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Note

The hyper-Wiener index of the generalized hierarchical product of graphs

Mehdi Eliasi, Ali Iranmanesh *

Department of Pure Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P.O. Box: 14115-137, Tehran, Iran

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ABSTRACT

The hyper Wiener index of the connected graph G is $WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(d(u,v) + d(u,v)^2)$, where $d(u,v)$ is the distance between the vertices u and v of G. In this paper we compute the hyper-Wiener index of the generalized hierarchical product of two graphs and give some applications of this operation.

1. Introduction

A topological index is a numerical value associated with the chemical constitution purporting for the correlation of the chemical structure with various physical properties, chemical reactivity or biological activity. The Wiener index [18] is one of the oldest molecular-graph-based structure-descriptors. In fact let G be an undirected connected graph without loops or multiple edges. The set of vertices and edges of G are denoted by $V(G)$ and $E(G)$ respectively. For vertices x and y in $V(G)$, we denote by $d(x,y)$ (or $d_G(x,y)$ when we deal with more than one graph) the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. The Wiener index of G is the half sum of all distances in the graph G:

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

Mathematical properties and chemical applications of the Wiener index have been intensively studied over the past thirty years. For more information about the Wiener index in chemistry and mathematics see [1,5,6,8,10–12], respectively. 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. [15] generalized this extension to cyclic structures as:

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

$WW(G)$ has seen widespread use in correlations; references may be found in [9]. For information about the hyper-Wiener index in mathematics see [4,9,14]. Recently topological indices of many of composite graphs have been studied [7,13,17,20,21]. In particular Ashrafi et al. computed the hyper-Wiener index of Cartesian product, joint and other graph operations [13]. Here we compute the hyper-Wiener index of a generalized hierarchical product. Also we give some applications of this operation to compute the hyper-Wiener index of well-known graphs such as F-sum [7].

* Corresponding author. Fax: +98 21 88006544.
E-mail addresses: m.eliasi@modares.ac.ir (M. Eliasi), iranmanesh@modares.ac.ir (A. Iranmanesh).

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2. Generalized hierarchical product

The Cartesian product $G\Box H$ of 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

$$(g_1, h_1) \sim (g_2, h_2) \Leftrightarrow \begin{cases} g_1 = g_2 \quad \text{and} \quad h_1 \sim h_2 \quad \text{in } H, \\ \text{or} \\ h_1 = h_2 \quad \text{and} \quad g_1 \sim g_2 \quad \text{in } G. \end{cases}$$

Barriére et al. [2,3], defined a new product of graphs, namely the 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

$$(g, h) \sim (g', h') \Leftrightarrow \begin{cases} g = g' \in U \quad \text{and} \quad h \sim h' \quad \text{in } H \\ \text{or} \\ h = h' \quad \text{and} \quad g \sim g' \quad \text{in } G. \end{cases}$$

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

Lemma 1 (*See [3]*). *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,*
(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 $u, v \in V$ through U is a $u - v$ path in G containing some vertex $z \in U$ (vertex z could be the vertex u or v). The distance between u and v in through U, $d_{G(U)}(u, v)$, is the length of a shortest path between u and v through U. Note that, if one of the vertices u and v belongs to U, then $d_{G(U)}(u, v) = d_G(u, v)$. We define

$$W(G(U)) = \frac{1}{2}\sum_{(u,v)} d_{G(U)}(u, v),$$
$$WW(G(U)) = \frac{1}{4}\sum_{(u,v)} [d_{G(U)}(u, v)^2 + d_{G(U)}(u, v)].$$

Using this notation, in the following theorem, we compute the Wiener index of the generalized hierarchical product.

