where equality holds if and only if G is a tree or $g(G) \geq 7$.

Proof. Let $D_3(G) = \{\{u, v\} | d(u, v) = 3, u, v \in V(G)\}$, then $W_P(G) = |D_3(G)|$. Suppose $xy \in E(G)$, let $A(xy) = \{(u, v)|u \in N(x)\backslash\{y\}$ and $v \in N(y)\backslash\{x\}\}$, where (u, v) is an ordered vertex pair. Clearly, $|A(yx)| = |A(xy)| = (d(x) - 1)(d(y) - 1)$. If $\{u, v\} \in D_3(G)$, then there must exist some $xy \in E(G)$ such that $(u, v) \in A(xy)$. Since $\{u, v\} = \{v, u\}$, then

$$\begin{aligned} W_P(G) = |D_3(G)| &\leq \sum_{xy \in E} |A(xy)| \qquad (4) \\ &= \sum_{xy \in E} (d(x) - 1)(d(y) - 1) \\ &= \sum_{xy \in E} d(x)d(y) - \sum_{xy \in E} (d(x) + d(y)) + \sum_{xy \in E} 1 \\ &= \sum_{xy \in E} d(x)d(y) - \sum_{x \in V} d(x)^2 + m \\ &= M_2(G) - M_1(G) + m. \end{aligned}$$

This yields the inequality (3).

The equality holds in inequality (3) if and only if the equality holds in inequality (4). If G is a tree or $g(G) \geq 7$, it is easy to see that equality holds in inequality (4). If $g(G) = 6$, suppose $V(C_6) = \{v_1, v_2, v_3, v_4, v_5, v_6\}$ such that $\{v_1v_2, v_2v_3, v_3v_4, v_4v_5, v_5v_6, v_1v_6\} = E(C_6)$. Note that $(v_1, v_4) \in A(v_2v_3)$ and $(v_1, v_4) \in A(v_6v_5)$, then the inequality (4) is strict. By the same method, we can prove that inequality (4) is strict when $g(G) = 3$, 4, or 5.

By combining the above discussions, the result follows.

Suppose G is a connected (n,m) graph, by the proof of Theorem 2.1 it follows that

$$M_2(G) - M_1(G) + m = \sum_{xy \in E} (d(x) - 1)(d(y) - 1). \tag{5}$$

The *diameter* of G, denoted by $diam(G)$, is $diam(G) = max\{d(u,v) : u, v \in V(G)\}$.

Theorem 2.2 *If G is a triangle- and quadrangle-free connected (n,m) graph, then*

$$W_P(G) \geq 2n(n-1) - m - M_1(G) - W(G),$$

where equality holds if and only if $diam(G) \leq 4$.

Proof. Since G is a triangle- and quadrangle-free graph, then $\gamma(G,1) = m$, $\gamma(G,2) = \frac{1}{2}M_1(G) - m$ and $\sum_{k \geq 1} \gamma(G,k) = \binom{n}{2}$ (see [12]), by Eq. (1) it follows that

$$\begin{aligned} W(G) &= m + 2\left(\frac{1}{2}M_1(G) - m\right) + 3W_P(G) + \sum_{k \geq 4} k\gamma(G,k) \\ &\geq M_1(G) - m + 3W_P(G) + 4\left(\binom{n}{2} - \frac{1}{2}M_1(G) - W_P(G)\right) \\ &= 2n(n-1) - M_1(G) - m - W_P(G). \end{aligned}$$

Thus, we have the required inequality. Moreover, it is easy to see the equality holds if and only if $diam(G) \leq 4$.

The next result gives another lower bound for $W_P(G)$ in term of hyper-Wiener index.

Theorem 2.3 *If G is a triangle- and quadrangle-free connected (n,m) graph, then*

$$W_P(G) \geq \frac{5}{4}n(n-1) - \frac{1}{2}m - \frac{7}{8}M_1(G) - \frac{1}{4}WW(G),$$

where equality holds if and only if $diam(G) \leq 4$.

