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REMARKS ON THE WIENER POLARITY INDEX OF SOME GRAPH OPERATIONS†

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Abstract. The Wiener polarity index $W_p(G)$ of a graph G of order n is the number of unordered pairs of vertices u and v of G such that the distance $d_G(u, v)$ between u and v is 3. In this paper the Wiener polarity index of some graph operations are computed. As an application of our results, the Wiener polarity index of a polybuckyball fullerene and C_4 nanotubes and nanotori are computed.

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1. Introduction

Let $G = (V, E)$ be a connected simple graph in which V and E are the set of vertices and edges respectively. As usual the distance between the vertices u and v is denoted by $d_G(u, v)$ (or $d(u, v)$ for short) and it is the length of a shortest path connecting u and v. The number of unordered pairs of vertices u and v of G such that $d_G(u, v) = k$ is denoted by $d(G, k)$. A topological index $Top(G)$ for G is a number with this property that for every graph H isomorphic to G, $Top(G) = Top(H)$. The Wiener index is the first distance-based and most studied topological indices, both from theoretical point of view and applications. It is equal to the sum of distances between all pairs of vertices of the respective graph [29].

The Wiener polarity index of an organic molecule with molecular graph $G = (V, E)$ is defined as $W_p(G) = d(G, 3)$. Using the Wiener polarity index, Lukovits and Linert demonstrated quantitative structure property relationships in a series of acyclic and cycle-containing hydrocarbons [25]. In [12] Hosoya, one of the

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pioneers of chemical graph theory, found a physico-chemical interpretation of $W_p(G)$.

Recently, Du, Li and Shi [7] described a linear time algorithm for computing the Wiener polarity index of trees and characterized the trees maximizing the index among all trees of given order. Deng, Xiao and Tang [3] characterized the extremal trees with respect to this index among all trees of order n and diameter d. Deng [4] also gave the extremal Wiener polarity index of all chemical trees with order n. Xiao and Deng [30] found the maximum Wiener polarity index of chemical trees with n vertices and k pendants. Tong and Deng [27] characterized the trees with the first three smallest Wiener polarity indices among all trees of order n and diameter d. Mathematical properties and chemical meaning of the Wiener polarity index and its applications in chemistry can be found in [3, 4, 7, 9, 10, 12, 25, 27, 30] and the references cited therein.

The Wiener index of Cartesian product graphs was studied in [8, 21]. In [20], Klavzar et al computed the Szeged index of Cartesian product graphs and in [21] the PI index of the Cartesian product graphs is computed. In a series of papers [1, 2, 11, 13, 15, 16, 17, 18, 19, 31, 33], Ashrafi and his co-authors considered PI, vertex PI, hyper-Wiener, edge Wiener, edge frustration, Szeged, edge Szeged and Zagreb group indices into account under some graph operations. Here we continue this progress to compute the Wiener polarity index of some graph operations.

Throughout this paper our notation is standard and taken mainly from [5, 14, 28]. For a graph G and two vertices $u, v \in V(G)$, we define the odd distance $od_G(u, v)$ as the length of the shortest odd walk joining $u, v \in G$, and the even distance $ed_G(u, v)$ as the length of the shortest even walk joining $u, v \in G$. If there are no walk of odd (even) length between u and v, then we set $od_G(u, v) = \infty(ed_G(u, v) = \infty)$.

Definition 1.1. Let G and H be simple connected graphs. The join $G + H$, symmetric difference $G\Delta H$, disjunction $G \vee H$, composition $G[H]$, Cartesian product $G \times H$, strong product $G \odot H$ and tensor product $G \otimes H$ of G and H are defined as follows:

$$V(G+H) = V(G) \cup V(H),$$
$$E(G+H) = E(G) \cup E(H) \cup \{uv : u \in V(G), v \in V(H)\}$$
$$V(G\Delta H) = V(G) \times V(H),$$
$$E(G\Delta H) = \{(a,b)(c,d) : \ ac \in E(G) \ or \ bd \in E(H) \ not \ both\}$$
$$E(G \vee H) = \{(a,b)(c,d) \ : \ ac \in E(G) \ or \ bd \in E(H)\}$$
$$E(G[H]) = \{(a,b)(c,d) \ : \ ac \in E(G) \ or \ a = c \ and \ bd \in E(H)\}$$
$$E(G \times H) = \{(a,b)(c,d) \ : \ [ac \in E(G) \ and \ b = d] \ or \ [a = c \ and \ bd \in E(H)]\}$$
$$E(G \odot H) = \{(a,b)(c,d) \ : \ [ac \in E(G) \ and \ b = d] \ or \ [a = c \ and \ bd \in E(H)] \ or \ [ac \in E(G) \ and \ bd \in E(H)]\}$$
$$E(G \otimes H) = \{(a,b)(c,d) \ : \ [ac \in E(G) \ and \ bd \in E(H)]\}$$

