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A Survey on the Wiener Polarity Index

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Abstract

The *Wiener polarity index* $W_p(G)$ of a graph G, proposed by Wiener in 1947, is the number of unordered pairs of vertices $\{u, v\}$ of G such that the distance between u and v is 3. As one of the classic topological indices, properties of $W_p(G)$ have been extensively studied for various graphs. We survey some recent development on the Wiener polarity index and related results.

1 Introduction

A (chemical) topological index is a real number calculated from chemical graphs. Graphs are used to model chemical compounds and drugs. In the graphs, each vertex represents an atom of molecule and edges between the corresponding vertices are used to represent covalent bounds between atoms. The topological indices have received much attention in recent years, as they provide a strong correlation between a chemical compound's molecular structure and its properties. There exist several types of such indices, especially those based on vertex and edge distances. One of the oldest and well-studied such indices

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is the *Wiener index*, defined as the sum of distances over all unordered vertex pairs in a graph G [55] and denoted by

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

where $d_G(u,v)$ (or simply $d(u,v)$) is the distance between u and v in G.

Throughout the years the Wiener index has been extensively studied and has become one of the best known topological indices. For more results on the Wiener index, we refer the readers to the survey paper [21] written by Dobrynin, Entringer and Gutman. In the same paper, another topological index was also introduced by Wiener, called the *Wiener polarity index* $W_p(G)$, which is defined as the number of unordered pairs of vertices that are at distance 3 in G:

$$W_p(G) = |\{(u,v)|d_G(u,v) = 3, u, v \in V(G)\}|. \tag{1}$$

Like the Wiener index, the Wiener polarity index has attracted much attention in recent years. By using the Wiener polarity index, Lukovits and Linert [43] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya [30] found a physical-chemical interpretation of the Wiener polarity index. Du, Li and Shi [24] described a linear time algorithm for computing the Wiener polarity index of trees and characterized the trees maximizing the index among all the trees of the given order. Later, the extremal Wiener polarity index of (chemical) trees with given different parameters (e.g. order, diameter, maximum degree, the number of leaves, etc.) were studied, see [17, 18, 20, 37, 38, 40]. While for cycle-containing graphs, the maximum Wiener polarity index of unicyclic graphs and the corresponding extremal graphs were determined in [31]. For other classes of graphs, such as fullerenes, hexagonal systems, lattices and cactus graphs, we refer to [8, 14, 15, 19, 44, 46]. There are some results of the Wiener polarity index of the graph operations and the relations with other indices, such as [32, 45, 58]. In addition, the more results on bounding the Wiener polarity index were described in [57].

In this paper, We survey the results on the Wiener polarity index. Section 2 discusses the Wiener polarity index for trees and trees with certain restrictions. In Section 3, we consider the unicyclic graphs and the extremal problem with respect to the Wiener polarity index. Section 4 presents some results on the Wiener polarity index of graph products and the Nordhaus-Gaddum-type inequality. In Section 5 we discuss the Wiener polarity index in terms of other graph invariants such as the Wiener index, hyper-Wiener index, first Zagreb index, second Zagreb index, etc.. Finally in Section 6 we summarize the generalization of the Wiener polarity index and related extremal problems.

Additional notation is as follows. Given a graph $G = (V(G), E(G))$, we use $|G|$ to denote the number of vertices, $e(G)$ the number of edges, $\delta(G)$ the minimum degree, $\Delta(G)$ the maximum degree, and $\overline{G}$ the complement graph of G, respectively. For any $v \in V(G)$, let $d_G(v)$ and $N_G(v)$ denote the degree and neighborhood of v in G, respectively. The *girth* of a graph with a cycle is the length of its shortest cycle. A graph with no cycle has infinite girth. For $u, v \in V(G)$, the *distance* from u to v (i.e., the length of a shortest $u-v$ path) in G is denoted by $d(u, v)$; 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 $[k] = \{1, 2, \ldots, k\}$. We use S_n, P_n and C_n to denote the star, the path and the cycle on n vertices, respectively. Let $K_{m,n}$ denote the complete bipartite graph in which the orders of its bipartition sets are m and n. A *tree* is a connected acyclic graph. We call a tree *nontrivial*, if it is not an isolated vertex. The vertices with degree 1 in a tree are its *leaves*. A *unicyclic graph* is a connected graph containing exactly one cycle.

Let G be a graph with t components $G_1, G_2, \ldots, G_t$. Obviously, $W_p(G) = \sum_{i=1}^{t} W_p(G_i)$. So it suffices to consider the Wiener polarity index of connected graphs. Some graph transformations that decrease or increase the Wiener polarity index of connected graphs are very useful for studying Wiener polarity index, see [57].

2 The Wiener polarity index of trees

It is well known that for any two vertices u and v in a tree T, there exists exactly one path between u and v in T. Thus, the distance between two vertices u and v in T is the length of the path between u and v in T. By the good property, Du, Li and Shi [24] get a linear time algorithm and a formula for computing the Wiener polarity index of a tree.

Lemma 2.1 ([24]) *Let $T = (V, E)$ be a tree. Then* $W_p(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1)$.

Let $\mathcal{T}(n)$ denote the set of the trees on n vertices. By the definition of Wiener polarity index, one can readily check that $W_p(S_n) = 0$ and $W_p(T) > 0$ for any $T \in \mathcal{T}(n)\backslash\{S_n\}$. Du, Li, Shi [24] and Liu, Liu [40] obtained the maximum and the second smallest Wiener polarity index in $\mathcal{T}(n)$, respectively. To state their results, we define some specific trees.

Let $T(k_1, k_2, k_3, l_1, \ldots, l_m)$ be a tree with diameter 4 as in Figure 1, with $k_i \geq 0$ $(i = 1, 2, 3)$, $m \geq 1$ and $k_1 + k_2 + k_3 + l_1 + \cdots + l_m = n - 5 - m$. Let $\mathrm{T}_3(n) := \{T \in \mathcal{T}(n) |\ diam(T) = 3, W_p(T) = \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil\}$ and $\mathrm{T}_4(n) := \{T(k_1, k_2, k_3, l_1, \ldots, l_m) \in \mathcal{T}(n) |\ m + k_2 + 1 = \lfloor \frac{n-2}{2} \rfloor$ or $\lceil \frac{n-2}{2} \rceil\}$. A *double star* $S_{a,b}$ is obtained from S_a and S_b by connecting the center of S_a with that of S_b. A *general double star* $P(k; a, b)$ is a tree obtained from a path $P_k = v_1 \ldots v_k$ $(k \geq 3)$ by attaching a pendent vertices and b pendent vertices to the vertices v_1 and v_k, respectively. A *capillary tree* $CT(x_1, \ldots, x_{k-1})$ is a tree obtained from a path $P_{k+1} = v_0 v_1 \ldots v_k$ by attaching x_i pendent vertices to the vertices v_i for $i \in [k-1]$.

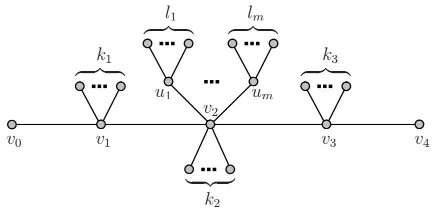


Figure 1: The tree $T(k_1, k_2, k_3, l_1, \ldots, l_m)$.

