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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 $G_1, \cdots, G_n$ are graphs then we denote $G_1 \times \cdots \times G_n$ by $\bigotimes_{i=1}^n G_i$. In the case that $G_1 = ... = G_n = G$, 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 $A = \underbrace{H + \cdots + H}_{n\ times}$, 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 $u_1u_2 \in E(G)$ or $v_1v_2 \in E(H)$.

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:

$$d_{G[H]}((u_1, v_1), (u_2, v_2)) = \begin{cases} d_G(u_1, u_2) & u_1 \neq u_2 \\ 0 & u_1 = u_2 \ \& \ v_1 = v_2 \\ 1 & u_1 = u_2 \ \& \ v_1v_2 \in E(H) \\ 2 & u_1 = u_2 \ \& \ v_1v_2 \notin E(H) \end{cases} .$$

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

(g) If G and H are connected graphs then

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

(h) If G and H are connected graphs then

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

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

(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 $WW(G_1[G_2], x) = n_2^2 WW(G_1, x) + \frac{1}{2}n_2m_2x^2 + \frac{1}{2}n_1(\binom{n_2}{2} - m_2)x^6$.

Proof. By Theorem 1-1(e),

$$\begin{aligned}
WW(G_1[G_2], x) &= \frac{1}{2}\sum_{\{(u_1,v_1),(u_2,v_2)\}} x^{d_{G_1[G_2]}((u_1,v_1),(u_2,v_2))+d^2_{G_1[G_2]}((u_1,v_1),(u_2,v_2))} \\
&= \frac{1}{2}\sum_{u_1\neq u_2} x^{d_{G_1[G_2]}((u_1,v_1),(u_2,v_2))+d^2_{G_1[G_2]}((u_1,v_1),(u_2,v_2))} \\
&+ \frac{1}{2}\sum_{\substack{v_1v_2\in E(G_2)\\ u_1=u_2}} x^2 + \frac{1}{2}\sum_{\substack{v_1v_2\notin E(G_2)\\ u_1=u_2}} x^6 \\
&= \frac{1}{2}\sum_{u_1\neq u_2} n_2^2 x^{d_{G_1}(u_1,u_2)+d^2_{G_1}(u_1,u_2)} + \frac{1}{2}n_1m_2x^2 \\
&+ \frac{1}{2}n_1(\binom{n_2}{2} - m_2)x^6 \\
&= n_2^2 WW(G_1, x) + \frac{1}{2}n_2m_2x^2 + \frac{1}{2}n_1(\binom{n_2}{2} - m_2)x^6. \qquad \square
\end{aligned}$$

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

$$WW(G\vee H, x) = \frac{1}{2}(n_1^2m_2 + n_2^2m_1 - 2m_1m_2)x^2 + \frac{1}{2}\left[\binom{n_1n_2}{2} - n_1^2m_2 - n_2^2m_1 + 2m_1m_2\right]x^6.$$

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

$$WW(G\oplus H, x) = \frac{1}{2}(n_1^2m_2 + n_2^2m_1 - 4m_1m_2)x^2 + \frac{1}{2}\left[\binom{n_1n_2}{2} - n_1^2m_2 - n_2^2m_1 + 4m_1m_2\right]x^6.$$

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

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

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

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

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. □

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) $WW(K_{n_1,n_2,\cdots,n_k}, x) = \frac{1}{2}\binom{k}{2}x^2 + \frac{1}{2}[\sum_{i=1}^{k}\binom{n_i}{2}]x^6$,
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,

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

which completes the proof. □

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

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

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

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 $d_G(a, b) \le k$. There are $n_G(1)$ pair of vertices at distance 1 (edges), $n_G(2)$ vertices at distance 2, $\cdots$ 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 $A_i = \{ik + j, j = 1, 2, ..., k\}$, where $0 \le i \le [n/k] - 1$. There are $n_G(ik+1)+\cdots+n_G(ik+k)$ 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 $n_G(ik+1)+\cdots+n_G(ik+k)$ 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:

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

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

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

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. □

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:

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

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