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Hosoya Polynomial of Hierarchical Product of Graphs

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Abstract. The Hosoya polynomial of a graph G is a graphical invariant polynomial that its first derivative at $x = 1$ is equal to the Wiener index. In this paper we compute the Hosoya polynomial of the hierarchical product of graphs and give some applications of this operation.

1 Introduction

Let G be a simple connected graph, with vertex and edge sets $V(G)$ and $E(G)$, respectively. The distance between the vertices u and v of G is denoted by $d_G(u,v)$ or $d(u,v)$ which is defined as the length of a shortest path between u and v in G. The Wiener index of G is a distance-based graph invariant defined as:

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v).$$

For details on mathematical properties of the Wiener index and its chemical applications see [2, 3] and [7, 8, 17]. Motivated by the Wiener index Randić in [16] introduced an extension of the Wiener index for trees, and this has come to be known as the hyper Wiener index. Klein et al. [14] generalized this extension to cyclic structures as:

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4} \sum_{(u,v) \in V(G) \times V(G)} d(u,v)^2.$$

In [12], Hosoya introduced a distance-based graph polynomial, is called Wiener polynomial or Hosoya polynomial, as:

$$H(G,x) = \frac{1}{2} \sum_{u \in V(G)} \sum_{u \neq v \in V(G)} x^{d(u,v)}.$$

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As you see the first derivative of $H(G,x)$ at $x = 1$ is equal to the Wiener index. This polynomial is very attractive for some mathematicians and mathematical chemists [4, 5, 9, 11, 13, 15, 18]. Computing the Wiener index and the Hosoya polynomial of the graph operations have been the object of some papers. For instance, Yeh and Gutman et al. in [22] computed the Wiener index in the case of graphs that are obtained by means of certain binary operations (such as product, join, and composition) on pairs of graphs. Stevanović in [19] and Sagan et al. in [18] generalized their results and computed the Wiener polynomial of product, join, and composition of graphs. Recently in [6] Eliasi et al. introduced four new sums of graphs(is called $F-$sums) and computed the Winer indices of these new graphs. In this paper we compute the Hosoya polynomial of the hierarchical product of graphs and give some applications of this operation. For example we obtain the Hosoya polynomial of $F-$sums. Also at the end of paper we give a new proof of a result of Zhang et al. [20] on the Hosoya polynomial of hexagonal chains.

2 Generalized Hierarchical Product

The cartesian product $G\Box H$ of the graphs G and H has the vertex set $V(G\Box H) = V(G) \times V(H)$ and two vertices (g_1, h_1) and (g_2, h_2) adjoint by an edge if and only if [$g_1 = g_2$ and $h_1h_2 \in E(H)$] or [$h_1 = h_2$ and $g_1g_2 \in E(G)$].

L. Barrire, et al. in [1], defined a new product of graphs, namely generalized hierarchical product, as follows:

Definition 1. *Let G and H be two graphs with nonempty vertex subset $U \subseteq V(G)$. Then the generalized hierarchical product $G(U) \sqcap H$ is the graph with the vertex set $V(G) \times V(H)$ and two vertices (g,h) and (g',h') adjoint by an edge if and only if [$g = g' \in U$ and $hh' \in E(H)$] or [$h = h'$ and $gg' \in E(G)$].*

The following lemma gives some basic properties of the generalized hierarchical product of graphs.

Lemma 1. *(See [1]) Let G and H be graphs with $U \subseteq V(G)$. Then we have*

(a) If $U = V(G)$, then the generalized hierarchical product $G(U) \sqcap H$ is the Cartesian product of G and H,

(b) $|V(G(U) \sqcap H)| = |V(G)||V(H)|$, $|E(G(U) \sqcap H)| = |E(G)||V(H)| + |E(H)||U|$,

(c) $G(U) \sqcap H$ is connected if and only if G and H are connected,

$$\textit{(d)}\ d_{G(U)\sqcap H}((g,h),(g',h')) = \begin{cases} d_{G(U)}(g,g') + d_H(h,h') & \text{if } h \neq h' \\ d_G(g,g') & \text{if } h = h'. \end{cases}$$