Theorem 2.1 ([24]) *Let T be a tree of order n. Then*

$$W_p(T) \leq \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil$$

with equality if and only if $T \in \mathrm{T}_3(n) \cup \mathrm{T}_4(n)$.

Theorem 2.2 ([40]) *Suppose that $T \in \mathcal{T}(n)\backslash\{S_n\}$. Then*

$$W_p(T) \geq n - 3$$

with equality if and only if $T \cong P(k; a, b)$, where $a + b = n - k$.

In the following, we introduce some results of the Wiener polarity index of trees with given different parameters, such as maximum degree, diameter and the number of leaves.

2.1 Maximum degree

Let $\mathcal{T}^M(n,\Delta)$ be the set of all trees with n vertices and maximum degree Δ. Given $T \in \mathcal{T}^M(n,\Delta)$, let $V^{(\Delta)}(T) = \{v \in V(T)|\ d_T(v) = \Delta\}$ and $N^{(\Delta)}(T) = \cup_{v\in V^{(\Delta)}(T)} N_T(v)$. Let $h = n - (\Delta + 1)$ and $T_0 = S_{\Delta+1}$, we construct T_i from T_{i-1} by attaching a vertex to one vertex of $N^{(\Delta)}(T_{i-1})\backslash V^{(\Delta)}(T_{i-1})$ for $i = 1, 2, \ldots, h$. The set of all possible T_h after h steps is denoted by $\mathcal{T}_{\max}(n,\Delta)$.

Liu, Hou and Huang [38] characterized the trees minimizing (resp. maximizing) the Wiener polarity index among all trees $T \in \mathcal{T}^M(n,\Delta)$.

Theorem 2.3 ([38]) *(1)* $\mathcal{T}^M(n,2) = \{P_n\}$, *and* $W_p(P_n) = n-3$;
(2) $\mathcal{T}^M(n,n-1) = \{S_n\}$, *and* $W_p(S_n) = 0$;
(3) $\mathcal{T}^M(n,n-2) = \{P(2;n-3,1)\}$, *and* $W_p(P(2;n-3,1)) = n-3$.

Theorem 2.4 ([38]) *Let* $T \in \mathcal{T}^M(n,\Delta)$, *where* $3 \le \Delta \le n-3$. *Then*

$$n - 3 \le W_p(T) \le (n - \Delta - 1)(\Delta - 1).$$

The left equality holds if and only if $T \cong P(n-\Delta+1-l;\Delta-1,l)$ *where* $0 \le l \le min\{\Delta-1, n-\Delta-2\}$, *while the right equality holds if and only if* $T \in \mathcal{T}^M_{\max}(n,\Delta)$.

Note that Theorem 2.1 can be regarded as a corollary of Theorem 2.4.

2.2 Diameter

Let $T \in \mathcal{T}^D(n,d)$ be the set of trees of order n with diameter d. It is easy to see that $W_p(G) = 0$ if $diam(G) \le 2$. For $3 \le diam(G) \le n-1$, we have the following theorems.

Theorem 2.5 ([20]) *Let* $T \in \mathcal{T}^D(n,d)$, *where* $3 \le d \le n-1$. *Then*

$$W_p(T) \ge n - 3$$

with equality if and only if $T \cong P(d-1;r,t)$ *where* $r > 0$, $t > 0$, $r+t = n-d+1$ *if* $d > 3$ *and* $T \cong P(2;n-3,1)$ *if* $d = 3$.

Tang and Deng [50] characterized the trees with the first three smallest Wiener polarity indices in $T^D(n,d)$.

Note that the trees with the maximal Wiener polarity index among all trees of order n and diameter $d = 3, 4$ were characterized in Theorem 2.1.

Theorem 2.6 ([20]) *Let $T \in \mathcal{T}^D(n,d)$, where $5 \le d \le n-1$. Then*

$$W_p(T) \le \left\lfloor \frac{n-d-1}{2} \right\rfloor \left\lceil \frac{n-d-1}{2} \right\rceil + 2n - d - 4.$$

Moreover, the equality holds if and only if $T \cong CT(0,\ldots,0,x_i,x_{i+1},x_{i+2},0,\ldots,0)$, where $2 \le i \le d-4$, $x_i + x_{i+1} + x_{i+2} = n-d-1$, $x_i \ge 0$, $x_{i+2} \ge 0$ and $x_{i+1} = \lfloor \frac{n-d-1}{2} \rfloor$ or $\lceil \frac{n-d-1}{2} \rceil$.

2.3 The number of leaves

Let $\mathcal{T}^L(n,k)$ be the set of all trees with n vertices and k leaves. It is obvious that $2 \le k \le n-1$. The trees minimizing and maximizing $W_p(T)$ in $\mathcal{T}^L(n,k)$ were characterized by Liu, Hou, Huang [38] and Deng, Xiao [18], respectively.

Theorem 2.7 ([18, 38]) *(1) $\mathcal{T}^L(n,2) = \{P_n\}$, and $W_p(P_n) = n-3$;*
(2) $\mathcal{T}^L(n,n-1) = \{S_n\}$, and $W_p(S_n) = 0$;
(3) $\mathcal{T}^L(n,n-2) = \{P(2;n_1,n_2) \mid n_1 + n_2 = n-2$ and $n_1 \ge n_2 > 0\}$. Then for $T \in \mathcal{T}^L(n,n-2)$, $n-3 \le W_p(T) \le \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$, where the left equality holds if and only if $T \cong P(2;n-3,1)$, and the right equality holds if and only if $T \cong P(2;\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$.

Theorem 2.8 ([38]) *Let $T \in \mathcal{T}^L(n,k)$, where $3 \le k \le n-3$. Then*

$$W_p(T) \ge n-3$$

with equality if and only if $T \cong P(n-k;n_1,k-n_1)$, where $0 < n_1 \le k-n_1$.

Theorem 2.9 ([18]) *Let $T \in \mathcal{T}^L(n,k)$, where $k+2 \le n \le 2k$ and $n \ge 4$. Then*

$$W_p \le \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil$$

with equality if and only if (i) $T \cong T(k_1,k_2,k_3,l_1,\ldots,l_s)$ where $k_2 = k+1-\lfloor \frac{n}{2} \rfloor$ or $k_2 = k+1-\lceil \frac{n}{2} \rceil$), or (ii) $T \cong P(2;\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)$.

This result shows that the maximum Wiener polarity index is independent of k when $k+2 \le n \le 2k$.

Theorem 2.10 ([18]) *Let $T \in \mathcal{T}^L(n,k)$. If $n \ge 2k+1$, then*

$$W_p(T) \le k^2 - 3k + n - 1$$

with equality if and only if T is a star-like tree of order n in which the lengths of all pendant chains are at least 2.

2.4 Chemical trees

A *chemical graph* is a graph with maximum degree no more than 4. Deng [17] obtained the maximum Wiener polarity index among chemical trees on n vertices.

