

## The Hyper-Wiener Polynomial of Graphs

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ABSTRACT. The distance  $d(u, v)$  between two vertices  $u$  and  $v$  of a graph  $G$  is equal to the length of a shortest path that connects  $u$  and  $v$ . Define  $WW(G, x) = 1/2 \sum_{\{a,b\} \subseteq V(G)} x^{d(a,b)+d^2(a,b)}$ , where  $d(G)$  is the greatest distance between any two vertices. In this paper the hyper-Wiener polynomials of the Cartesian product, composition, join and disjunction of graphs are computed.

**Keywords:** Hyper-Wiener polynomial, graph operation.

**2000 Mathematics subject classification:** 05C12, 05A15, 05A20, 05C05.

### 1. INTRODUCTION

All graphs we consider are assumed to be finite, connected, and to have no loops or multiple edges. The vertex and the edge sets of a graph  $G$  are denoted by  $V(G)$  and  $E(G)$ , respectively. The distance between any two vertices  $u$  and  $v$  in  $V(G)$  is denoted by  $d(u, v)$  and it is defined as the number of edges in a minimal path connecting the vertices  $u$  and  $v$ . The greatest distance between any two vertices of  $G$  is called diameter of  $G$ . It is denoted by  $d(G)$ . The Wiener index is one of the most studied topological indices defined as the sum of distances between all pairs of vertices of the respective graph, [5 – 8, 22]. In 1993, Milan Randić proposed a generalization of the Wiener index for trees. Then Klein *et al.* [18], generalized the Randić's definition for all connected

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graphs. It is defined as  $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d^2(u,v)$ , where  $d^2(u,v) = d(u,v)^2$ .

The Cartesian product  $G \times H$  of graphs  $G$  and  $H$  has the vertex set  $V(G \times H) = V(G) \times V(H)$  and  $(a,x)(b,y)$  is an edge of  $G \times H$  if  $a = b$  and  $xy \in E(H)$ , or  $ab \in E(G)$  and  $x = y$ . If  $G_1, \dots, G_n$  are graphs then we denote  $G_1 \times \dots \times G_n$  by  $\bigotimes_{i=1}^n G_i$ . In the case that  $G_1 = \dots = G_n = G$ , we denote  $\bigotimes_{i=1}^n G_i$  by  $G^n$ . The hypercube  $Q_n$  and the ladder graph  $L_n$  are defined as the Cartesian product of  $n$  copies of  $K_2$  and  $K_2 \times P_n$ , respectively. Let  $G$  and  $H$  be two graphs with disjoint vertex sets  $V(G)$  and  $V(H)$  and edge sets  $E(G)$  and  $E(H)$ . The join  $G + H$  is the graph with vertex set  $V(G + H) = V(G) \cup V(H)$  together with all the edges joining vertices  $V(G)$  and  $V(H)$ . If  $A = \underbrace{H + \dots + H}_{n \text{ times}}$ ,

then we denote  $A$  by  $nH$ . The composition  $G[H]$  is the graph with vertex set  $V(G) \times V(H)$  and  $u = (u,v)$  is adjacent with  $v = (a,b)$  whenever  $(u$  is adjacent with  $a)$  or  $(u = a$  and  $v$  is adjacent with  $b)$ , see [10, p. 22].

The power graph  $G^{(k)}$  of graph  $G$  has vertex set  $V(G^{(k)}) = V(G)$  and  $xy \in E(G^{(k)})$  if  $d_G(x,y) \leq k$ .

Consider two arbitrary graphs  $G$  and  $H$ . The disjunction  $G \vee H$  is the graph with vertex set  $V(G) \times V(H)$  and  $(u_1, v_1)$  is adjacent with  $(u_2, v_2)$  whenever  $u_1 u_2 \in E(G)$  or  $v_1 v_2 \in E(H)$ .