Proof. Since G is a triangle- and quadrangle-free graph, by Eq. (2) it follows that

$$\begin{aligned} WW(G) &= m + 3\left(\frac{1}{2}M_1(G) - m\right) + 6W_P(G) + \sum_{k \geq 4} \frac{1}{2}k(k+1)\gamma(G,k) \\ &\geq \frac{3}{2}M_1(G) - 2m + 6W_P(G) + 10\left(\binom{n}{2} - \frac{1}{2}M_1(G) - W_P(G)\right) \\ &= 5n(n-1) - \frac{7}{2}M_1(G) - 2m - 4W_P(G). \end{aligned}$$

Thus, we have the required inequality. Moreover, it is easy to see the equality holds if and only if $diam(G) \leq 4$.

3 The second smallest Wiener polarity index among all trees of order n

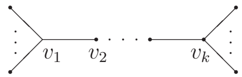

Fig. 1. A general double star $P(k;a,b)$, where $k \geq 3$.

As shown in Fig. 1, a *general double star* $P(k;a,b)$, is a tree obtained from a path $P_k = v_1v_2\cdots v_k$ ($k \geq 3$) by attaching a pendant vertices and b pendant vertices to the vertices v_1 and v_k, respectively. By the definition, $P(n;0,0) = P(n-1;1,0) = P(n-2;1,1)$ ($n \geq 5$) is just a path of order n. Suppose v is a vertex of G, let $G - v$ be the new graph obtained from G by deleting the vertex v and the edges adjacent to v in G. Let $\mathcal{T}_n$ denote the class of trees on n vertices.

Theorem 3.1 *Suppose* $T \in \mathcal{T}_n \setminus \{K_{1,n-1}\}$, *then* $W_P(T) \geq n-3$. *Moreover, the equality holds if and only if* $T \cong P(k;n-k-b,b)$, *where* $k \geq 3$, $n-k \geq b \geq 0$.

Proof. We prove this result by induction on n. Since $T \ncong K_{1,n-1}$, then $n \geq 4$. When $n = 4$, then $T \cong P_4 = P(3;1,0)$, it is easy to see that $W_P(T) = 1 = n-3$, thus the result holds. When $n = 5$, then $T \cong P_5 = P(4;1,0)$ or $T \cong P(3;2,0)$ (see [13, p 273-275]), it is easily checked the result follows. Now suppose that T has n vertices and that result holds for all trees with less than $n \geq 6$ vertices.

Since $T \ncong K_{1,n-1}$, then $\Delta(T) \leq n-2$. If $\Delta(T) = n-2$, then $T \cong P(3;n-3,0)$, it is easy to see that $W_P(T) = n-3$, thus the result follows. Next we consider the case of $\Delta(T) \leq n-3$. Since $\Delta(T) \leq n-3$, there exists one pendant vertex, says u_0, such that $T - u_0 \ncong K_{1,n-2}$, then $W_P(T-u_0) \geq (n-1)-3 = n-4$ by the induction hypothesis. Denote by v_0 the unique neighbor of u_0 in T, and let $N(v_0)$ denote the first neighbor vertex set of v_0 in T. Let $V_{u_0} = \{\{x,u_0\}|\ x \in V(U) \text{ and } d(x,u_0) = 3\}$. Since T is a tree, then $|V_{u_0}| = \sum\limits_{x \in N(v_0)} (d(x)-1)$. Since $T - u_0 \ncong K_{1,n-2}$, then there exists at least one vertex $x \in N(v_0)$ such that $d(x) \geq 2$. Thus,

$$\begin{aligned} W_P(T) &= W_P(T-u_0) + |V_{u_0}| \\ &= W_P(T-u_0) + \sum_{x \in N(v_0)} (d(x)-1) \end{aligned}$$

$$\geq n-4+1$$
$$= n-3.$$

If $W_P(T) = n-3$, then either $T \cong P(3; n-3, 0)$ or $\Delta(T) \leq n-3$ with $W_P(T-u_0) = n-4$ and $\sum_{x \in N(v_0)} (d(x)-1) = 1$, where u_0 is a pendant vertex of T and v_0 is the unique neighbor of u_0. Since $T - u_0 \ncong K_{1,n-2}$ and $W_P(T-u_0) = (n-1)-3$, by the induction hypothesis it follows that $T - u_0 \cong P(k; n-1-k-c, c)$, where $k \geq 3$, $n-1-k \geq c \geq 0$. Moreover, since $\sum_{x \in N(v_0)} (d(x)-1) = 1$, then exactly one neighbor of v_0 (in T) is of degree two, and $d(v)-1$ neighbors of v_0 (in T) are pendant vertices. This implies that $T \cong P(k; n-k-c, c)$ or $T \cong P(k; n-k-a, a)$, where $a = c+1$. Thus, we can conclude that if $W_P(T) = n-3$, then $T \cong P(k; n-k-b, b)$, where $k \geq 3$, $n-k \geq b \geq 0$.