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

$$\begin{aligned} WW(G(U) \sqcap H) = {} & |V(H)|WW(G) + |V(G)|^2 WW(H) \\ & + |V(H)|\Big(|V(H)| - 1\Big)WW(G(U)) + 2W(H)W(G(U)). \end{aligned}$$

Proof. Set $V(G) = \{g_1, g_2, \ldots, g_n\}$ and $V(H) = \{h_1, h_2, \ldots, h_m\}$, we have

$$\begin{aligned} WW(G(U) \sqcap H) &= \frac{1}{4}\sum_{(u,v)\in V(G(U)\sqcap H)} \left(d_{G(U)\sqcap H}(u, v) + d_{G(U)\sqcap H}(u, v)^2\right) \\ &= \frac{1}{4}\sum_{(g_j,h_l)}\sum_{(g_i,h_k)} \left(d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_l)) + d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_l))^2\right) \\ &= \frac{1}{4}\left[\sum_{k=1}^{m}\sum_{i,j=1}^{n} \left(d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_k)) + d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_k))^2\right)\right. \\ &\quad \left. + \sum_{k\neq l=1}^{m}\sum_{i,j=1}^{n} \left(d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_l)) + d_{G(U)\sqcap H}((g_i, h_k), (g_j, h_l))^2\right)\right] \\ &= \frac{1}{4}\left[\sum_{k=1}^{m}\sum_{i,j=1}^{n} \left(d_G(g_i, g_j) + d_G(g_i, g_j)^2\right)\right. \end{aligned}$$

$$+\sum_{k\neq l=1}^{m}\sum_{i,j=1}^{n}\Big([d_{G(U)}(g_i,g_j)+d_H(h_k,h_l)]+[d_{G(U)}(g_i,g_j)+d_H(h_k,h_l)]^2\Big)\Bigg]$$

$$=\frac{1}{4}\Bigg[\sum_{k=1}^{m}\sum_{i,j=1}^{n}\Big(d_G(g_i,g_j)+d_G(g_i,g_j)^2\Big)+\sum_{k\neq l=1}^{m}\sum_{i,j=1}^{n}\Big(d_{G(U)}(g_i,g_j)+d_{G(U)}(g_i,g_j)^2\Big)$$

$$+\sum_{i,j=1}^{n}\sum_{k\neq l=1}^{m}\Big(d_H(h_k,h_l)+d_H(h_k,h_l)^2\Big)+2\sum_{i,j=1}^{n}\sum_{k\neq l=1}^{m}\Big(d_{G(U)}(g_i,g_j)d_H(h_k,h_l)\Big)\Bigg]$$

$$=|V(H)|WW(G)+|V(G)|^2WW(H)+|V(H)|\Big(|V(H)|-1\Big)WW(G(U))+2W(H)W(G(U))$$

which completes the proof. □

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

$$WW(G\Box H)=|V(H)|^2W(G)+|V(G)|^2W(H)+2W(H)W(G).$$

Proof. Let $U := V(G)$. Then $WW(G(U)) = WW(G)$ and $W(G(U)) = W(G)$ and the desired result obtains from Theorem 1. □

Let G be a graph and u be a vertex of G. We denote the summation of distances between u and all vertices in the G by $d_G(u)$. Also we let $dd_G(u)=\sum_{x\in V(G)}[d_G(u,x)+d_G(u,x)^2]$.

Proposition 1. *Let G be a graph and $U = \{u\}$ be a singleton vertex of G. Then $W(G(U)) = |V(G)|d_G(u)$ and $WW(G(U)) = \frac{|V(G)|}{2}dd_G(u)+\frac{1}{2}d_G(u)^2$.*

Proof. We have

$$W(G(U))=\frac{1}{2}\sum_{(x,y)}d_{G(U)}(x,y)=\frac{1}{2}\sum_{(x,y)}(d_G(x,u)+d_G(u,y))=|V(G)|d_G(u),$$

$$\begin{aligned}WW(G(U)) &= \frac{1}{4}\sum_{(x,y)}[d_{G(U)}(x,y)+d_{G(U)}(x,y)^2]\\ &= \frac{1}{4}\sum_{(x,y)}[d_G(x,u)+d_G(u,y)+(d_G(x,u)+d_G(u,y))^2]\\ &= \frac{1}{4}\Bigg[\sum_{(x,y)}[d_G(x,u)+d_G(x,u)^2]+\sum_{(x,y)}[d_G(y,u)+d_G(y,u)^2]+\sum_{(x,y)}2d_G(x,u)d_G(u,y)\Bigg]\\ &= \frac{|V(G)|}{2}dd_G(u)+\frac{1}{2}d_G(u)^2,\end{aligned}$$

which gives the result. □

By Theorem 1 and Proposition 1, we have the following corollary:

Corollary 3. *If G and H are two graphs and $U = \{u\}$ is a singleton vertex of G, then*

$$\begin{aligned}WW(G(U)\sqcap H) &= |V(H)|WW(G)+|V(G)|^2+2W(H)|V(G)|d_G(u)WW(H)\\ &\quad+|V(H)|\Big(|V(H)|-1\Big)\left(\frac{|V(G)|}{2}dd_G(u)+\frac{1}{2}d_G(u)^2\right).\end{aligned}$$

3. Hyper-Wiener index of *F*-sum of graphs

As an application of Theorem 1, we give a new method to compute the hyper-Wiener index of graphs which was introduced in [7]. First we recall some definitions and notations (See [19]). 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).