The Wiener index of the Cartesian product graphs was studied in [9, 20]. Klavžar, *et al.* [15] computed the Szeged index of the Cartesian product graphs and one of us (ARA) computed exact formulae for the vertex PI, edge PI, first Zagreb, second Zagreb, hyper-Wiener and edge Szeged indices of Cartesian product, composition, join, disjunction and symmetric difference of graphs, see [11 – 14, 23] for details.

Sagan *et al.* [20] computed exact expressions for the Wiener polynomial of various graph operations. The aim of this paper is to continue this program by computing the hyper-Wiener index of these operations on graphs.

We encourage the reader to consult [2 – 4] and [16, 17, 19, 24] for the mathematical properties of hyper-Wiener index and its applications in chemistry. We state without proof the following theorem which is crucial throughout the paper.

**Theorem 1-1.** Let  $G$  and  $H$  be graphs. Then we have:

- (a)  $|V(G \times H)| = |V(G \vee H)| = |V(G[H])| = |V(G \oplus H)| = |V(G)||V(H)|$  and  $|E(G \times H)| = |E(G)||V(H)| + |V(G)||E(H)|$ ,
- (b)  $G \times H$  is connected if and only if  $G$  and  $H$  are connected,
- (c) If  $(a,x)$  and  $(b,y)$  are vertices of  $G \times H$  then  $d_{G \times H}((a,x), (b,y)) = d_G(a,b) + d_H(x,y)$ ,

(d) The Cartesian product, join, composition, disjunction and symmetric difference of graphs are associative and all of them are commutative except for composition.

(e) If  $G$  is connected and  $|V(G)| > 1$  then for every vertices  $(u_1, v_1), (u_2, v_2) \in V(G[H])$  we have:

$$d_{G[H]}((u_1, v_1), (u_2, v_2)) = \begin{cases} d_G(u_1, u_2) & u_1 \neq u_2 \\ 0 & u_1 = u_2 \text{ \& } v_1 = v_2 \\ 1 & u_1 = u_2 \text{ \& } v_1 v_2 \in E(H) \\ 2 & u_1 = u_2 \text{ \& } v_1 v_2 \notin E(H) \end{cases} .$$

$$(f) \quad d_{G+H}(u, v) = \begin{cases} 0 & u = v \\ 1 & uv \in E(G) \cup E(H) \text{ or } (u \in V(G) \text{ \& } v \in V(H)) \\ 2 & \text{otherwise} \end{cases} .$$

(g) If  $G$  and  $H$  are connected graphs then

$$d_{G \oplus H}((a, b), (c, d)) = \begin{cases} 0 & a = c \text{ \& } b = d \\ 1 & ac \in E(G) \text{ or } bd \in E(H) \text{ but not both} \\ 2 & \text{otherwise} \end{cases} .$$

(h) If  $G$  and  $H$  are connected graphs then

$$d_{G \vee H}((a, b), (c, d)) = \begin{cases} 0 & a = c \text{ \& } b = d \\ 1 & ac \in E(G) \text{ or } bd \in E(H) \\ 2 & \text{otherwise} \end{cases} .$$

**Definition 1-2.** Let  $G$  be a graph. The hyper-Wiener polynomial of  $G$  is defined as  $WW(G, x) = \frac{1}{2} \sum_{\{a,b\} \subseteq V(G)} x^{d(a,b)+d^2(a,b)}$ .

It is easy to see that  $WW'(G, 1) = WW(G)$ ,  $WW(G, 1) = \binom{n}{2}$  and  $WW(G, x) = \sum_{j=1}^{d(G)} n_G(j) x^{j(j+1)}$ , where  $n_G(j) = |\{a, b\} | d(a, b) = j\}$ .