On conversely, if $T \cong P(k; n-k-b, b)$, where $k \geq 3$ and $n-k \geq b \geq 0$, by Theorem 2.1 and Eq. (5), we have

$$W_P(T) = \sum_{xy \in E} (d(x)-1)(d(y)-1)$$
$$= n-3.$$

This proves the theorem.

By Theorem 2.1, it follows that $W_P(T) = M_2(T) - M_1(T) + n - 1$ for a tree T of order n. Thus, by Theorem 3.1 we have

Corollary 3.1 *Suppose $T \in \mathcal{T}_n \setminus \{K_{1,n-1}\}$, then $M_2(T) - M_1(T) \geq -2$. Moreover, the equality holds if and only if $T \cong P(k; n-k-b, b)$, where $k \geq 3$, $n-k \geq b \geq 0$.*

4 The smallest and second smallest Wiener polarity indices among all unicyclic graphs of order n

A *unicyclic graph* of order n is a connected graph with n vertices and n edges. It is well-known that every unicyclic graph has exactly one cycle. Let $\mathcal{U}_n$ denote the class of unicyclic graphs on n vertices. Let $S(n, 1)$ be the unicyclic graph obtained from $K_{1,n-1}$ by adding one edge to two pendant vertices of $K_{1,n-1}$. Especially, $S(3, 1) = C_3$.

Theorem 4.1 *Suppose $U \in \mathcal{U}_n$, then $W_P(U) \geq 0$, where equality holds if and only if $U \cong S(n, 1)$ or $U \cong C_4$ or $U \cong C_5$.*

Proof. By the definition of $W_P(U)$, $W_P(U) = 0$ if and only if $1 \leq diam(U) \leq 2$. Note that a unicyclic graph U with $1 \leq diam(U) \leq 2$ if and only if $U \cong S(n,1)$ or $U \cong C_4$ or $U \cong C_5$. This completes the proof of this result.

Next we consider the second smallest Wiener polarity index among $\mathcal{U}_n$. We need some more lemmas as follows.

Lemma 4.1 [14] *If $U \in \mathcal{U}_n$, then $M_2(U) \geq M_1(U)$.*

Suppose $uv \in E$, the notion $G - uv$ denotes the new graph yielded from G by deleting the edge uv. Similarly, if $uv \notin E$, then $G + uv$ denotes the new graph obtained from G by adding the edge uv. A *non-pendant vertex* of G is a vertex of G, which is not a pendant vertex. Suppose U is a unicyclic graph with unique cycle C_t, in the sequel, we agree that $V(C_t) = \{v_1, v_2, ..., v_t\}$ and $E(C_t) = \{v_1v_2, v_2v_3, ..., v_{t-1}v_t, v_1v_t\}$. For $1 \leq i \leq t$, let $l_i = max\{d(v_i, w)$, where w is a non-pendant vertex and there is exactly one path connecting v_i with $w\}$. If u_i is a non-pendant vertex of U such that $d(v_i, u_i) = l_i$ and there exists unique path from v_i to u_i, then we call u_i a *matching point* of v_i, where $1 \leq i \leq t$. The next lemma is useful in the sequel.

Lemma 4.2 *Suppose $U \in \mathcal{U}_n$ and $d(v_i, u_i) = l_i$, where v_i is one vertex of the cycle in U and u_i a matching point of v_i. If $d(v_i, u_i) \geq 1$ and w_i is a pendant vertex such that $w_iu_i \in E(U)$, then*

$$W_P(U) = W_P(U - w_i) + \sum_{x \in N(u_i)} (d(x) - 1). \tag{6}$$

Proof. Let $V_{w_i} = \{\{x, w_i\} | \ x \in V(U)$ and $d(x, w_i) = 3\}$. By the definition of u_i, there exists unique path from u_i to v_i. Since $d(v_i, u_i) \geq 1$, then

$$|V_{w_i}| = \sum_{x \in N(u_i)} (d(x) - 1).$$

It is easy to see that $W_P(U) = W_P(U - w_i) + |V_{w_i}|$, the result follows.