Theorem 2.11 ([17]) *Let T be a chemical tree of order n (≥ 7). Then*

$$W_p(T) \leq 3n - 15.$$

Du and Ali [23] determined all chemical trees on n vertices having maximum W_p.

Theorem 2.12 ([23]) *For every $n \geq 8$, only chemical trees which satisfy every vertex of degree 2 (if exists) is adjacent to one vertex of degree 1 and one vertex of degree 4, and every vertex of degree 3 (if exists) is adjacent to two vertices of degree 1 and one vertex of degree 4 have maximum Wiener polarity index $3n - 15$.*

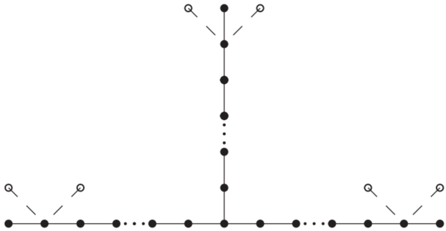
Ashrafi and Ghalavand [6] determined the first three minimum W_p values and characterized the trees attaining the first two minimum W_p values among n-vertex chemical trees for $n \geq 7$. Subsequently, Ali, Du and Ali [4] characterized the chemical trees with the third minimum W_p value in the collection of all n-vertex chemical trees for $n \geq 7$. Note that the chemical trees attaining the first minimum W_p values have been characterized in Theorem 2.4.

Theorem 2.13 ([4, 6]) *For fixed $n \geq 8$, Figures 2 and 3 are the only chemical trees with the second, the third minimum W_p values, which are $n-2$, $n-1$, respectively, among all the n-vertex chemical trees.*

Figure 2: The chemical trees with the second minimum W_p value.

(a)

(b)



(c)

(d)

Figure 3: The chemical trees with the third minimum W_p value.

Furthermore, Du and Ali [22] proved that for every integer $n-3 \leq t \leq 3n-15$, there exists an n-vertex chemical tree T such that $W_p(T) = t$.

Deng and Xiao [19] also identified the maximum Wiener polarity index of chemical trees with n vertices and k leaves.

Theorem 2.14 ([19]) *Let T be a chemical tree with $n \geq 7$ vertices and $k \geq 2$ leaves.*

Then

$$W_p(T) = \begin{cases} n-3, & \textit{if } k=2; \\ n-1, & \textit{if } k=3; \\ n+5k-17, & \textit{if } k \textit{ is even and } 4 \le k \le \frac{2}{5}(n+1); \\ 3n-15, & \textit{if } k \textit{ is even and } k \ge \frac{2}{5}(n+1); \\ n+5k-18, & \textit{if } k \textit{ is odd and } 5 \le k \le \frac{2n+1}{5}; \\ 3n-16, & \textit{if } k \textit{ is odd and } k = \frac{2n+3}{5} \ge 5; \\ 3n-15, & \textit{if } k \textit{ is odd and } k \ge \frac{2n+5}{5}. \end{cases}$$

A vertex of degree greater than 2 is called a *branching vertex.* A *segment* of a tree T is a path-subtree S whose terminal vertices have degrees different from 2 in T and every internal vertex (if exists) of S has degree 2 in T. Rencently, Noureena, Bhattia and Ali [48] obtained the best possible sharp upper and lower bounds on the Wiener polarity index W_p for the chemical trees of order n with a given number of branching vertices or segments, and characterized the corresponding extremal chemical trees.

2.5 Other results

2.5.1 Hückel trees

The trees with perfect matching, of which all vertices have degrees not greater than 3, are referred to as the Hückel trees. Wang [54] considered the smallest and the largest Wiener polarity index among all Hückel trees on $2n$ vertices and characterized the corresponding extremal graphs.

Let $TH(2n)$ denote the set of Hückel trees on $2n$ vertices satisfying the following properties:

(i) All the lengths of pendent chains are no more than 2.

(ii) If P is a path of a Hückel tree with both ends of degree 3, then all internal vertices of P are of degree 3.

(iii) All the vertices of degree 2 are on the pendent chains.

Theorem 2.15 ([54]) *Suppose T is a Hückel tree on $2n$ vertices. Then*

$$2n-3 \le W_p(T) \le 4n-8,$$

the left equality holds if and only if $T = P_{2n}$ and the right equality holds if and only if $T \in TH(2n)$.

2.5.2 Given degree sequences

Liu, Liu [41] and Lei, Li, Shi, Wang [37] studied trees with a given degree sequence, and characterized the extremal graphs attaining the maximum value of the Wiener polarity index. Lei, Li, Shi and Wang [37] also characterized the extremal graphs attaining the minimum value of the Wiener polarity index.

Definition 2.1 (Greedy Tree) *With given vertex degrees, the greedy tree is constructed through the following "greedy algorithm":*

(i) *Label the vertex with the largest degree as v (the root);*

(ii) *Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them such that $d(v_1) \geq d(v_2) \geq \ldots$;*

(iii) *Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$, such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \ldots$, then do the same for $v_2, v_3, \ldots$;*

(iv) *Repeat (iii) for all the newly labeled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.*

Figure 4 shows an example of a greedy tree.

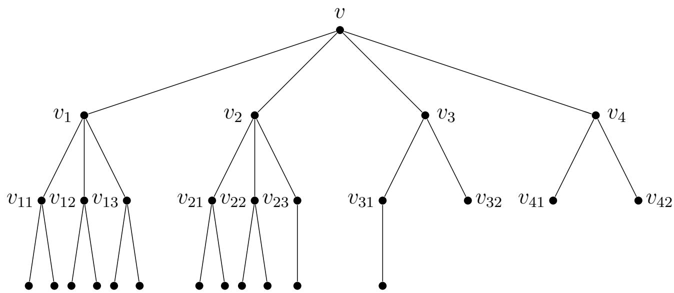


Figure 4: A greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$.

Definition 2.2 (Alternating greedy tree) *Given the non-increasing sequence $(d_1, d_2, \ldots, d_m)$ of internal vertex degrees, the alternating greedy tree is constructed through the following recursive algorithm:*

- *If $m-1 \leq d_m$, then the alternating greedy tree is simply obtained by a tree rooted at r with d_m children, $d_m - m + 1$ of which are leaves and the rest with degrees $d_1, \ldots, d_{m-1}$;*
- *Otherwise, $m-1 \geq d_m+1$. We produce a subtree T_1 rooted at r with d_m-1 children with degrees $d_1, \ldots, d_{d_{m-1}}$;*
- *Consider the alternating greedy tree S with degree sequence $(d_{d_m}, \ldots, d_m - 1)$, let v be a leaf with the smallest neighbor degree. Identify the root of T_1 with v.*

Theorem 2.16 ([37, 41]) *Among all trees with a given degree sequence, $W_p(T)$ is maximized by the greedy tree and is minimized by the alternating greedy tree.*

2.5.3 Quasi-trees

A connected graph $G = (V, E)$ is called a *quasi-tree*, if there exists $u_0 \in V(G)$ such that $G - u_0$ is a tree. Denote $\mathcal{QT}(n, d_0) = \{G\colon G$ is a quasi-tree graph of order n with $G - u_0$ being a tree and $d_G(u_0) = d_0\}$. The concept of quasi-tree graphs was first introduced by Liu and Lu [42].