It is an easy fact that the Wiener polarity index of any graph with diameter less than 3 such as the complete graph K_n, the star graph S_n, the Wheel W_n, the Petersen graph $P_{2,5}$, the complete bipartite graph $K_{m,n}$, join $G+H$, symmetric difference $G\Delta H$ and the disjunction $G \vee H$ are zero.

Example 1.2. The Wiener polarity index of the $n-$vertex path P_n is $n-3$ and for the cycle C_n, $n \geq 7$ is n.

Example 1.3. Consider the path P_n with vertex set $V(P_n) = \{x_1, x_2, ..., x_n\}$. We form a graph G with vertices correspond to each vertex of P_n as follows: for each i, $1 \leq i \leq n$ we define a set $M_i = \{x_{i_1}, x_{i_2}, ..., x_{i_{m_i}}\}$ and connect any vertex x_i to all vertices in M_i. The resulting graph is called a caterpillar denoted by $G = Cat_{n,m_1,m_2,...,m_n}$. To compute the Wiener polarity index of G we notice that there are three types of pair of vertices with distance three. At first, we count the number of vertices $u \in M_i$, $v \in M_{i+1}$ and $d_G(u,v) = 3$. The number of such pairs is $\sum_{i=1}^{n} m_i.m_{i+1}$. Secondly, the number of vertices with $u = x_i$, $v \in M_{i+2}$ and $d_G(u,v) = 3$ is $[m_3 + m_4 + ... + m_n] + [m_1 + m_2 + ... + m_{n-2}]$. Finally, if $u, v \in \{x_1, x_2, ..., x_n\}$ then the number of vertices with distance 3 is $n-3$. Hence we have:

$$\begin{aligned} W_p(Cat_{n,m_1,m_2,...,m_n}) = &\sum_{i=1}^{n}[m_i.m_{i+1}] + 2 \times [m_3 + m_4 + ... + m_{n-2}] \\ &+ [m_1 + m_2 + m_{n-1} + m_n] + n - 3. \end{aligned}$$

Let G and H be two graphs. We consider n copies of H and connect the i-th vertex of G to all vertices of i-th copy of H. This graph is called the corona product of G and H denoted by GoH.

2. Main results

In this section, the Wiener polarity index of some graph operations are computed. For further details the interested reader can be consulted [1, 16, 19, 20, 26, 31, 32]. First of all it is clear that for any two vertices u and v in disjunction graph $G \vee H$ we have $d_{G\vee H}(u,v) \leq 2$ and so the Wiener polarity index of $G \vee H$ is equal to zero. We now consider the composition graph $G[H]$. We have:

Theorem 2.1. *Let $G_1, G_2, ..., G_k$ be connected graphs then we have:*

$$W_P(G_1[G_2[...[G_k]...]]) = W_p(G_1)\prod_{i=2}^{k}|V(G_i)|.$$

Proof. It is clear that,

$$d_{G_1[G_2]}((a,b),(c,d)) = \begin{cases} 0 & \text{if } a = c,\ b = d \\ 1 & \text{if } (a = c),\ bd \in E(G_2), or, ac \in E(G_1) \\ 2 & \text{if } (a = c),\ bd \notin E(G_2) \\ d_{G_1}(a,c) & \text{if } (a \neq c) \end{cases}$$

The proof is by induction on k. If $k = 2$ then we have: $d_{G_1[G_2]}((a,b),(c,d)) = 3$ if and only if $d_{G_1}(a,c) = 3$. Therefore, $W_P(G_1[G_2]) = W_P(G_1).|V(G_2)|^2$. Now assume that the result holds for k. Then,

$$\begin{aligned} W_P(G_1[G_2[...[G_k[G_{k+1}]]...]]) &= W_p(G_1)[(\prod_{i=2}^{k}|V(G_i)|)|V(G_{k+1})|] \\ &= W_p(G_1)\prod_{i=2}^{k+1}|V(G_i)|. \end{aligned}$$