Some graph operations have been defined in [7] as follows.

Definition 2. 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 [7]. 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* $WW(G +_F H) =$

$$\begin{cases} |V(H)|WW(F(G)) + |V(F(G))|^2 WW(H) + |V(H)|\Big(|V(H)|-1\Big)\Big(WW(F(G)) \\ \quad + W(L(G)) + \frac{1}{4}[|E_1|^2 + 6|E_1|]\Big) + 2W(H)\Big(W(F(G)) + W(L(G)) + |E_1| + |E_1|^2\Big) & F = Q, T \\ |V(H)|WW(F(G)) + |V(F(G))|^2 WW(H) \\ \quad + |V(H)|\Big(|V(H)|-1\Big)\Big(WW(F(G)) + \frac{3}{2}|E_1|\Big) + 2W(H)(W(F(G)) + |E_1|) & F = S, R. \end{cases}$$

Proof. Let $F = S, R$. 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

$$\begin{aligned} WW(F(G)(U)) &= \frac{1}{4}\Bigg(\sum_{y\in V(F(G))}\sum_{y\neq x\in V(F(G))}[d_{F(G)(U)}(x,y) + d_{F(G)(U)}(x,y)^2] + \sum_{x\in V(F(G))\setminus U}[d_{F(G)(U)}(x,x) \\ &\quad + d_{F(G)(U)}(x,x)^2] + \sum_{x\in U}[d_{F(G)(U)}(x,x) + d_{F(G)(U)}(x,x)^2]\Bigg) \\ &= \frac{1}{4}\Bigg(\sum_{y\in V(F(G))}\sum_{y\neq x\in V(F(G))}[d_{F(G)}(x,y) + d_{F(G)}(x,y)^2]\Bigg) + \frac{1}{4}\sum_{x\in V(F(G))\setminus U}[d_{F(G)(U)}(x,x) + d_{F(G)(U)}(x,x)^2] \\ &\quad + \frac{1}{4}\sum_{x\in U}[d_{F(G)(U)}(x,x) + d_{F(G)(U)}(x,x)^2] \\ &= \frac{1}{4}\Big(4WW(F(G)) + 6|V(F(G))\setminus U| + 0\Big) \\ &= WW(F(G)) + \frac{3}{2}|E_1|. \end{aligned} \tag{1}$$

A similar argument shows that

$$W(F(G)(U)) = W(F(G)) + |E_1|. \tag{2}$$

Combining (1), (2) and Theorem 1, we obtain the desired result when $F = S, R$.

Now let $F = Q, T$. Then clearly for every $y \neq x$ where $\{x, y\} \subset (V(F(G)) \setminus U) = E(G)$, we have: $d_{F(G)(U)}(x, y) = d_{F(G)}(x, y) + 1 = d_{L(G)}(x, y) + 1$ and for other pair vertices of $F(G)$, $d_{F(G)(U)}(x, y) = d_{F(G)}(x, y)$. Also note that for every $x \in V(F(G)) \setminus U$, $d_{F(G)(U)}(x, x) = 2$. So by using these facts, we obtain

$$\begin{aligned} WW(F(G)(U)) &= \frac{1}{4}\Bigg[\sum_{y\in V(F(G))\setminus U}\sum_{y\neq x\in V(F(G))\setminus U}[d_{F(G)(U)}(x,y) + d_{F(G)(U)}(x,y)^2] \\ &\quad + \sum_{y\in V(F(G))}\sum_{y\neq x\in U}[d_{F(G)(U)}(x,y) + d_{F(G)(U)}(x,y)^2] \\ &\quad + \sum_{x\in V(F(G))\setminus U}[d_{F(G)(U)}(x,x) + d_{F(G)(U)}(x,x)^2] + \sum_{x\in U}[d_{F(G)(U)}(x,x) + d_{F(G)(U)}(x,x)^2]\Bigg] \\ &= \frac{1}{4}\Bigg[\sum_{y\in V(F(G))\setminus U}\sum_{y\neq x\in V(F(G))\setminus U}[d_{F(G)}(x,y) + 1 + (d_{F(G)}(x,y)+1)^2] \end{aligned}$$