Let $G = (V, E)$ be a graph and $\emptyset \neq U \subseteq V$. A path between vertices u and v through U, denoted by $\rho_{G(U)}(u,v)$, is simply a $u-v$ path of G containing some vertex $z \in U$ (vertex z could be the vertex u or v). Then, the distance through U, denoted by $d_{G(U)}(u,v)$, between u and v is the length of the shortest path $\rho_{G(U)}(u,v)$. Note that, if one of the vertices u or v belong to U, then $d_{G(U)}(u,v) = d_G(u,v)$. We define

$$\overline{H}(G(U),x) = \sum_{(u,v)\in V(G)\times V(G)} x^{d_{G(U)}(u,v)}.$$

As [18], it is sometimes more natural to express our results in terms of the ordered Hosoya polynomial defined by

$$\overline{H}(G,x) = \sum_{(u,v)} x^{d(u,v)},$$

where the sum is now over all ordered pairs (u,v) of vertices, including those $u = v$. Thus

$$\overline{H}(G,x) = 2H(G,x) + |V(G)|.$$

Using this notation, in the following theorem, we compute the Hosoya polynomial of the generalized hierarchical product.

Theorem 1. *Let G and H be graphs with $U \subseteq V(G)$. Then we have*

$$\overline{H}(G(U)\sqcap H,x) \;=\; |V(H)|\overline{H}(G,x) + \Big(\overline{H}(H,x) - |V(H)|\Big)\overline{H}(G(U),x).$$

Proof. Set $V(G) = \{g_1, g_2, \ldots, g_n\}$ and $V(H) = \{h_1, h_2, \ldots, h_m\}$. Also let $\Gamma = G(U)\sqcap H$. We have

$$\begin{aligned}
\overline{H}(\Gamma,x) &= \sum_{(u,v)\in V(\Gamma)\times V(\Gamma)} x^{d_\Gamma(u,v)} \\
&= \sum_{(g_j,h_l)}\sum_{(g_i,h_k)} x^{d_\Gamma((g_i,h_k),(g_j,h_l))} \\
&= \left[\sum_{k=1}^{m}\sum_{i,j=1}^{n} x^{d_\Gamma((g_i,h_k),(g_j,h_k))} + \sum_{k\neq l=1}^{m}\sum_{i,j=1}^{n} x^{d_\Gamma((g_i,h_k),(g_j,h_l))}\right] \\
&= \left[\sum_{k=1}^{m}\sum_{i,j=1}^{n} x^{d_G(g_i,g_j)} + \sum_{k\neq l=1}^{m}\sum_{i,j=1}^{n} x^{[d_{G(U)}(g_i,g_j)+d_H(h_k,h_l)]}\right]
\end{aligned}$$

$$= \left[\sum_{k=1}^{m}\sum_{i,j=1}^{n} x^{d_G(g_i,g_j)} + \sum_{k\neq l=1}^{m} x^{d_H(h_k,h_l)} \sum_{i,j=1}^{n} x^{d_{G(U)}(g_i,g_j)}\right]$$

$$= |V(H)|\overline{H}(G,x) + \Big(\overline{H}(H,x) - |V(H)|\Big)\overline{H}(G(U),x),$$

which completes the proof. ■

Corollary 2. *Let G and H be two connected graphs. Then*

$$\overline{H}(G\Box H) = \overline{H}(G,x)\overline{H}(H,x).$$

Proof. Let $U = V(G)$. Then $\overline{H}(G(U),x) = \overline{H}(G,x)$ and the desired result obtains from Theorem 1. ■

3 Hosoya polynomial of $F-$sum of graphs

In [6], the authors introduced four new sums of graphs and obtained their Wiener index. Here we obtain the Hosoya polynomials of these operations and as an application, we give a new method to compute the Wiener index of these graphs. At first we recall some definitions and notations. Let G be a connected graph.

(a) $S(G)$ is obtained from G by replacing each edge of G by a path of length two.

(b) $R(G)$ is obtained from G by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge.

(c) $Q(G)$ is obtained from G by inserting a new vertex into each edge of G, then joining with edges those pairs of new vertices on adjacent edges of G.

(d) $T(G)$ has as its vertices the edges and vertices of G. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G. (This graph is called total graph of G).

Definition 2. *(See [6]) Let F be one of the symbols S, R, Q or T. The F-sum $G_1 +_F G_2$ is a graph with the set of vertices $V(G_1 +_F G_2) = (V(G_1) \cup E(G_1)) \times V(G_2)$ and two vertices (g_1, g_2) and (g_1', g_2') of $G_1 +_F G_2$ are adjacent if and only if $[g_1 = g_1'$ and $g_2 \sim g_2'$ in $G_2]$ or $[g_2 = g_2'$ and $g_1 \sim g_1'$ in $F(G_1)]$.*

The Wiener index of $G +_F H$ has been computed in [6]. Note that if we set $U = V(G) \subseteq V(F(G))$, then $G +_F H = F(G)(U) \sqcap H$. Thus we have a new and short method in computing the Wiener index of $G +_F H$.