This completes the proof. □

There are many graph operations with vertex set $V(G) \times V(H)$. Let us consider the Cartesian product of graphs. We have:

Lemma 2.2. *Let $G_1, G_2, ..., G_k$ be connected graphs. Then*

$$(a)\quad d_{\prod_{i=1}^{k} G_i}[\ (x_1, x_2..., x_k), (y_1, y_2, ..., y_k)\ ] = \sum_{i=1}^{k} d_{G_i}\ (x_i, y_i)$$

$$(b)\quad d(\prod_{i=1}^{k} G_i, 2) = \ [\ \sum_{i=1}^{k} d_i \prod_{j=1, j\neq i}^{k} v_j\ ] + 2[\sum_{i,j\in A_k, i<j} e_i e_j \prod_{l\neq i,j} v_l\ ]$$

$$(c)\quad |E(\prod_{i=1}^{k} G_i)| = \sum_{i=1}^{k}(e_i \prod_{i=1, i\neq j}^{k} v_j),$$

in which $A_k = \{1, 2, ..., k\}$, $e_i = |E(G_i)|$, $d_i = d(G_i, 2)$, and $v_i = |V(G_i)|$.

Proof. We first notice that the following equality holds:

$$d_{G_1\times G_2}[\ (a,b),(c,d)\ ] = d_{G_1}(a,c) + d_{G_2}(b,d)$$

see [26] for details. We proceed by induction on k. The equality (a) is obvious and (c) holds by the definition of Cartesian product of graphs. To prove (b), we notice that $d_{G_1\times G_2}[\ (a,b),(c,d)\ ] = 2$ if and only if

$$d_{G_1}(a,c) + d_{G_2}(b,d) = 2.$$

It implies that $d(G_1 \times G_2, 2) = d_1 v_2 + d_2 v_1 + 2e_1 e_2$.

Assume that the result holds for k. Then

$$\begin{aligned} d(\prod_{i=1}^{k+1} G_i, 2) &= d(\prod_{i=1}^{k} G_i, 2)v_{k+1} + \ d(G_{k+1}, 2)(\prod_{j=1}^{k} v_j) + 2e(\prod_{i=1}^{k} G_i)(e_{k+1}) \\ &= \sum_{i=1}^{k}[d_i \prod_{j=1, j\neq i}^{k} v_j]v_{k+1} + (d_{k+1})(\prod_{j=1}^{k} v_j) \\ &\quad + 2v_{k+1}[\sum_{i,j\in A_k, i<j} e_i e_j \prod_{l\neq i,j} v_l\ ] + 2[\sum_{i=1}^{k}(e_i \prod_{i=1, i\neq j}^{k} v_j)](e_{k+1}) \\ &= \ [\ \sum_{i=1}^{k+1} d_i \prod_{j=1, j\neq i}^{k+1} v_j\ ] + 2[\sum_{i,j\in A_{k+1}, i<j} e_i e_j \prod_{l\neq i,j} v_l\ ], \end{aligned}$$

proving the lemma. $\square$

Theorem 2.3. *Let $G_1, G_2, ..., G_k$ be connected graphs. Then we have:*

$$W_P(\prod_{i=1}^{k} G_i) = \sum_{i=1}^{k}(w_i \prod_{j=1,j\neq i}^{k} v_j) + 2\sum_{i\neq j,i,j\in A_k}(e_i d_j \prod_{l\in A_k-\{i,j\}} v_l) + 4\sum_{(i,j,l\in A_k),i<j<l}(e_i e_j e_l \prod_{p\in A_k-\{i,j,l\}} v_p)$$

in which $A_k = \{1, 2, ..., k\}$, $e_i = |E(G_i)|$, $d_i = d(G_i, 2)$, $v_i = |V(G_i)|$ and $w_i = W_p(G_i)$.