**Lemma 1-3.** (a)  $WW(K_n, x) = \binom{n}{2} x^2$ .

$$(b) \quad WW(P_n, x) = \sum_{j=1}^{n-1} (n-j) x^{j(j+1)}.$$

$$(c) \quad WW(C_n, x) = \begin{cases} \sum_{j=1}^{\frac{n}{2}-1} n x^{j(j+1)} + \frac{n}{2} x^{n(n+2)/4} & n \text{ is even} \\ \sum_{j=1}^{\frac{n+1}{2}} x^{j(j+1)} & n \text{ is odd} \end{cases} .$$

$$(d) \quad WW(L_n, x) = (3n-2)x^2 + \sum_{k=2}^n (2k-3)x^{(n-k-2)(n-k-1)}.$$

$$(e) \quad WW(Q_n, x) = \sum_{k=1}^n \binom{n}{k} x^{k(k+1)}.$$

Throughout this paper our notation is standard and taken mainly from the standard books of graph theory and [4, 21].  $K_n$ ,  $P_n$ ,  $C_n$  denote the complete graph, The path and the cycle on  $n$  vertices respectively. For a real number  $x$ ,  $[x]$  denotes the greatest integer less than or equal to  $x$ .

## 2. MAIN RESULTS

In this section, exact expressions for the hyper-Wiener polynomials of composition, Cartesian product, join, disjunction symmetric difference and power of graphs are computed.

**Theorem 2-1.** Suppose  $G_1$  and  $G_2$  are graphs with  $|V(G_1)| = n_1$ ,  $|V(G_2)| = n_2$ ,  $|E(G_1)| = m_1$  and  $|E(G_2)| = m_2$ . If  $G_1$  is connected then  $WW(G_1[G_2], x) = n_2^2 WW(G_1, x) + \frac{1}{2}n_2m_2x^2 + \frac{1}{2}n_1\left(\binom{n_2}{2} - m_2\right)x^6$ .

**Proof.** By Theorem 1-1(e),

$$\begin{aligned}
 WW(G_1[G_2], x) &= \frac{1}{2} \sum_{\{(u_1, v_1), (u_2, v_2)\}} x^{d_{G_1[G_2]}((u_1, v_1), (u_2, v_2)) + d_{G_1[G_2]}^2((u_1, v_1), (u_2, v_2))} \\
 &= \frac{1}{2} \sum_{u_1 \neq u_2} x^{d_{G_1[G_2]}((u_1, v_1), (u_2, v_2)) + d_{G_1[G_2]}^2((u_1, v_1), (u_2, v_2))} \\
 &+ \frac{1}{2} \sum_{\substack{v_1 v_2 \in E(G_2) \\ u_1 = u_2}} x^2 + \frac{1}{2} \sum_{\substack{v_1 v_2 \notin E(G_2) \\ u_1 = u_2}} x^6 \\
 &= \frac{1}{2} \sum_{u_1 \neq u_2} n_2^2 x^{d_{G_1}(u_1, u_2) + d_{G_1}^2(u_1, u_2)} + \frac{1}{2} n_1 m_2 x^2 \\
 &+ \frac{1}{2} n_1 \left( \binom{n_2}{2} - m_2 \right) x^6 \\
 &= n_2^2 WW(G_1, x) + \frac{1}{2} n_2 m_2 x^2 + \frac{1}{2} n_1 \left( \binom{n_2}{2} - m_2 \right) x^6. \quad \square
 \end{aligned}$$

**Theorem 2-2.** Let  $G$  and  $H$  be graphs with  $n_1 = |V(G)|$ ,  $n_2 = |V(H)|$ ,  $m_1 = |E(G)|$  and  $m_2 = |E(H)|$ . Then

$$WW(G \vee H, x) = \frac{1}{2} (n_1^2 m_2 + n_2^2 m_1 - 2m_1 m_2) x^2 + \frac{1}{2} \left[ \binom{n_1 n_2}{2} - n_1^2 m_2 - n_2^2 m_1 + 2m_1 m_2 \right] x^6.$$

**Proof.** The proof is straightforward and follows from Lemma 1-1(h).  $\square$

**Theorem 2-3.** Let  $G$  and  $H$  be graphs with  $n_1 = |V(G)|$ ,  $n_2 = |V(H)|$ ,  $m_1 = |E(G)|$  and  $m_2 = |E(H)|$ . Then

$$WW(G \oplus H, x) = \frac{1}{2} (n_1^2 m_2 + n_2^2 m_1 - 4m_1 m_2) x^2 + \frac{1}{2} \left[ \binom{n_1 n_2}{2} - n_1^2 m_2 - n_2^2 m_1 + 4m_1 m_2 \right] x^6.$$