Tang and Liang [51] obtained the maximal and the second smallest Wiener polarity index of quasi-tree graphs of order n. Note that the smallest Wiener polarity index among all quasi-tree graphs of order n is 0.

Theorem 2.17 ([51]) *Let $G \in \mathcal{QT}(n, d_0)$ with $n \geq 4$ and $d_0 \geq 2$.*

(1) If $n \in \{4, 5, 6\}$, then $W_p(G) \leq n - 3$.

(2) If $n = 7$, then $W_p(G) \leq 7$.

(3) If $n = 8$, then $W_p(G) \leq 9$.

(4) If $n = 9$, then $W_p(G) \leq 12$.

(5) If $n \geq 10$, then $W_p(G) \leq \lfloor \frac{n^2-6n+9}{3} \rfloor$.

Theorem 2.18 ([51]) *Let $G \in \mathcal{QT}(n, d_0)$. If $W_p(G) > 0$ and $d_0 \leq n - 3$, then*

$$W_p(G) \geq n - d_0 - 2.$$

3 The Wiener polarity index of unicyclic graphs

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 $C_g = u_1u_2\dots u_gu_1$ be a cycle of order $g(\geq 3)$. Let $C_g(k_1,\dots,k_g)$ denote a caterpillar cycle, which is a unicyclic graph obtained from C_g by attaching k_i vertices to vertex u_i, where $k_i \geq 0$ for $i \in [g]$. When there is exactly one $i \in [g]$ such that $k_i \neq 0$, we write $C_g(k_i)$ for short. Let EC_3 denote the caterpillar cycle $C_3(k_1,k_2,k_3)$ with $|k_i - k_j| \leq 1$ $(i,j = 1,2,3)$ of order n.

We first present a formula of the Wiener polarity index of unicyclic graphs.

Lemma 3.1 ([40]) *Let $U = (V,E)$ be a unicyclic graph and let C denote the unique cycle of U. If $g(U) = 3$ with $V(C) = \{u_1,u_2,u_3\}$, then*

$$W_p(U) = \sum_{uv\in E}(d_U(u)-1)(d_U(v)-1) + 9 - 2d_U(u_1) - 2d_U(u_2) - 2d_U(u_3).$$

If $g(U) = 4$ and $V(C) = \{u_1,u_2,u_3,u_4\}$, then

$$W_p(U) = \sum_{uv\in E}(d_U(u)-1)(d_U(v)-1) + 4 - d_U(u_1) - d_U(u_2) - d_U(u_3) - d_U(u_4).$$

If $g(U) \geq 5$, then

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

To illustrate the following results, we define some special unicyclic graphs.

- Let C^j_{g,l_1,l_2} be a unicyclic graph obtained from C_g by attaching l_1 and l_2 pendant vertices to u_i and u_{i+j} respectively, where $i, i+j \in \{1,\dots,g \pmod g\}$.
- Let $C_g(P_{n-g+1})$ be the unicyclic graph on n vertices formed by attaching one pendent vertex of P_{n-g+1} to one vertex of C_g.
- Let $C_g(P(t+1;0,n-g-t))$ be a unicyclic graph obtained from a cycle C_g and $P(t+1;0,n-t-g)$ by identifying a vertex of C_g and v_1.

- Let $C_g^j(P(t+1;0,n-g-t-s),s)$ be a unicyclic graph obtained from a cycle C_g by attaching the vertex v_1 of $P(t+1;0,n-g-t-s)$ and s pendant vertices to u_i and u_{i+j} respectively, where $i, i+j \in \{1,\ldots,g \pmod g\}$.

Liu and Liu [40] considered the smallest and second smallest Wiener polarity indices among all unicyclic graphs of order n.

Theorem 3.1 ([40]) *Suppose $U \in \mathcal{U}(n)$, then $W_p(U) \geq 0$, where the equality holds if and only if $U \cong C_3(n-3)$ or C_4 or C_5.*

Theorem 3.2 ([40]) *Suppose $U \in \mathcal{U}(n)\backslash\{C_3(n-3), C_4, C_5\}$, then $W_p(U) \geq n-4$, where the equality holds if and only if $U \cong C_3(n-4,1,0)$ or $C_4(n-4)$ or $C^2_{4,\ell,n-4-\ell}$ $(1 \leq \ell \leq n-5)$ or $C_5(1)$.*

Fang, Ma, Chen and Dong [26] determined the third smallest Wiener polarity index of unicyclic graphs and characterized the corresponding extremal graphs.

Theorem 3.3 ([26]) *Suppose $U \in \mathcal{U}(n)$. Then the third smallest Wiener polarity index $W_p(U) = n-3$, the equality holds if and only if $U \cong C_6, C_3(2,2,0), C_3^j(P(t;0,s), n-t-s-2)$ with $j = 0,1$, $C^1_{4,1,1}$, $C_4^2(P(t;0,s), n-t-s-3)$, $C_5(2)$, $C^2_{5,1,1}$, $C_5((P(t;0,,n-t-4))$, where $t \geq 3$.*

Hou, Liu and Huang [31] first obtained an upper bound for the Wiener polarity index of unicyclic chemical graphs.

Theorem 3.4 ([31]) *Let U be a unicyclic chemical graph with $n(\geq 5)$ vertices. Then*

$$W_p(U) \leq 3n+12.$$

Recently, an ordering of chemical unicyclic graphs of order n with respect to the Wiener polarity index was given by Ghalavand and Ashrafi [27].

Hou, Liu and Huang [31] determined the maximum Wiener polarity index of unicyclic graphs and characterized the corresponding extremal graphs. In particular, they proved the following result for $n \geq 12$.

Theorem 3.5 ([31]) *Let U be a unicyclic graph of order $n \geq 12$. Then*

$$W_p(U) \leq W_p(EC_3)$$

with equality if and only if $U \cong EC_3$.

In the following, Huang, Hou, Liu [34] and Ma, Shi, Yue [44] considered the Wiener polarity index of unicyclic graphs with given different parameters, girth, the number of leaves, the maximum degree and diameter.

Now for unicyclic graphs with a given girth, let $\mathcal{U}^G(n,g)$ be the set of unicyclic graphs of order n with girth g.

Theorem 3.6 ([34]) *Suppose $n \geq 9$. Then*

(1) $\mathcal{U}^G(n,n) = \{C_n\}$, and $W_p(C_n) = n$;

(2) $\mathcal{U}^G(n,n-1) = \{C_{n-1}(1)\}$, and $W_p(C_{n-1}(1)) = n+1$;

(3) $\mathcal{U}^G(n,n-2) = \{C_{n-2}(P_3), C_{n-2}(2), C^j_{n-2,1,1}\}$, where $1 \leq j \leq \lfloor \frac{n-2}{2} \rfloor$.

And $W_p(C^1_{n-2,1,1}) = n+3 > n+2 = W_p(C_{n-2}(P_3)) = W_P(C_{n-2}(2)) = W_p(C^j_{n-2,1,1})$, where $1 < j \leq \lfloor \frac{n-2}{2} \rfloor$.