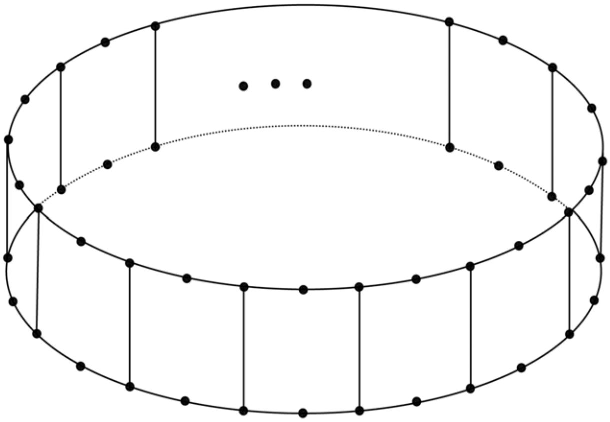

Fig. 1. $TUHC_6[2n, 2]$ zig-zag polyhex nanotube.

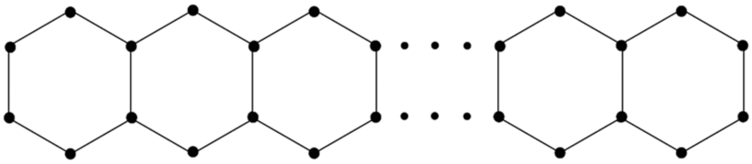

Fig. 2. The hexagonal chain L_n.

$$+ \sum_{y\in V(F(G))} \sum_{y\neq x\in U} [d_{F(G)}(x,y) + d_{F(G)}(x,y)^2] + \sum_{x\in V(F(G))\setminus U} 6 + \sum_{x\in U} 0 \Bigg]$$

$$= \frac{1}{4}\left[4WW(F(G)) + 2\sum_{y\in E(G)} \sum_{y\neq x\in E(G)} d_{L(G)}(x,y) + |E(G)|^2 + 6|E(G)|\right]$$

$$= WW(F(G)) + W(L(G)) + \frac{1}{4}[|E_1|^2 + 6|E_1|]. \tag{3}$$

A similar argument shows that

$$W(F(G)(U)) = W(F(G)) + W(L(G)) + |E_1| + |E_1|^2. \tag{4}$$

Again by Theorem 1, (4) and (3) we obtain the result. □

Let C_n and P_n be cycle and path with n vertices, respectively.

Example 1. If $G' = S(C_n)(U) \sqcap P_2$, the zig-zag polyhex nanotube $TUHC_6[2n, 2]$ (See Fig. 1), then

$$WW(G') = \frac{1}{3}n\left(4n^3 + 15 + 14n + 12n^2\right).$$

Proof. It is easy to see $W(P_n) = \frac{n(n^2-1)}{6}$ and $WW(P_n) = \frac{1}{24}(n^4 + 2n^3 - n^2 - 2n)$. Also $W(C_n) = \begin{cases} \frac{n^3}{8} & 2 \mid n \\ \frac{n(n^2-1)}{8} & 2 \nmid n. \end{cases}$ and

$$WW(C_n) = \begin{cases} \frac{n^2(n+1)(n+2)}{48} & 2 \mid n \\ \frac{n(n^2-1)(n+3)}{48} & 2 \nmid n. \end{cases}.$$

So by Theorem 1, we obtain the desired result. □

Example 2. Let L_n be a hexagonal chains with n hexagonal, Fig. 2. Then

$$WW(L_n) = \frac{8n^4 + 32n^3 + 46n^2 + 37 + 3}{3}.$$

Proof. Since $L_n = S(P_{n+1})(U) \sqcap P_2$, where $U = V(P_{n+1})$, so by Theorem 1, we obtain the result. □

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