**Proof.** The proof is straightforward and follows from Lemma 1-1(g).  $\square$

**Theorem 2-4.** Let  $G_1, G_2, \dots, G_k$  be graphs with  $n_i = |V(G_i)|$  and  $m_i = |E(G_i)|$ ,  $1 \leq i \leq k$ . Then

$$WW(G_1 + G_2 + \dots + G_k) = \frac{1}{2} \left[ \sum_{i=1}^k m_i + \sum_{i \neq j} n_i n_j \right] x^2 + \frac{1}{2} \sum_{i=1}^k \left[ \binom{n_i}{2} - m_i \right] x^6.$$

In particular, if  $G$  is a graph with  $n$  vertices and  $m$  edges then  $WW(kG, x) = \frac{1}{2}[km + \binom{k}{2}n^2]x^2 + \frac{1}{2}[\binom{n}{2} - m]x^6$ .

**Proof.** By Lemma 1-1(f), we have  $WW(G_1 + G_2, x) = \frac{1}{2} \sum_{u \in V(G_1), v \in V(G_2)} x^2 + \frac{1}{2} \sum_{uv \in E(G_1)} x^2 + \frac{1}{2} \sum_{uv \in E(G_2)} x^2 + \frac{1}{2} \sum_{uv \notin E(G_1)} x^6 + \frac{1}{2} \sum_{uv \notin E(G_2)} x^6 = \frac{1}{2}[n_1n_2 + m_1 + m_2]x^2 + \frac{1}{2}[(\binom{n_1}{2}) + (\binom{n_2}{2}) - m_1 - m_2]x^6$ . We now apply an inductive argument to complete the proof.  $\square$

**Corollary 2-5.** The following equations hold:

- a)  $WW(W_{n+1}, x) = nx^2 + \frac{1}{2}[\binom{n}{2} - n]x^6$ ,
- b)  $WW(S_{n+1}, x) = \frac{1}{2}nx^2 + \frac{1}{2}\binom{n}{2}x^6$ ,
- c)  $WW(K_{n_1, n_2, \dots, n_k}, x) = \frac{1}{2}\binom{k}{2}x^2 + \frac{1}{2}[\sum_{i=1}^k \binom{n_i}{2}]x^6$ ,
- d)  $WW(C_n + C_n), x) = \frac{1}{2}(2n + n^2)x^2 + [\binom{n}{2} - n]x^6$

**Theorem 2-6.** Suppose  $G$  and  $H$  are graphs and  $d = d(G) + d(H)$ . Then

$$WW(G \times H, x) = \frac{1}{2} \sum_{k=1}^d \left[ \sum_{j=1}^{k-1} 2n_G(j)n_H(k-j) + |V(G)|n_H(k) + |V(H)|n_G(k) \right] x^{k(k+1)},$$

where  $n_G(k)$  denotes the number of pairs in  $G$  with distance  $k$ . The quantity  $n_H(k)$  is defined analogously.

**Proof.** By Lemma 1-1(a), we have  $d_{G \times H}((a, x), (b, y)) = d_G(a, b) + d_H(x, y)$ . Thus,

$$\begin{aligned} n_{G \times H}(k) &= |\{(a, x), (b, y) \mid d_{G \times H}((a, x), (b, y)) = k\}| \\ &= |\{(a, x), (b, y) \mid d_G(a, b) + d_H(x, y) = k\}| \\ &= |\{(a, x), (b, y) \mid d_G(a, b) = j, d_H(x, y) = k - j, j = 0, 1, \dots, k\}| \\ &= \sum_{j=0}^k 2n_G(j)n_H(k-j) \\ &= |V(G)|n_H(k) + |V(H)|n_G(k) + \sum_{j=1}^{k-1} 2n_G(j)n_H(k-j), \end{aligned}$$