Theorem 3.2 together with Theorem 3.7 determined the minimum Wiener polarity index together with its corresponding unicyclic graphs of $\mathcal{U}^G(n,g)$ for $3 \leq g \leq n-3$.

Theorem 3.7 ([34]) *Let $U \in \mathcal{U}^G(n,g)$, where $5 \leq g \leq n-3$. Then*

$$W_p(U) \geq \begin{cases} n+2, & \text{if } \ g \geq 7; \\ n-1, & \text{if } \ g = 6; \\ n-3, & \text{if } \ g = 5, \end{cases}$$

with all equalities if and only if $U \cong C_g(P(t+1; 0, n-t-g))$ with $t \geq 2, n-t-g \geq 1$.

As for maximizing the Wiener polarity index, we have the following.

Theorem 3.8 ([34]) *Let $U \in \mathcal{U}^G(n,g)$, where $5 \leq g \leq n-3$. Then*

$$W_p(U) \leq \left\lfloor \frac{n-g}{2} \right\rfloor \left\lceil \frac{n-g}{2} \right\rceil + \begin{cases} 2n-10, & \text{if } \ g(U) = 5; \\ 2n-9, & \text{if } \ g(U) = 6; \\ 2n-g, & \text{if } \ g(U) \geq 7. \end{cases}$$

with equality if and only if $U \cong C_g(k_1, k_2, k_3, 0, \ldots, 0)$, where $k_1, k_2, k_3 \geq 0$, $\sum_{i=1}^{3} k_i = n-g$, and $k_2 = \lfloor \frac{n-g}{2} \rfloor$ or $\lceil \frac{n-g}{2} \rceil$.

Let $C_4(k_1,k_2,k_3,0) \bigotimes (t)$ denote the unicyclic graph obtained from t isolated vertices and $C_4(k_1,k_2,k_3,0)$ by attaching each of the t isolated vertices to any pendant vertices of $N_{C_4(k_1,k_2,k_3,0)}(u_2)$, where $k_1,k_2,k_3 \geq 0$ and $t \geq 1$.

Theorem 3.9 ([34]) *Let $U \in \mathcal{U}^G(n,4)$. Then*

$$W_p(U) \le \left\lfloor \frac{n-4}{2} \right\rfloor \left\lceil \frac{n-4}{2} \right\rceil + n - 4$$

with equality if and only if $U \cong C_4(k_1,k_2,k_3,k_4)$, where $k_1,k_2,k_3,k_4 \ge 0$ and $n-4-k_1-k_3 = k_2+k_4 = \lfloor \frac{n-4}{2} \rfloor or \lceil \frac{n-4}{2} \rceil$, or $U \cong C_4(k_1,k_2,k_3,0) \bigotimes (t)$, where $k_1,k_2,k_3 \ge 0$, $t \ge 1$, and $n-4-k_1-k_3-t = k_2 = \lfloor \frac{n-4}{2} \rfloor$ or $\lceil \frac{n-4}{2} \rceil$.

Theorem 3.10 ([34]) *Let $U \in \mathcal{U}^G(n,3)$, where $n \ge 11$. Then*

$$W_p(U) \le \begin{cases} \frac{1}{3}(n-3)^2, & \text{if } n = 0 \pmod 3; \\ \frac{1}{3}(n-2)(n-4), & \text{if } n \ne 0 \pmod 3, \end{cases}$$

with equality if and only if $U \cong EC_3$.

Let $\mathcal{U}^L(n,k)$ be the set of unicyclic graphs on n vertices with k leaves. The next result determined the minimum Wiener polarity index in $\mathcal{U}^L(n,k)$ for any k.

Theorem 3.11 ([34]) *Suppose $n \ge 9$. Then*

(1) $\mathcal{U}^L(n,0) = \{C_n\}$, and $W_p(U) = n$;

(2) $\mathcal{U}^L(n,1) = \{C_g(P_{n-g+1})\}$ $(n > g \ge 3)$, where $W_p(C_{n-1}(1)) = n+1$ and $W_p(C_g(P_{n-g+1})) = n+2$ for $g \le n-2$;

(3) Let $U \in \mathcal{U}^L(n,n-3)$. Then $W_p(U) \ge 0$ with equality if and only if $U \cong C_3(n-3)$;

(4) Let $U \in \mathcal{U}^L(n,n-4)$. Then $W_p(U) \ge n-4$ with equality if and only if $U \cong C_4(n-4)$ or $C^2_{4,l,n-4-l}$, where $1 \le l \le n-5$;

(5) If $2 \le k \le n-5$ and $U \in \mathcal{U}^L(n,k)$, then $W_p(U) \ge n-3$.

It is worth noting that, for $2 \le k \le n-5$, the extremal unicyclic graphs of Theorem 3.11 were also characterized in [34].

Now let $\mathcal{U}^M(n,\Delta)$ be the set of unicyclic graphs on n vertices with maximum degree Δ. Clearly, $2 \le \Delta \le n-1$. It is easy to see that $\mathcal{U}^M(n,2) = \{C_n\}$ and $\mathcal{U}^M(n,n-1) = \{C_3(n-3)\}$. For $3 \le \Delta \le n-2$, we have the following theorem.

Theorem 3.12 ([34]) *Let $U \in \mathcal{U}^M(n,\Delta)$ and $n \ge 7$.*

(1) If $3 \le \Delta < \lceil \frac{n}{2} \rceil$, then $W_p(U) \ge n-3$.

(2) If $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$, then $W_p(U) \ge n-4$ with equality if and only if $U \cong C^1_{3,n-4,1}$ or $C_4(n-4)$ if $\Delta = n-2$, and $U \cong C^2_{4,\Delta-2,n-2-\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta \le n-3$.

Since $W_p(C_n) = n$ and $W_p(C_3(n-3)) = 0$ for $n \geq 7$, Theorem 3.12 determines the minimum Wiener polarity index in $\mathcal{U}^M(n, \Delta)$ for arbitrary Δ. The extremal unicyclic graphs for $3 \leq \Delta < \lceil \frac{n}{2} \rceil$ of Theorem 3.12 were also characterized in [34].

Next let $\mathcal{U}^D(n, d)$ be the set of unicyclic graphs with order n and diameter d. For $d \geq 3$, we first introduce the following graphs defined in [44]:

Let $U_3(s, t)$ $(s+t = n-d-3)$ be a unicyclic graph, obtained from a path $P = v_0v_1 \ldots v_d$ of length d by adding s pendant vertices to v_1, t pendant vertices to v_{d-1}, and identifying a vertex of a triangle with v_1 or v_{d-1} (see Figure 5).

Figure 5: The unicyclic graphs $U_3(s, t)$.

Let $U_3'(a_1', a_2', a_3')$ $(a_1' + a_2' + a_3' = n - d - 2)$ be a unicyclic graph in $\mathcal{U}^D(n, d)(d \geq 4)$, which is obtained from a path $P = v_0v_1 \ldots v_d$ by identifying two vertices u_2 and u_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 $a_i'(i \in [3])$ pendant vertices to w_i (see Figure 6).