Theorem 2. *Let $G = (V_1, E_1)$ and $H = (V_2, E_2)$ be two connected graphs. Suppose that $U = V(G) \subseteq V(F(G))$. Then if $F = Q$ or T, then the Wiener index of graph $G +_F H$ is equal to:*

$$|V_2|\overline{H}(F(G), x) + \Big(\overline{H}(H, x) - |V_2|\Big)\Big(x[\overline{H}(F(G), x) - |V(F(G))|] + |E_1|x^2 + |V_1|\Big).$$

Also if $F = S$ or R, then the Wiener index of graph $G +_F H$ is equal to:

$$|V_2|\overline{H}(F(G), x) + \Big(\overline{H}(H, x)| - |V_2|\Big)\Big(\overline{H}(F(G), x) + |E_1|x^2 - |E_1|\Big).$$

Proof. At first suppose that $F = S$ or R. Then for every $y \neq x \in V(F(G))$ we have $d_{F(G)(U)}(x, y) = d_{F(G)}(x, y)$. Also for every $x \in V(F(G)) \setminus U$, $d_{F(G)(U)}(x, x) = 2$. So we obtain

$$\begin{aligned}
\overline{H}(F(G)(U), x) &= \Big(\sum_{y \in V(F(G))} \sum_{y \neq x \in V(F(G))} x^{d_{F(G)(U)}(x,y)} \\
&\quad + \sum_{x \in V(F(G)) \setminus U} x^{d_{F(G)(U)}(x,x)} + \sum_{x \in U} x^{d_{F(G)(U)}(x,x)} \Big) \\
&= \sum_{y \in V(F(G))} \sum_{y \neq x \in V(F(G))} x^{d_{F(G)}(x,y)} + \sum_{x \in V(F(G)) \setminus U} x^2 + \sum_{x \in U} x^0 \\
&= \Big(\overline{H}(F(G), x) - |V(F(G))|\Big) + |V(F(G)) \setminus U|x^2 + |V_1| \\
&= \overline{H}(F(G), x) + |E_1|x^2 - |E_1|. \qquad (1)
\end{aligned}$$

Combining (1) and Theorem 1, we obtain the desired result when $F = S, R$.

Now suppose that $F = Q$ or T. Then clearly for every $y \neq x \in V(F(G)) \setminus U$ we have $d_{F(G)(U)}(x, y) = d_{F(G)}(x, y) + 1$ and for other vertices of $F(G)$ $d_{F(G)(U)}(x, y) = d_{F(G)}(x, y)$. Also note that for every $y \neq x \in V(F(G)) \setminus U$ we have $d_{F(G)}(x, y) = d_{L(G)}(x, y)$ and for every $x \in V(F(G)) \setminus U$, $d_{F(G)(U)}(x, x) = 2$. Hence, we obtain

$$\begin{aligned}
\overline{H}(F(G)(U), x) &= \Big(\sum_{y \in V(F(G))} \sum_{y \neq x \in V(F(G))} x^{d_{F(G)(U)}(x,y)} \\
&\quad + \sum_{x \in V(F(G)) \setminus U} x^{d_{F(G)(U)}(x,x)} + \sum_{x \in U} x^{d_{F(G)(U)}(x,x)} \Big)
\end{aligned}$$

$$
\begin{aligned}
&= x \sum_{y\in V(F(G))} \sum_{y\neq x\in V(F(G))} x^{d_{F(G)}(x,y)} + \\
&\quad \sum_{x\in V(F(G))\setminus U} x^0 + \sum_{x\in U} x^2 \\
&= x\Big(\overline{H}(F(G),x) - |V(F(G))|\Big) + |V(F(G))\setminus U|x^2 + |V_1| \\
&= x\Big(\overline{H}(F(G),x) - |V(F(G))|\Big) + |E_1|x^2 + |V_1|. \qquad (2)
\end{aligned}
$$

Again by Theorem 1 and (2) we obtain the result. ■

Corollary 3. *Let $G = (V_1, E_1)$ and $H = (V_2, E_2)$ be two connected graphs. Suppose that $U = V(G) \subseteq V(F(G))$. Then $W(G +_F H) =$*

$$
\begin{cases}
|V_2|^2 W(F(G)) + \Big(|V_1| + |E_1|\Big)^2 W(H) + \frac{1}{2}(|E_1|^2 + |E_1|)(|V_2|^2 - |V_2|)) & F = Q, T \\
|V_2|^2 W(F(G)) + \Big(|V_1| + |E_1|\Big)^2 W(H) + |E_1||V_2|(|V_2)| - 1) & F = S, R.
\end{cases}
$$