which completes the proof.  $\square$

**Theorem 2-7.** Let  $G$  be a graph then the hyper Wiener polynomial of  $G^{(k)}$  is given by

$$\begin{aligned} WW(G^{(k)}) &= \sum_{i=0}^{\lfloor n/k \rfloor - 1} \sum_{j=1}^k n_G(j + ik)x^{(i+1)(i+2)} \\ &\quad + (n_G(1 + \lfloor n/k \rfloor k) + \dots + n_G(n))x^{(\lfloor n/k \rfloor + 1)(\lfloor n/k \rfloor + 2)}, \end{aligned}$$

where  $n \geq k$ , and  $n_G(n+1) = n_G(n+2) = \dots = 0$ . If  $k|n$  then the hyper Wiener polynomial of  $G^k$  becomes  $\sum_{i=1}^{\lfloor n/k \rfloor} \sum_{(i-1)k+1 \leq j \leq ik} n_G(j)x^{i(i+1)}$ .

**Proof.** By definition of the power graph  $G^{(k)}$ ,  $V(G^{(k)}) = V(G)$  and for every vertex  $a, b \in V(G)$   $a$  and  $b$  are adjacent if and only if  $d_G(a, b) \leq k$ . There are  $n_G(1)$  pair of vertices at distance 1 (edges),  $n_G(2)$  vertices at distance 2,  $\dots$  and,  $n_G(k)$  vertices that are at distance  $k$ . These vertices become at distance one in  $G^{(k)}$ . Hence the coefficient of  $x$  is  $\sum_{j=1}^k n_G(j)$  in  $G^{(k)}$ . One can generalize this idea by taking the distinct pairs of vertices in  $G$  whose distances are in the set  $A_i = \{ik + j, j = 1, 2, \dots, k\}$ , where  $0 \leq i \leq \lfloor n/k \rfloor - 1$ . There are  $n_G(ik + 1) + \dots + n_G(ik + k)$  distinct pairs of vertices in  $G$  whose distances are in  $A_i$ . These distinct pairs of vertices become at distance  $i + 1$  in  $G^{(k)}$ . Hence we have  $n_G(ik + 1) + \dots + n_G(ik + k)$  distinct pairs of vertices in  $G^{(k)}$  that are at distance  $i + 1$ . This gives the hyper Wiener polynomial of  $G^{(k)}$ .  $\square$

**Corollary 2-8.** The hyper Wiener polynomials of the graphs  $P_n^{(k)}$ ,  $C_{2n+1}^{(k)}$ ,  $C_{2n}^{(k)}$ ,  $L_n^{(k)}$  and  $Q_n^{(k)}$  are given by the following polynomials:

$$\begin{aligned}
 a) \quad & WW(P_n^{(k)}; x) = \sum_{i=1}^{\lfloor (n-1)/k \rfloor} \frac{k}{2} (2n - (2i-1)k - 1) x^{i(i+1)} \\
 & + \frac{1}{2} (n-1 - \lfloor \frac{n-1}{k} \rfloor k) (n - \lfloor \frac{n-1}{k} \rfloor k) x^{(\lfloor \frac{n-1}{k} \rfloor k + 1)(\lfloor \frac{n-1}{k} \rfloor k + 2)}, \\
 b) \quad & WW(C_{2n+1}^{(k)}; x) = \sum_{i=1}^{\lfloor n/k \rfloor} (2n+1) k x^{i(i+1)} \\
 & + (n - \lfloor \frac{n}{k} \rfloor k) (2n+1) x^{(\lfloor n/k \rfloor + 1)(\lfloor n/k \rfloor + 2)}, \\
 c) \quad & WW(C_{2n}^{(k)}; x) = \sum_{i=1}^{\lfloor \frac{n-1}{k} \rfloor} (2n) k x^{i(i+1)} \\
 & + (n - \lfloor \frac{n-1}{k} \rfloor k) (2n) x^{(\lfloor \frac{n-1}{k} \rfloor + 1)(\lfloor \frac{n-1}{k} \rfloor + 2)}, \\
 d) \quad & WW(L_n^{(k)}; x) = \frac{1}{2} [2k(2n-k) - nx^2 \\
 & + \sum_{i=2}^{\lfloor \frac{n}{k} \rfloor} 2k(2n + (1-2i)k) x^{i(i+1)} + 2(n - \lfloor \frac{n}{k} \rfloor k)^2 x^{(\lfloor n/k \rfloor + 1)(\lfloor \frac{n}{k} \rfloor + 2)}], \\
 e) \quad & WW(Q_n^{(k)}; x) = \sum_{i=0}^{\lfloor \frac{n}{k} \rfloor - 1} \sum_{j=1}^k \binom{n}{j+ik} 2^{n-1} x^{i(i+1)} \\
 & + \left( \binom{n}{1+k\lfloor \frac{n}{k} \rfloor} + \binom{n}{2+k\lfloor \frac{n}{k} \rfloor} + \dots + \binom{n}{n} \right) x^{(\lfloor \frac{n}{k} \rfloor + 1)(\lfloor \frac{n}{k} \rfloor + 2)}.
 \end{aligned}$$