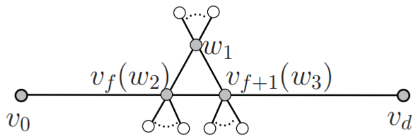


Figure 6: The unicyclic graphs $U_3'(a_1', a_2', a_3')$.

Ma, Shi and Yue [44] characterized the extremal graphs among all the unicyclic graphs with order n and diameter d.

Theorem 3.13 **([44])** *Let U be a unicyclic graph in $\mathcal{U}^D(n, d)$ $(d \geq 3)$.*

(1) If $d = 3$, then $W_p(U) \geq n - 3$ with equality if and only if $U \cong U_3(0, t)$ $(t = n - 6)$.

(2) If $d = 4$, then $W_p(U) \geq n-3$ with equality if and only if $U \cong U_3(s, t)$ $(s+t = n-7)$.

(3) If $d \geq 5$, *then* $W_p(U) \geq n-3$ *with equality if and only if* $U \cong U_3(s,t)$ $(s+t = n-d-3), C_4(P(d-2;0,n-d-1)), C_5(P(d-2;0,n-d-2))$.

Theorem 3.14 ([44]) *Let* U *be a unicyclic graph in* $\mathcal{U}^D(n,d)$ $(d \geq 4, n \geq d+8)$, *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* $|a_1' + 1 - a_i'| \leq 1$ $(i = 2, 3)$, $|a_2' - a_3'| \leq 1$, *and*

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

(2) If $d \geq 5$, *then* $U^* \cong U_3'(a_1', a_2', a_3')$ *with* $|a_i' - a_j'| \leq 1$ $(i, j \in [3])$, *and*

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

Ou, Feng and Liu [49] also determined the minimum Wiener polarity index of unicyclic graphs with any given maximum degree and girth, and characterized extremal graphs. In [54], the following theorem was shown by Wang.

Theorem 3.15 ([54]) *Let* U *be a unicyclic Hückel graph of* $2n$ *vertices, where* $n \geq 4$. *Then*

$$2n - 7 \leq W_p(U) \leq 4n + 4.$$

Du, Li and Shi [24] presented an algorithm which computes the index $W_p(G)$ for any given connected graph G on n vertices in time $O(M(n))$, where $M(n)$ denotes the time necessary to multiply two $n \times n$ matrices of small integers (which is currently known to be $O(n^2.376)$ [16]). For further results on the Wiener polarity index of other classes of graphs, one may see [46] (bicyclic graphs), [15] (cactus graphs), [8] (fullerenes and hexagonal systems), [14] (various lattices), [33,36] (some chemical structures), [5](silicate and oxide networks), [39](dendrimers), [2](polyomino chains), [3](nanostar dendrimers).

4 Graph products and the Nordhaus-Gaddum-type inequalities

4.1 Graph products

Various products of graphs often appear in the study of chemical graphs. Let G and H be two simple connected graphs. The *join* $G+H$ is defined as $V(G+H) = V(G) \cup V(H)$ and $E(G+H) = E(G) + E(H) + \{uv | u \in V(G), v \in V(H)\}$.

Definition 4.1 *Let G and H be two simple connected graphs. The Cartesian product $G \Box H$, strong product $G \boxtimes H$, lexicographic product $G[H]$, direct product $G \times H$, symmetric difference $G \triangle H$, and disjunction $G \vee H$ are defined with vertex set $V(G) \times V(H)$ and edge set as follows:*

- $E(G \Box H) = \{(a,x)(b,y) : ab \in E(G) \text{ and } x = y, \text{ or } xy \in E(G) \text{ and } a = b\}$;
- $E(G \boxtimes H) = \{(a,x)(b,y) : a = b \text{ and } xy \in E(H), \text{ or } ab \in E(G) \text{ and } x = y,$
  $\text{or } ab \in E(G) \text{ and } xy \in E(H)\}$;
- $E(G[H]) = \{(a,x)(b,y) : ab \in E(G), \text{ or } a = b \text{ and } xy \in E(H)\}$;
- $E(G \times H) = \{(a,x)(b,y) : ab \in E(G) \text{ and } xy \in E(H)\}$;
- $E(G \triangle H) = \{(a,x)(b,y) : ab \in E(G) \text{ or } xy \in E(H) \text{ not both } \}$;
- $E(G \vee H) = \{(a,x)(b,y) : ab \in E(G) \text{ or } xy \in E(H)\}$.

The *corona product* of two graphs G and H is the graph $G \circ H$ formed from one copy of G and $|G|$ copies of H where the i^{th} vertex of G is adjacent to every vertex in the i^{th} copy of H.

It is an easy fact that the Wiener polarity index of any graph with diameter less than 3 is zero. So the Wiener polarity index of join $G+H$, symmetric difference $G \triangle H$ and the disjunction $G \vee H$ are zero.

Faghani, Ashrafi, Ori [25] and Ma, Shi, Yue [45] studied the Wiener polarity index on the graph products of two non-trivial connected graphs. We list some results as follows.

For a given connected graph G, we define $W_2(G) := |\{\{u,v\} \mid d(u,v) = 2, u,v \in V(G)\}|$, which is the number of unordered pairs of vertices $\{u,v\}$ of G such that $d_G(u,v) = 2$. Note that $W_2(G)$ can be computed in polynomial time.

Theorem 4.1 ([45]) *Let G and H be two non-trivial connected graphs. Then*

(1) $W_p(G\Box H) = W_p(G)|H| + W_p(H)|G| + 2W_2(G)e(H) + 2W_2(H)e(G)$.

(2) $W_p(G \boxtimes H) = W_p(G)[2W_p(H) + 2W_2(H) + 2e(H) + |H|] + W_p(H)[2W_2(G) + 2e(G) + |G|]$.

(3) $W_p(G \times H) = 2W_p(G)W_p(H) + 2W_p(H)e(G) + 2W_p(G)e(H)$.

(4) $W_p(G[H]) = W_p(G)|H|^2$.

Theorem 4.2 ([25]) *Let G and H be two graphs. Then $W_p(G\circ H) = W_p(G)+\sum_{i=1}^{|G|} t_i + e(G)|G|^2$ in which $t_i = |\bigcup_{b\in N_G(v_i)}[N_G(b) - N_G(v_i)]| - 1$.*

4.2 The Nordhaus-Gaddum-type inequalities

Nordhaus-Gaddum-type results are bounds of the sum or the product of a parameter for a graph and its complement. For the Wiener polarity index, by Lemma 4.1, it is nontrival to consider the Nordhaus-Gaddum-type inequality of a graph G and its complement $\overline{G}$ in the case both $diam(G) = 3$ and $diam(\overline{G}) = 3$.

Lemma 4.1 ([9]) *Let G be a graph. If $diam(G) > 3$, then $diam(\overline{G}) < 3$.*

Denote by G^* and G^{**} the graphs of order $n \geq 5$ obtained from joining $n-4$ vertices to each internal vertex of the path P_4 such that $V(G^*)\setminus V(P_4)$ is a clique and $V(G^{**})\setminus V(P_4)$ is any graph of order $n-4$, respectively. Let $S^*_{a,b}$ be a graph containing a double star $S_{a,b}$, such that any two vertices both in $V(S_a)$ or both in $V(S_b)$ may be adjacent. From the definition of the Wiener polarity index, we easily obtain that

$$W_p(G^*) = 1, \quad W_p(\overline{G^*}) = 1$$

and

$$W_p(S^*_{a,b}) = (a-1)(b-1), \quad W_p(\overline{S^*_{a,b}}) = 1.$$

Zhang and Hu [58] first established the Nordhaus-Gaddum-type inequality for the Wiener polarity index of a graph G and its complement $\overline{G}$, in terms of the order of G.