Proof. By induction on k. If $k = 2$ then $d_{G_1\times G_2}[\ (a,b),(c,d)\ ] = 3$. Therefore, one of the following holds:

(1) Let $[d_{G_1}(a,c) = 3, b = d]$. In this case the number of pairs in $G_1 \times G_2$ with distance 3 is equal to $w_1.v_2$.
(2) Let $d_{G_2}(b,d) = 3, a = c$. In this case the number of pairs in $G_1 \times H_2$ with distance 3 is equal to $w_2.v_1$.
(3) Let $[d_{G_1}(a,c) = 2, bd \in E(G_2)]$. In this case the number of pairs in $G_1 \times G_2$ at distance 3 is equal to $2e_2.d_1$.
(4) Let $[d_{G_2}(b,d) = 2, ac \in E(G_1)]$. In this case the number of pairs in $G_1 \times G_2$ at distance 3 is equal to $2e_1.d_2$.

Therefore, $W_P(G_1 \times G_2) = w_2.v_1 + w_1.v_2 + 2e_2.d_1 + 2e_1d_2$. Assume that the result holds for k. Then the Lemma 2.2 implies that

$$\begin{aligned}
W_p(\prod_{i=1}^{k+1} G_i) &= W_p(G_{k+1})[|V(\prod_{i=1}^{k} G_i)|] + [W_p(\prod_{i=1}^{k} G_i)]v_{k+1} + 2[e_{k+1}].d(\prod_{i=1}^{k} G_i, 2) + 2d_{k+1}|E(\prod_{i=1}^{k} G_i)| \\
&= w_{k+1}(\prod_{i=1}^{k} v_i) + \{\sum_{i=1}^{k}(w_i \prod_{j=1,j\neq i}^{k} v_j) + 2\sum_{i\neq j,i,j\in A_k}(e_i d_j \prod_{l\in A_k-\{i,j\}} v_l) \\
&\quad + 4\sum_{(i,j,l\in A_k),i<j<l}(e_i e_j e_l \prod_{p\in A_k-\{i,j,l\}} v_p)\}v_{k+1} + 2e_{k+1}\{\sum_{i=1}^{k}[d_i \prod_{j=1,j\neq i}^{k} v_j\ ] \\
&\quad + 2\sum_{i,j\in A_k,i<j}[e_i e_j \prod_{l\neq i,j} v_l\ ]\} + 2d_{k+1}\{\sum_{i=1}^{k}[e_i \prod_{i=1,i\neq j}^{k} v_j]\} \\
&= \{w_{k+1}(\prod_{i=1}^{k} v_i) + v_{k+1}\sum_{i=1}^{k} w_i[\prod_{j=1,j\neq i}^{k} v_j]\} + [2v_{k+1}\sum_{i\neq j,i,j\in A_k}(e_i d_j \prod_{l\in(A_k-\{i,j\})} v_l)] \\
&\quad + [\ 2d_{k+1}\sum_{i=1}^{k} e_i \prod_{j=1,j\neq i}^{k} v_j\ ] + \{4e_{k+1}[\sum_{i,j\in A_k,i<j} e_i e_j \prod_{l\neq i,j} v_l\ ] \\
&\quad + [2e_{k+1}\sum_{i=1}^{k} d_i \prod_{j=1,j\neq i}^{k} v_j] + 4v_{k+1}[\sum_{(i,j,l\in A_k),i<j<l}(e_i e_j e_l \prod_{p\in[(A_k)-i,j,l]} v_p)]\} \\
&= \sum_{i=1}^{k+1}(w_i \prod_{j=1,j\neq i}^{k+1} v_j) + 2\sum_{i\neq j,i,j\in A_{k+1}}(e_i d_j \prod_{l\in A_{k+1}-\{i,j\}} v_l) \\
&\quad + 4\sum_{(i,j,l\in A_{k+1}),i<j<l}(e_i e_j e_l \prod_{p\in A_{k+1}-\{i,j,l\}} v_p).
\end{aligned}$$

This completes the proof. $\square$

Define Q_n to be the $n-$dimentional cube. Then Q_n is isomorphic to the Cartesian product of n copies of K_2. Apply Theorem 2.3, we have:

$$\begin{aligned} W_p(Q_n) = W_p(\prod_{i=1}^{n} K_2) &= 4 \sum_{(i,j,l \in A_n), i<j<l} (e_i e_j e_l \prod_{p \in A_n - \{i,j,l\}} v_p) \\ &= 4 \sum_{(i,j,l \in A_n), i<j<l} (2^{n-3}) = 4\binom{n}{3} \times 2^{n-3} = \binom{n}{3} \times 2^{n-1}. \end{aligned}$$

We now define $R = P_m \times C_n$ and $S = C_m \times C_n$. The graphs R and S are called C_4-nanotube and C_4-nanotorus.

