

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.

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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 $n_G(j) = |\{a, b\} \mid d(a, b) = j\}|$.

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

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

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

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

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

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),

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

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

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

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 $WW(G_1 + G_2, x) = \frac{1}{2} \sum_{u \in V(G_1), v \in V(G_2)} x^2 + \frac{1}{2} \sum_{uv \in E(G_1)} x^2 + \frac{1}{2} \sum_{uv \in E(G_2)} x^2 + \frac{1}{2} \sum_{uv \notin E(G_1)} x^6 + \frac{1}{2} \sum_{uv \notin E(G_2)} x^6 = \frac{1}{2}[n_1 n_2 + m_1 + m_2]x^2 + \frac{1}{2}[\binom{n_1}{2} + \binom{n_2}{2} - m_1 - m_2]x^6$. 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,

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

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 $x^{([\frac{n-1}{k}]+1)([\frac{n-1}{k}]+2)}$ is

$$(n - [\frac{n-1}{k}]k)(n - [\frac{n-1}{k}]k - 1) + \cdots + 1 = \frac{1}{2}(n - [\frac{n-1}{k}]k)(n - [\frac{n-1}{k}]k + 1).$$

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:

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

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