Theorem 4.3 ([58]) *Let G be a graph of order $n \geq 4$, and $\overline{G}$ be its complement. If $diam(G) = 3$ and $diam(\overline{G}) = 3$, then*

$$2 \leq W_p(G) + W_p(\overline{G}) \leq \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - n + 2.$$

Moreover, the lower bound is achieved if and only if $G \cong P_4$ or G is isomorphic to some G^*; the upper bound is achieved if and only if $G \cong S^*_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ or $\overline{G} \cong S^*_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

A better lower bound was given by Hua and Das [32].

Theorem 4.4 ([32]) *Let G be a connected graph with a connected complement $\overline{G}$. Then* $d + \overline{d} - 4 \leq W_p(G) + W_p(\overline{G}) \leq \frac{n(n-1)(n-2)^2}{2} + 2m^2 + (n - \frac{3}{2})[\frac{2(m-\Delta)^2}{n-2} - \Delta(n - \Delta)] - \frac{m}{2}(4n^2 - 19n + 17) - 2[\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)(\Delta_2-\delta)^2}{(n-1)^2}]$, *where d and $\overline{d}$ are the diameter of G and $\overline{G}$, Δ, Δ_2 and δ are the maximum degree, the second maximum degree and the minimum degree in G, respectively. Moreover, the lower bound holds if and only if $G \cong P_n$ or $G \cong G^{**}$ or $d = \overline{d} = 2$.*

By Theorem 2.1, One can easily check that $W_p(T) + W_p(\overline{T}) \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - n + 2$ among all trees of order n. In addition, Zhang and Hu [58] proved

$$W_p(G) + W_p(\overline{G}) \leq \begin{cases} \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - n + 2, & \text{if } \ n \leq 8; \\ \lfloor \frac{(n-3)^2}{3} \rfloor, & \text{if } \ n \geq 9 \end{cases}$$

for any unicyclic graph of order n.

5 The relation between the Wiener polarity index and other indices

First we recall some of the best known chemical indices. The *Wiener index* $W(G)$ is defined as [30]

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

and the *hyper-Wiener index* $WW(G)$ is defined as [47]

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

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as [29]

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v) \text{ and } M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The *Hosoya index* of a graph, denoted by $Z(G)$, is defined to be the total number of matchings, that is,

$$Z(G) = \sum_{k \geq 0} m(G;k),$$

where $m(G;k)$ is the number of k-matchings in G for $k \geq 1$, and $m(G;0) = 1$.

Liu and Liu [40] discussed the relation between the Wiener polarity index and the Zagreb, Wiener, hyper-Wiener indices.

Theorem 5.1 ([40]) *Let G be a graph with order n and size m. Then*

$$W_p(G) \leq M_2(G) - M_1(G) + m$$

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

Theorem 5.2 ([40]) *If G is a triangle- and quadrangle-free connected graph, whose order is n and size is m, then*

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

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

Theorem 5.3 ([40]) *If G is a triangle- and quadrangle-free connected graph, whose order is n and size is m, then*

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

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

Behmarama, Yousefi-Azari, Ashrafi [8] and Tratnik [52] determined the relation between the Wiener polarity index and the first and second Zagreb indices of connected graphs.

Theorem 5.4 ([8]) *Suppose G is a connected triangle- and quadrangle- free graph such that its different cycles have at most one common edge. Let $N_p(G)$ and $N_h(G)$ denote the number of pentagons and hexagons of G. Then*

$$W_p(G) = M_2(G) - M_1(G) - 5N_p(G) - 3N_h(G) + e(G).$$

The set of all cycles of length k in G is denoted as $C_k(G)$. Let G be a graph without cycles of length 3. If G has at least one cycle of length 4, then we define

$$f(G) = \sum_{C=u_1u_2u_3u_4u_1 \in C_4(G)} (d_G(u_1) + d_G(u_2) + d_G(u_3) + d_G(u_4) - 8).$$

Otherwise, $f(G) = 0$.

Theorem 5.5 ([52]) *Let G be a connected graph without cycles of length 3. Moreover, suppose that any two distinct cycles $C_1, C_2 \in C_4(G) \cup C_5(G) \cup C_6(G)$ have at most two common edges and any two cycles $C_1', C_2' \in C_4(G)$ have at most one common edge. Then it holds*

$$W_p(G) = M_2(G) - M_1(G) - f(G) - 4|C_4(G)| - 5|C_5(G)| - 3|C_6(G)| + e(G).$$

By Theorems 5.4 and 5.5, Behmarama, Yousefi-Azari, Ashrafi [8] and Tratnik [52] determined the Wiener polarity index for some special graphs, such as catacondensed hexagonal systems, hexagonal cacti, polyphenylene chains, phenylenes and catacondensed benzenoid graphs.

Hua and Das [32] established some upper bounds on the Wiener polarity index in terms of the Hosoya index, independence number and the first Zagreb index.

Theorem 5.6 ([32]) *Let G be a connected triangle-free graph of order n and size m with independence number $\alpha(G)$. Then*

$$W_p(G) < \frac{1}{3}\left[\frac{n(n-1)}{2}\alpha(G) + m - M_1(G)\right].$$

Theorem 5.7 ([32]) *Let G be a connected graph of order n and size m. Then*

$$W_p(G) \leq Z(G) - 1 - m$$

with equality if and only if $G \cong C_3$ or S_n or a double-star.

Theorem 5.8 ([32]) *Let G be a connected graph of size m. Then $W_p(G) = Z(G) - m - 2$ with equality if and only if $G \cong P_5$ or $C_3(1)$.*

In [7], the relation between the Wiener polarity index and the Zagreb indices, the Wiener index are also considered for various graphs.

6 Generalizations of the Wiener polarity index

For $k \geq 1$, the *generalized Wiener polarity index* is defined as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is k [35]. This is denoted by

$$W_k(G) = |\{(u, v)|d(u, v) = k, u, v \in V\}|.$$

To generalize Theorem 5.1 for $k \geq 4$. Lei, Li, Shi and Wang [37] defined a generalization of the Zagreb indices

$$M_k(G) = \sum_{d(u,v)=k-1} d_G(u)d_G(v)$$

for $k \geq 3$. and proved the following result.

Theorem 6.1 **([37])** *For a tree T and integer $k \geq 3$, we have*

$$W_k(T) = (-1)^k \left(\frac{k-1}{2} M_1(T) + \sum_{i=2}^{k-1} (-1)^{i+1}(k-i)M_i(T) - (n-1) \right).$$

Given a positive integer $k \geq 3$, we define a t-*broom* ($t \geq 2$) as follows. For even $k \geq 4$, define a t-broom to be a graph consisting of a central vertex v with t 'brooms' attached, each consisting of a path of length $(k-2)/2$ with leaves attached to the ends opposite v. In this way, the leaves of different brooms will be at distance k. For odd $k \geq 3$, to define a t-broom, take a copy of K_t and attach a broom to each vertex, adjusting the length of the path (See Figure 7).