Corollary 2.4. *$W_P(R) = nm + n(m-3) + 2(m-2)n + 2n(m-1) = 6mn - 9n$ and $W_P(S) = 6mn - 3(m+n)$.*

Theorem 2.5. *Let G and H be two connected graphs. Then*

$$\begin{aligned} W_p(G \odot H) = W_p(G).&\left\{|V(H)| + |E(H)| + \sum_{i=1}^{|H|} \binom{(d_i)}{2}\right\} \\ &+ W_p(H).\left\{|V(G)| + |E(G)| + \sum_{i=1}^{|G|} \binom{(d_i)}{2}\right\} + W_p(G).W_p(H). \end{aligned}$$

Proof. We first notice that the following equality holds:

$$d_{G \odot H}((a,b),(c,d)) \quad = \quad Max[d_G(a,c), d_H(b,d)],$$

see [26] for details. Next we assume that $d_{G \odot H}[(a,b),(c,d)] = 3$. Therefore at least one of the following holds:

(1) Let $d_H(b,d) = 3, a = c$. In this case the number of pairs in $G \odot H$ by distance 3 is equal to $W_p(H).|V(G)|$.
(2) Let $d_H(b,d) = 3, ac \in E(G)$. In this case the number of pairs in $G \odot H$ with distance 3 is equal to $W_p(H).|E(G)|$.
(3) Let $d_H(b,d) = 3, d_G(a,c) = 2$. In this case the number of pairs in $G \odot H$ at distance 3 is equal to $W_p(H).[\sum_{i=1}^{|G|} \binom{d_i}{2}]$.
(4) Let $d_G(a,c) = 3, b = d$. In this case the number of pairs in $G \odot H$ at distance 3 is equal to $W_p(G)|V(H)|$.
(5) Let $d_G(a,c) = 3, bd \in E(H)$. In this case the number of pairs in $G \odot H$ at distance 3 is equal to $W_p(G)|E(H)|$.
(6) Let $d_H(b,d) = 2, d_G(a,c) = 3$. In this case the number of pairs in $G \odot H$ at distance 3 is equal to $W_p(G).[\sum_{i=1}^{i=|H|} \binom{d_i}{2}]$.
(7) Let $d_G(a,c) = 3, d_H(b,d) = 3$. In this case the number of pairs in $G \odot H$ at distance 3 is equal to $W_p(G).W_p(H)$.

Therefore,

$$W_p(G \odot H) = W_p(G).\left\{|V(H)| + |E(H)| + \sum_{i=1}^{|H|} \binom{d_i}{2}\right\}$$
$$+ W_p(H).\left\{|V(G)| + |E(G)| + \sum_{i=1}^{|G|} \binom{d_i}{2}\right\} + W_p(G).W_p(H).$$

This completes the proof. □

The graph H is called strongly triangular if for every pair $u, v \in V(H)$ there exists a vertex w adjacent to both of them. The number of triangles in G is denoted by t_G.

Theorem 2.6. *Let G and H be simple connected graphs, where H is a strongly triangular graph. Then the Wiener polarity index of tensor product $G \otimes H$ is equal to $W_P(G).|V(H)|^2 + [(|E(G)| - 3t_G)(|V(H)^2 - |E(H)|)]$.*

Proof. By [22, Theorem 2], $d_{G\otimes H}((a,b),(c,d))$ is computed as follows:

$$d_{G\otimes H}((a,b),(c,d)) = \begin{cases} 2 & [(ac \in E(G))\ ,\ (bd \notin E(H))\ ,\ (ac \in Tri(G))] \\ & or\ [(ac \in E(G))\ ,\ (b = d)\ ,\ (ac \in Tri(G))]\ or\ [a = c] \\ 3 & [(ac \in E(G))\ ,\ (bd \notin E(H))\ ,\ (ac \notin Tri(G))] \\ & or\ [(ac \in E(G))\ ,\ (b = d)\ ,\ (ac \notin Tri(G))] \\ d_G(a,c) & Otherwise \end{cases},$$

in which $Tri(G)$ is the set of all edges in triangles in G. Our main proof will consider the following two cases:

Case 1: Suppose $d_{G\otimes H}((a,b),(c,d)) = 3$. Then $[(ac \in E(G))\ ,\ (bd \notin E(H))\ ,\ (ac \notin Tri(G))]$ or $[(ac \in E(G))\ ,\ (b = d)\ ,\ (ac \notin Tri(G))]$. Let t_G be the number of triangles in G. If $ac \notin Tri(G)$ then the number of such edges are equal to $3 \cdot t_G$. This implies that the number of pairs $a, c \in E(G)$ is equal to $|E(G)| - 3t_G$. Similarly, the number of vertices b and d such that $bd \in E(H)$ is $(|V(H)^2) - |E(H)|$. Therefore, the number of pairs $(a,c),(b,d)$ with $W_P(G \otimes H) = 3$ is $[|E(G)| - 3t_G][(|V(H)^2) - |E(H)|]$.

Case 2: Suppose $d_{G\otimes H}((a,b),(c,d)) = d_G(a,c) = 3$. Then the number of pairs $(a,c),(b,d)$ such that $W_P(G \otimes H) = 3$ is $W_P(G).|V(H)|^2$. So, $W_p(G \otimes H) = W_P(G).|V(H)|^2 + [(|E(G)| - 3t_G)(|V(H)^2 - |E(H)|)]$, proving the theorem. □

We now consider the corona product of graphs.

Theorem 2.7. *Let G and H be graphs. Then the Wiener polarity index of GoH is equal to $W_p(G) + \sum_{i=1}^{|G|} t_i + |E(G)|.|V(G)|^2$ in which $t_i = |(\bigcup_{b\in N(v_i)}[N(b) - N(v_i)])| - 1$.*

Proof. We note that $d_{GoH}(a,b)$ is computed as follows:

$$d_{GoH}(a,b)=\begin{cases} 0 & a=c \\ d_G(a,b) & (a\neq b)\ ,\ (a,b\in V(G)) \\ 2, or, 1 & (a\neq b)\ ,\ (a,b\in H_i) \\ d_G(a,v_i)+1 & (a\in V(G))\ ,\ (b\in H_i) \\ d_G(v_i,v_j)+2 & (b\in V(H_j))\ ,\ (a\in H_i) \end{cases}.$$

We now assume that $d_{GoH}(a,b)=3$. Therefore at least one of the following hold:

(1) Let $(a\neq b)$, $(a,b\in V(G))$. In this case the number of pairs in GoH at distance 3 is equal to $W_P(G)$.

(2) Let $(a\in V(G))$, $(b\in H_i)$. In this case the number of pairs in GoH with distance 3 is equal to $\sum_{i=1}^{|G|} t_i$ in which t_i is the number of vertices in G by distance 3 from v_i, it is equal to $t_i=|(\bigcup_{b\in N(v_i)}[N(b)-N(v_i)])|-1$.

(3) Let $(b\in V(H_j))$, $(a\in H_i)$. In this case the number of pairs in GoH at distance 3 is equal to $|E(G)|.|V(G)|^2$.

Therefore, $W_p(GoH)=W_p(G)+\sum_{i=1}^{|G|} t_i+|E(G)|.|V(G)|^2$. □

Let G and H be two connected graphs, $u\in V(G)$ and $v\in V(H)$. The linked graph K is a graph with $V(K)=[(V(G))\cup(V(H))]$ and $E(K)=(E(G))\cup(E(H))\cup\{uv\}$, Figure 1. We end the paper by the following theorem:

Theorem 2.8. $W_p(K)=W_p(G)+W_p(H)+deg_G(u)deg_H(v)+d_G(u,2)+d_H(v,2)$.

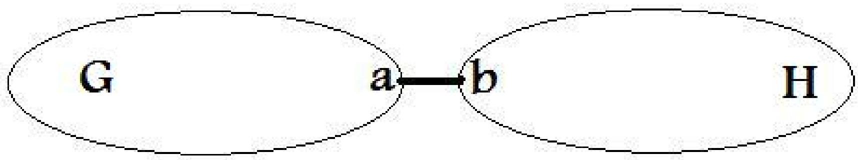

Figure 1. The Link of the Graphs G and H.

The link is an important graph operation with some application in chemistry. The models of some complex molecules can be built from simpler building block by iterating combining the link operation, see [6]. Let G and H be two simple and connected graphs with disjoint vertex sets and $a,b\in V(G)$ and $c,d\in V(H)$. A link of G and H by a and c is defined as the graph $(G\ H)(a;c)$ obtained by joining the vertices a and c by an edge. Similarly, a double link of G and H by (a,c) and (b,d) is defined as the graph $(G\ H)(a,b:c,d)$ obtained by joining a and c by an edge and b and d by another edge. A link and double link of two graphs are shown schematically in Figures 1 and 2.