**Proof.** a) By Theorem 2-2, the coefficient of  $x^{i(i+1)}$  in  $P_n^{(k)}$  is as follows:

$$n - (i-1)k - 1 + (n - (i-1)k - 2) + \dots + (n - ik) = \frac{k}{2} (2n - (2i-1)k - 1).$$

Also, the coefficient of  $x^{(\lfloor \frac{n-1}{k} \rfloor + 1)(\lfloor \frac{n-1}{k} \rfloor + 2)}$  is

$$(n - \lfloor \frac{n-1}{k} \rfloor k)(n - \lfloor \frac{n-1}{k} \rfloor k - 1) + \dots + 1 = \frac{1}{2}(n - \lfloor \frac{n-1}{k} \rfloor k)(n - \lfloor \frac{n-1}{k} \rfloor k + 1).$$

Proof of other parts are the same.  $\square$

**Corollary 2-9.** The hyper Wiener indices of the graphs  $P_n^{(k)}$ ,  $C_{2n+1}^{(k)}$ , and  $C_{2n}^{(k)}$  are given by the following formulae:

$$\begin{aligned} a ) \quad WW(P_n^{(k)}) &= \frac{k(k-1)}{2} \lfloor \frac{n-1}{k} \rfloor^4 + (\frac{3}{2}k^2 + \frac{2}{3}n - kn - \frac{5}{6}k - \frac{1}{3}) \lfloor \frac{n-1}{k} \rfloor^3 \\ &+ (k^2 + \frac{1}{2}n^2 + k - 1 + \frac{3}{2}n - 3kn) \lfloor \frac{n-1}{k} \rfloor^2 \\ &+ (k + \frac{3}{2}n^2 - \frac{1}{6}n - 2kn - \frac{2}{3}) \lfloor \frac{n-1}{k} \rfloor - n \\ b ) \quad WW(C_{2n+1}^{(k)}) &= \frac{-2}{3}kn(\lfloor \frac{n}{k} \rfloor + 1) - \frac{1}{3}k(\lfloor \frac{n}{k} \rfloor + 1) + \frac{2}{3}kn(\lfloor \frac{n}{k} \rfloor + 1)^3 \\ &+ (1/3)k(\lfloor \frac{n}{k} \rfloor + 1)^3 + (n - \lfloor \frac{n}{k} \rfloor k)(2n + 1)(\lfloor \frac{n}{k} \rfloor^2 + 3\frac{n}{k} + 2) \\ c ) \quad WW(C_{2n}^{(k)}) &= \frac{-2}{3}kn(\lfloor \frac{n-1}{k} \rfloor + 1) \\ &+ \frac{2}{3}kn(\lfloor \frac{n-1}{k} \rfloor + 1)^3 + 2(n - 1 - \lfloor \frac{n-1}{k} \rfloor k)n + n(\lfloor \frac{n-1}{k} \rfloor + 1)(\lfloor \frac{n-1}{k} \rfloor + 2) \end{aligned}$$

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