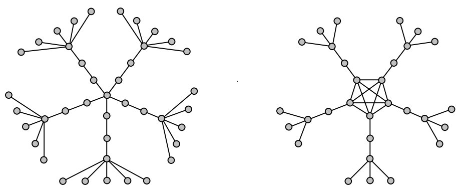


Figure 7: A 5-broom for $k = 8$ and a 5-broom for $k = 7$.

For a tree T, $W_k(T)$ is just the number of paths with length k in T. If the diameter of T is less than k, then $W_k(T) = 0$. Thus the minimum value of $W_k(T)$ is zero, achieved by all trees with $diam(T) < k$. In [13, 35], the authors obtained the maximum value of $W_k(T)$. A linear algorithm for computing $W_k(T)$ was also designed by Ilić and Ilić [35].

Theorem 6.2 ([13, 35]) *For a tree T of order n and every integer k, there is a t such that the maximal value of $W_k(T)$ is attained for a t-broom. If k is odd, then $t = 2$. If k is even, then t is within 1 of* $\frac{1}{4} + \sqrt{\frac{1}{16} + \frac{n-1}{k-2}}$.

In [53], Tyomkyn and Uzzell independently introduced the same concept, where they considered it as a new Turán-type problem on distances of graphs: determining the maximum number of paths with length k in a tree T on n vertices. Bollobás et al. studied the case of path with a given length [1,10–13]. In [11], it is shown that if $10 \leq \binom{k}{2} \leq m < \binom{k+1}{2}$, then the number of paths of length three in graph G of size m is at most $2m(m-k)(k-2)/k$. In [12], the maximum number of paths of length four of graph G of size m, denoted by $p_4(m)$, is determined.

Theorem 6.3 ([12]) *If m is sufficiently large, then*

$$p_4(m) = p_4(G_m) = \begin{cases} \frac{m^3}{8} - \frac{3m^2}{4} + m, & \text{if } m \text{ is even;} \\ \frac{m^3}{8} - \frac{7m^2}{8} + \frac{15m}{8} - \frac{9}{8}, & \text{if } m \text{ is odd.} \end{cases}$$

and G_m is the unique extremal graph. Here G_m is the complete bipartite graph $K_{\frac{m}{2},2}(m \geq 2)$ if m is even; or the complete bipartite graph $K_{\frac{m-1}{2},2}(m \geq 3)$ if m is odd.

Yue, Lei and Shi [56] characterized the extremal trees with respect to the generalized Wiener polarity index among all trees of order n and diameter d.

Let G be a graph and v a vertex of G. A *hanging tree* on the vertex v of G, denoted by $T[v]$, is a rooted tree whose root is the vertex v, and all other vertices are not in $V(G)$. These vertices of $T[v]$ at distance t from v have *height* t and form the t-th *level* of T. Let $h_{\max}(T[v])$ be the maximum height of a rooted tree $T[v]$.

Suppose $d \geq 2k - 3$. We construct a family of graphs as follows. Take a underlying path of length d, say $P = v_0v_1 \ldots v_d$. Let $T[v_i]$ be a hanging tree on the vertex v_i of P with diameter at most $k-1$ for $i \in [d-1]$, and for any nontrivial $T[v_i]$ and $T[v_j]$ with $0 < j - i \leq k - 2$, the following hold:

(1) $h_{\max}(T[v_i]) + h_{\max}(T[v_j]) \leq k + i - j - 1$;

(2) $\min\{h_{\max}(T[v_i]) + i, h_{\max}(T[v_i]) + d - i\} \leq k - 1$;

(3) $s_1 + s_2 + \cdots + s_{d-1} = n - d - 1$, where s_i is the number of vertices of root tree $T[v_i]$ different from the root v_i for $i \in [d-1]$.

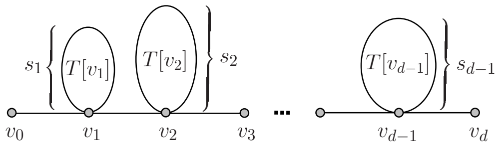


Figure 8: A graph in $\mathcal{T}^1(s_1, \ldots, s_{d-1})$.

Denoted the family of graphs by $\mathcal{T}^1(s_1, \ldots, s_{d-1})$, which is shown in Figure 8. Note that s_i may be 0.

Let $4 \leq k \leq d \leq 2k-4$, we construct another family of graphs as follows. Take a underlying path of length d, say $P = v_0 v_1 \ldots v_d$. Let $T[v_i]$ be a hanging tree on the vertex v_i of P with diameter at most $k-1$ for $i \in [d-1]$, and for any nontrivial $T[v_i]$ and $T[v_j]$ with $0 < j - i \leq k-2$, the following hold:

(1) $h_{\max}(T[v_i]) + h_{\max}(T[v_j]) \leq k + i - j - 1$;

(2) $\max\{h_{\max}(T[v_i]) + i, h_{\max}(T[v_i]) + d - i\} \leq k - 1$;

(3) $s_1 + s_2 + \cdots + s_{d-1} = n - d - 1$, where s_i is the number of vertices of root tree $T[v_i]$ different from the root v_i for $i \in [d-1]$.

The family of graphs is denoted by $\mathcal{T}^2(s_1, \ldots, s_{d-1})$.

Theorem 6.4 ([56]) *Let T be a tree on n vertices with a given diameter d.*

(1) If $d \geq 2k-3$, then

$$W_k(T) \geq n - k.$$

The equality holds if and only if $T \in \mathcal{T}^1(s_1, \ldots, s_{d-1})$.

(2) If $k \leq d \leq 2k-4$, then

$$W_k(T) \geq d + 1 - k.$$

The equality holds if and only if $T \in \mathcal{T}^2(s_1, \ldots, s_{d-1})$.

To state the maximum generalized Wiener polarity index of trees with a given diameter. First, we introduce a family of graphs, denoted by $\mathcal{T}(n,p)$, which is obtained from a p-broom ($p \geq 2$) with $n - (d - k + 2)$ vertices by attaching two pendant paths of length s and t, respectively, to two different ends opposite the central vertex in p-broom, where $s, t \geq k-1$, $s + t = d - k + 2$ and $p = 2$ when k is odd.

Theorem 6.5 **([56])** *Let T be a tree on n vertices with a given diameter $d \geq 3k-4$.*

(1) If k is odd, then $W_k(T) \leq \lfloor \frac{n-d-1}{2} \rfloor \lceil \frac{n-d-1}{2} \rceil + (2n-d-k-1)$. The equality holds when $T \in \mathcal{T}(n,p)$.

(2) If k is even, then $W_k(T) \leq W_k(T^*)$, where $T^* \in \mathcal{T}(n,p)$ and p is near to

$$\frac{1}{4} + \sqrt{\frac{17}{16} + \frac{n-d-1}{k-2}}.$$

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