Theorem 2.9. *Suppose that G and H are connected graphs and $a,b\in V(G)$ and $c,d\in V(H)$. Set $L_1=(G\ H)(a;c)$ and $(G\ H)(a,b:c,d)$. Then*

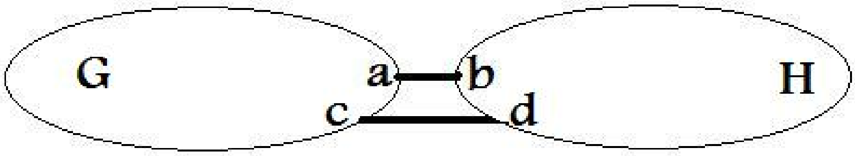

FIGURE 2. The Double Link of the Graphs G and H.

- $W_p(L_1) = W_p(G) + W_p(H) + d_G(a, 2) + d_H(b, 2) + deg_G(a)deg_H(b)$.
- $W_p(L_2) = W_p(G) + W_p(H) + d_G(a, 2) + d_H(b, 2) + d_G(c, 2) + d_H(d, 2) + deg_G(a)deg_H(b) + deg_G(c)deg_H(d) - |N_G(a) \cap N_G(c)| \cdot |N_G(c) \cap N_H(d)|$.

Proof. The first equality is a direct consequence of definition. To prove second, we consider three different cases as follows:

- *Two vertices are chosen from G.* The number of such pairs of distance 3 is equal to $W_p(G)$.
- *Two vertices are chosen from H.* The number of such pairs of distance 3 is equal to $W_p(H)$.
- *One vertex is chosen from G and another from H.* We have to count the number of pairs of vertices x, y of distance 3. To do this, we consider six subcases as follows:

  $x = a$ *and* $y \in H$. The number of such pairs are equal to $d_H(b, 2)$.
  $x \in G$ *and* $y = b$. The number of such pairs are equal to $d_G(a, 2)$.
  $x = c$ *and* $y \in H$. The number of such pairs are equal to $d_H(d, 2)$.
  $x \in G$ *and* $y = d$. The number of such pairs are equal to $d_G(c, 2)$.
  $x \in N_G(a)$ *and* $y \in N_H(b)$. The number of such pairs are equal to $deg_G(a) \cdot deg_H(b)$.
  $x \in N_G(c)$ *and* $y \in N_H(d)$. The number of such pairs are equal to $deg_G(c) \cdot deg_H(d)$.

Notice that in last two cases the vertices in $N_G(a) \cap N_G(c)$ and $N_G(b) \cap N_H(d)$ are counted twice. This completes our argument. □

Fullerenes are carbon cage molecules having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $20 \leq n(\neq 22)$ is an even integer. The discovery of the fullerene C_{60} in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [23, 24]. In the end of this paper, we apply Theorem 2.9 to compute the Wiener polarity index of a polybuckyball, Figure 3. The molecular graph of a polybuckyball is instructed by operations link or double link on the same IPR fullerene graphs on 60 vertices.

Corollary 2.10. *The Wiener polarity index of the first and second type polybuckyballs, that is made by n copies of C_{60} fullerene by operations link or double link is equal to* $561n - 615$ *and* $294n - 54$, *respectively.*

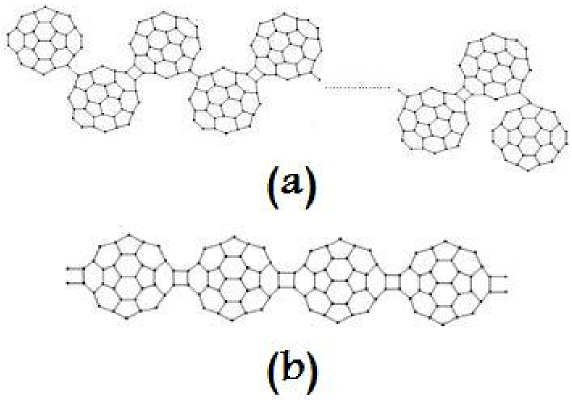

Figure 3. The Molecular Graph of a Polybuckyball a) of the first type; b) of the second type.

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