Lemma 4.3 *Suppose $U \in \mathcal{U}_n$.* (1) *If $g(U) = 3$ with $V(C_3) = \{v_1, v_2, v_3\}$, then $W_P(U) = M_2(U) - M_1(U) + n + 9 - 2d(v_1) - 2d(v_2) - 2d(v_3)$;* (2) *If $g(U) = 4$ with $V(C_4) = \{v_1, v_2, v_3, v_4\}$, then $W_P(U) = M_2(U) - M_1(U) + n + 4 - d(v_1) - d(v_2) - d(v_3) - d(v_4)$;* (3) *If $g(U) = 5$, then $W_P(U) = M_2(U) - M_1(U) + n - 5$;* (4) *If $g(U) = 6$, then $W_P(U) = M_2(U) - M_1(U) + n - 3$.*

Proof. We only prove the first assertion because the other assertions can be proved analogously. Next we prove the first assertion by induction on n. If $n = 3$, then $U = C_3$. It is easy to see that $W_P(C_3) = 0 = M_2(C_3) - M_1(C_3) + n + 9 - 2d(v_1) - 2d(v_2) - 2d(v_3)$, thus the result follows. Now assume the assertion holds for all unicyclic graphs with less than $n \geq 4$ vertices and a cycle C_3. Suppose U is a unicyclic graph with n vertices and a cycle C_3. We consider the next cases.

Case 1. $max\{l_1, l_2, l_3\} = 0$. This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 3$. By Eq. (5) we have $M_2(U) - M_1(U) + n + 9 - 2d(v_1) - 2d(v_2) - 2d(v_3) = (k_1 + 1)(k_2 + 1) + (k_1 + 1)(k_3 + 1) + (k_2 + 1)(k_3 + 1) + 9 - 2(k_1 + 2) - 2(k_2 + 2) - 2(k_3 + 2) = k_1k_2 + k_2k_3 + k_1k_3 = W_P(U)$, thus the result follows.

Case 2. $max\{l_1, l_2, l_3\} \geq 1$. Without loss of generality, suppose $d(v_1, u_1) = max\{l_1, l_2, l_3\}$, where u_1 is a matching point of v_1. By the definition of u_1, there exists one pendant vertex, says w_1, such that $w_1u_1 \in E(U)$. Let $E_1 = \{u_1x | \ x \in N(u_1)\}$, where $N(u_1)$ denotes the first neighbor vertex set of u_1 in U. By the induction hypothesis, Eq. (5) and Eq. (6), we have

$$
\begin{aligned}
W_P(U) &= W_P(U - w_1) + \sum_{x \in N(u_1)} (d(x) - 1) \\
&= \sum_{xy \in E \setminus E_1} (d(x) - 1)(d(y) - 1) + \sum_{x \in N(u_1)} (d(x) - 1)(d(u_1) - 2) + 9 \\
&- 2(d(v_1) + d(v_2) + d(v_3)) + \sum_{x \in N(u_1)} (d(x) - 1) \\
&= \sum_{xy \in E \setminus E_1} (d(x) - 1)(d(y) - 1) \\
&+ \sum_{xu_1 \in E_1} (d(x) - 1)(d(u_1) - 1) + 9 - 2(d(v_1) + d(v_2) + d(v_3)) \\
&= \sum_{xy \in E} (d(x) - 1)(d(y) - 1) + 9 - 2(d(v_1) + d(v_2) + d(v_3)) \\
&= M_2(U) - M_1(U) + n + 9 - 2d(v_1) - 2d(v_2) - 2d(v_3).
\end{aligned}
$$

By combining the above arguments, the result follows.

In the following, let $F_1(n)$, $F_2(n)$ and $H_1(n)$ be the unicyclic graphs of order $n \geq 5$ as shown in Fig. 2. Let $F_3(6)$ be the unicyclic graph of order 6 obtained from C_5 by attaching one pendant vertex to v_1 of $V(C_5)$.