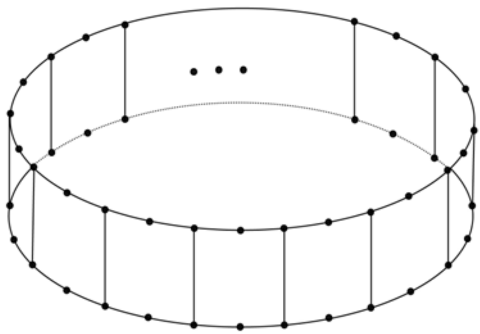

Figure 1: $G' = C_n +_S P_2$

4 Examples

Let C_n and P_n denote a cycle and path with n vertices respectively. Then

$$\overline{H}(P_n, x) = \frac{2x}{1-x}(n - [n]) + n,$$

$$\overline{H}(C_{2n}, x) = 4n([n] - 1) + 2nx^n + 2n,$$

$$\overline{H}(C_{2n+1}, x) = 2(2n+1)([n]-1) + (2n+1) = (2n+1)(2[n]-1),$$

where $[n] = 1 + x + x^2 + \cdots + x^{n-1} = \frac{x^n - 1}{x-1}$.

If $G = C_n$ and $H = K_2$, then by Theorem 2 for graph $G' = S(C_n)(U) \sqcap P_2$, shown in Fig. 1, $\overline{H}(G', x)$ is equal to

$$\begin{aligned}
& |V(P_2)|\overline{H}(S(C_n), x) + \Big(\overline{H}(P_2, x)| - |V(P_2)|\Big)\Big(\overline{H}(S(C_n), x) + |E(C_n)|x^2 - |E(C_n)|\Big) \\
= \;& 2\overline{H}(C_{2n}, x) + \Big(\overline{H}(P_2, x) - 2\Big)\Big(\overline{H}(C_{2n}, x) + nx^2 - n\Big) \\
= \;& 2\Big(4n([n]-1) + 2nx^n + 2n\Big) + 2x\Big(4n([n]-1) + 2nx^n + 2n + nx^2 - n\Big) \\
= \;& \frac{2n\,(2\,x^n - 3\,x + 4\,x^{n+1} - 2 - 3\,x^2 + 2\,x^{n+2} + x^4 - x^3)}{x-1}
\end{aligned}$$

Note that $S(C_n)(U) \sqcap P_2$ is called the Zig-Zag polyhex nanotube $TUHC_6[2n, 2]$.

Corollary 4. *Let n be an integer. Then the Wiener index and the hyper Wiener index of Zig-Zag polyhex nanotube $TUHC_6[2n, 2]$ are equal to*

$$\begin{aligned}
W(TUHC_6[2n,2]) &= 4\,n^3 + 4\,n^2 + 2\,n, \\
WW(TUHC_6[2n,2]) &= \frac{n}{3}\left(15 + 14\,n + 12\,n^2 + 4\,n^3\right).
\end{aligned}$$

Also for hexagonal chains with n hexagonal $L_n = S(P_{n+1})(U) \sqcap P_2$, where $U = V(P_{n+1})$, shown Fig. 2, we obtain

$$\overline{H}(L_n, x) = \frac{2\,(1+x)\,(nx^4 - 3\,nx^3 + nx^2 - x^2 - 2\,x + 2\,xx^{2\,n+1} - nx + 2\,n + 1)}{(x-1)^2}.$$

As a corollary of our results we compute the hyper Wiener index of linear hexagonal chain. This result, by a different method, was already obtained by Zhang et al. Theorem 3.1, [20].

Corollary 5. *Let n be an integer. Then the Wiener index and hyper the hyper Wiener index of a hexagonal chain with n hexagonal ,L_n, are equal to*

$$\begin{aligned}
W(L_n) &= \left(\frac{16n^3 + 36n^2 + 26n + 3}{3}\right) \\
WW(L_n) &= \frac{3 + 37n + 46n^2 + 32n^3 + 8n^4}{3}.
\end{aligned}$$

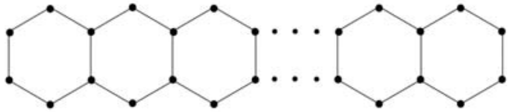

Figure 2: A linear hexagonal chain

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