Lemma 4.4 *Suppose $U \in \mathcal{U}_n \setminus \{S(n,1)\}$. If $g(U) = 3$ and $n \geq 5$, then $W_P(U) \geq n-4$, where equality holds if and only if $U \cong F_1(n)$.*

Proof. We prove this result by induction on n. When $n = 5$, then $U \cong F_1(5)$ or $U \cong H_1(5)$ (see [13, p 273-275]), it can be easily checked that result holds. Now assume the assertion holds for all unicyclic graphs with less than $n \geq 6$ vertices and a cycle C_3. Suppose U is a unicyclic graph with n vertices and a cycle C_3. Let $V(C_3) = \{v_1, v_2, v_3\}$. We consider the next cases.

Case 1. $max\{l_1, l_2, l_3\} = 0$. This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 3$. Without loss of generality, suppose $k_1 \geq k_2 \geq k_3 \geq 0$. Since $U \ncong S(n,1)$, then $k_2 \geq 1$.

If $k_2 = 1$ and $k_3 = 0$, then $k_1 = n-4$ and hence $U \cong F_1(n)$. It is easy to see that $W_P(U) = n-4$, the result follows.

If $k_2 = 1 = k_3$, then $k_1 = n-5$. It is easy to see that $W_P(U) = 2n-9 > n-4$, the result follows.

If $k_2 \geq 2$, by Lemma 4.3 and Eq. (5), we have $W_P(U) = M_2(U) - M_1(U) + n + 9 - 2d(v_1) - 2d(v_2) - 2d(v_3) = k_1k_2 + k_2k_3 + k_1k_3 = k_2(k_1+k_3) + k_1k_3 \geq 2(k_1+k_3) \geq k_1+k_2+k_3 = n-3 > n-4$, thus the result follows.

Case 2. $max\{l_1, l_2, l_3\} = 1$. Without loss of generality, suppose $d(v_1, u_1) = max\{l_1, l_2, l_3\}$, where u_1 is a matching point of v_1. By the definition of u_1, there exists one pendant vertex, says w_1, such that $w_1u_1 \in E(U)$.

Subcase 1. $U - w_1 \cong S(n-1,1)$. Then, $U \cong H_1(n)$ (see Fig. 2). It is easy to see that $W_P(U) = n-3 > n-4$, the result follows.

Subcase 2. $U - w_1 \ncong S(n-1,1)$. By Eq. (6) and the induction hypothesis, we have

$$\begin{aligned} W_P(U) &= W_P(U-w_1) + \sum_{x \in N(u_1)} (d(x)-1) \\ &\geq W_P(U-w_1) + d(v_1) - 1 \\ &\geq (n-1) - 4 + 2 \\ &= n-3. \end{aligned}$$

Case 3. $max\{l_1, l_2, l_3\} \geq 2$. Without loss of generality, suppose $d(v_1, u_1) = max\{l_1, l_2, l_3\}$, where u_1 is a matching point of v_1. By the definition of u_1, there exists one pendant vertex, says w_1, such that $w_1u_1 \in E(U)$. Since $d(v_1, u_1) \geq 2$, then $U - w_1 \ncong S(n-1,1)$ and

$U-w_1 \ncong F_1(n-1)$. By the suppose hypothesis, it follows that $W_P(U-w_1) \geq (n-1)-3 = n-4$. Note that there exists at least one vertex $x \in N(u_1)$ such that $d(x) \geq 2$, by Eq. (6) we have

$$\begin{aligned} W_P(U) &= W_P(U-w_1) + \sum_{x \in N(u_1)} (d(x)-1) \\ &\geq W_P(U-w_1) + 1 \\ &\geq n-3. \end{aligned}$$

The result follows by combining the above arguments.

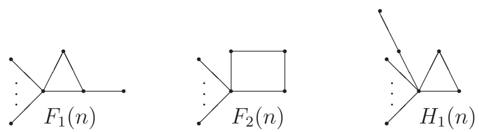

Fig. 2. The unicyclic graphs $F_1(n)$, $F_2(n)$ and $H_1(n)$, $n \geq 5$.

Lemma 4.5 *Suppose* $U \in \mathcal{U}_n$. *If* $g(U) = 4$ *and* $n \geq 5$, *then* $W_P(U) \geq n-4$, *where equality holds if and only if* $U \cong F_2(n)$.

Proof. We prove this result by induction on n. When $n = 5$, then $U \cong F_2(5)$ (see [13, p 273-275]), it can be easily checked the result holds. Now assume the assertion holds for all unicyclic graphs with less than $n \geq 6$ vertices and a cycle C_4. Suppose U is a unicyclic graph with n vertices and a cycle C_4. Let $V(C_4) = \{v_1, v_2, v_3, v_4\}$. Two cases occur.

Case 1. $max\{l_1, l_2, l_3, l_4\} = 0$. This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 4$. Without loss of generality, suppose $k_1 \geq k_2 \geq k_3 \geq k_4 \geq 0$.

If $k_2 = 0$, then $k_3 = k_4 = 0$ and $k_1 = n-4$. Thus, $U \cong F_2(n)$. It is easy to see that $W_P(U) = n-4$, the result follows.

If $k_2 \geq 1$, then by Lemma 4.3 and Eq. (5), we have $W_P(U) = M_2(U) - M_1(U) + n + 4 - d(v_1) - d(v_2) - d(v_3) - d(v_4) = k_1k_2 + k_2k_3 + k_3k_4 + k_1k_4 + k_1 + k_2 + k_3 + k_4 \geq k_1k_2 + k_1 + k_2 + k_3 + k_4 \geq 1 + n - 4 = n-3 > n-4$, thus the result follows.

Case 2. $max\{l_1, l_2, l_3, l_4\} \geq 1$. Without loss of generality, suppose $d(v_1, u_1) = max\{l_1, l_2, l_3, l_4\}$, where u_1 is a matching point of v_1. By the definition of u_1, there exists one pendant vertex, says w_1, such that $w_1u_1 \in E(U)$.

Subcase 1. $d(v_1, u_1) = 1$. Thus, from the induction hypothesis and Eq. (6), we have

$$\begin{aligned} W_P(U) &= W_P(U - w_1) + \sum_{x \in N(u_1)} (d(x) - 1) \\ &\geq W_P(U - w_1) + d(v_1) - 1 \\ &\geq n - 3. \end{aligned}$$

Subcase 2. $d(v_1, u_1) \geq 2$. Since $d(v_1, u_1) \geq 2$, then $U - w_1 \not\cong F_2(n-1)$. By the induction hypothesis, it follows that $W_P(U - w_1) \geq (n-1) - 3 = n - 4$. Note that there exists at least one vertex $x \in N(u_1)$ such that $d(x) \geq 2$, by Eq. (6) we have

$$\begin{aligned} W_P(U) &= W_P(U - w_1) + \sum_{x \in N(u_1)} (d(x) - 1) \\ &\geq W_P(U - w_1) + 1 \\ &\geq n - 3. \end{aligned}$$

Similarly with Lemma 4.5, we have the next result.

Lemma 4.6 *Suppose $U \in \mathcal{U}_n$. If $g(U) = 5$ and $n \geq 7$, then $W_P(U) \geq n - 3$.*

Now we give the main result of this section as follows.

Theorem 4.2 *Suppose $U \in \mathcal{U}_n \setminus \{S(n,1), C_4, C_5\}$, then $W_P(U) \geq n - 4$, where equality holds if and only if $U \cong F_1(n)$ or $U \cong F_2(n)$ or $U \cong F_3(6)$, where $F_1(n)$ and $F_2(n)$ are shown in Fig. 2.*

Proof. Since $U \in \mathcal{U}_n$, then U has unique cycle C_t. If $t \geq 7$, by Theorem 2.1 and Lemma 4.1, we have $W_P(U) = M_2(G) - M_1(G) + n \geq n$. If $t = 6$, by Lemmas 4.1 and 4.3, we have $W_P(U) = M_2(U) - M_1(U) + n - 3 \geq n - 3$. If $t = 5$, since $U \not\cong C_5$, then $n \geq 6$. When $n = 6$, then $U \cong F_3(6)$. It is easy to see that $W_P(F_3(6)) = 2 = n - 4$. When $n \geq 7$, by Lemma 4.6, it follows that $W_P(U) \geq n - 3$. If $t = 4$, since $U \not\cong C_4$, then $n \geq 5$. By Lemma 4.5, the result follows. If $t = 3$, since $U \not\cong S(n,1)$, then $n \geq 5$. By Lemma 4.4, the result follows. This proves the result.

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