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 \(\text{Top}(G)\) for \(G\) is a number with this property that for every graph \(H\) isomorphic to \(G\), \(\text{Top}(G) = \text{Top}(H)\). 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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Let the distance be defined as follows:

Definition 1.1. Let $G$ and $H$ be simple connected graphs. The join $G + H$, symmetric difference $G \Delta H$, disjunction $G \lor H$, 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:

$V(G + H) = V(G) \cup V(H)$,

$E(G + H) = E(G) \cup E(H) \cup \{uv : u \in V(G), v \in V(H)\}$

$V(G \Delta H) = V(G) \times V(H)$,

$E(G \Delta H) = \{(a, b)(c, d) : ac \in E(G) \text{ or } bd \in E(H) \text{ not both}\}$

$E(G \lor H) = \{(a, b)(c, d) : ac \in E(G) \text{ or } bd \in E(H)\}$

$E(G[H]) = \{(a, b)(c, d) : ac \in E(G) \text{ or } a = c \text{ and } bd \in E(H)\}$

$E(G \times H) = \{(a, b)(c, d) : [ac \in E(G) \text{ and } b = d] \text{ or } [a = c \text{ and } bd \in E(H)]\}$

$E(G \odot H) = \{(a, b)(c, d) : [ac \in E(G) \text{ and } b = d] \text{ or } [a = c \text{ and } bd \in E(H)]\}$

$E(G \otimes H) = \{(a, b)(c, d) : [ac \in E(G) \text{ and } bd \in E(H)]\}$
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 $GΔH$ and the disjunction $G ∨ H$ are zero.

**Example 1.2.** The Wiener polarity index of the $n$–vertex path $P_n$ is $n - 3$ and for the cycle $C_n$, $n ≥ 7$ 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 $1 ≤ i ≤ n$ we define a set $M_i = \{x_i, x_{i+1}, ..., x_{i+6}\}$ 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 $u ∈ M_i$, $v ∈ M_{i+1}$ 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 $u = x_i$, $v ∈ M_{i+2}$ and $d_G(u, v) = 3$ is $\sum_{i=1}^n m_i + m_4 + ... + m_n$. Finally, if $u, v ∈ \{x_1, x_2, ..., x_n\}$ then the number of vertices with distance 3 is $n - 3$. Hence we have:

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

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 $G ∨ H$ we have $d_{G ∨ H}(u, v) ≤ 2$ and so the Wiener polarity index of $G ∨ H$ 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,

$$d_{G_1[G_2]}((a, b), (c, d)) = \begin{cases} 
0 & \text{if } a = c, \ b = d \\
1 & \text{if } (a = c), \ bd ∈ E(G_2), \text{ or } ac ∈ E(G_1) \\
2 & \text{if } (a = c), \ bd \notin E(G_2) \\
d_{G_1}(a, c) & \text{if } (a \neq c)
\end{cases}$$
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, \( WP(G_1[G_2]) = WP(G_1)[|V(G_1)|^2] \). Now assume that the result holds for \( k \), then

\[
WP(G_1[G_2][\ldots[G_k[G_{k+1}]]\ldots]) = WP(G_1)[(\prod_{i=2}^{k} |V(G_i)|)|V(G_{k+1})|]
\]

\[
= WP(G_1) \prod_{i=2}^{k+1} |V(G_i)|.
\]

This completes the proof. \( \square \)

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 \( G_1, G_2, \ldots, G_k \) be connected graphs. Then

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

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

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

where \( A_k = \{1, 2, \ldots, k\} \), \( e_i = |E(G_i)| \), \( d_i = d(G_i, 2) \), 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 \( d(G_1 \times G_2, 2) = d_1 v_2 + d_2 v_1 + 2 e_1 e_2.\)

Assume that the result holds for \( k \) then

\[
d(\prod_{i=1}^{k+1} G_i, 2) = d(\prod_{i=1}^{k} G_i, 2)v_{k+1} + d(G_{k+1}, 2)(\prod_{j=1}^{k} v_j) + 2e(\prod_{i=1}^{k} G_i)(e_{k+1})
\]

\[
= \sum_{i=1}^{k+1} [d_i \prod_{j=1, j \neq i}^{k} v_j]v_{k+1} + (d_{k+1})(\prod_{j=1}^{k} v_j)
\]

\[+ 2v_{k+1}[\sum_{i,j \in A_{k+1}, i < j} e_i e_j \prod_{l \neq i,j} v_l] + 2[\sum_{i=1}^{k+1} (e_i \prod_{j=1, i \neq j}^{k} v_j)](e_{k+1})
\]

\[= \sum_{i=1}^{k+1} d_i \prod_{j=1, j \neq i}^{k+1} v_j + 2[\sum_{i,j \in A_{k+1}, i < j} e_i e_j \prod_{l \neq i,j} v_l].\]
proving the lemma.

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

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 \( 2 e_2 d_1 \).
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 \( 2 e_1 d_2 \).

Therefore, \( W_p(\bigwedge_{i=1}^k G_i) = w_1 v_2 + w_2 v_1 + 2 e_2 d_1 + 2 e_1 d_2 \). Assume that the result holds for \( k \). Then the Lemma 2.2 implies that

\[
W_p(\bigwedge_{i=1}^{k+1} G_i) = W_p(\bigwedge_{i=1}^k G_i)\left[|V(\bigwedge_{i=1}^k G_i)| + |W_p(\bigwedge_{i=1}^k G_i)|v_{k+1} + 2|e_{k+1}|d_{k+1} \bigwedge_{i=1}^k G_i\right]
\]

\[ = w_{k+1} \left( \prod_{i=1}^{k+1} v_i \right) + \left( \sum_{i=1}^k (w_i \prod_{j=1, j \neq i}^k v_j) + 2 \sum_{i \neq j, i, j \in A_k} (e_i d_j \prod_{l \in A_k - \{i, j\}} v_l) \right) \\
+ 4 \sum_{i, j \in A_k, i < j < l} (e_i e_j e_l \prod_{p \in A_k - \{i, j, l\}} v_p) v_{k+1} + 2 e_{k+1} \sum_{i=1}^k d_i \prod_{j=1, j \neq i}^k v_j \]

\[ + 2 \sum_{i, j \in A_k, i < j} (e_i e_j \prod_{p \in A_k - \{i, j\}} v_p) + 2 e_{k+1} \sum_{i=1}^k (e_i \prod_{j=1, j \neq i}^k v_j) \]

\[ = \left( w_{k+1} \left( \prod_{i=1}^{k+1} v_i \right) + v_{k+1} \sum_{i=1}^k w_i \left( \prod_{j=1, j \neq i}^k v_j \right) \right) + 2 e_{k+1} \sum_{i \neq j, i, j \in A_k} (e_i d_j \prod_{l \in A_k - \{i, j\}} v_l) \]

\[ + 2 d_{k+1} \sum_{i=1}^k e_i \prod_{j=1, j \neq i}^k v_j + \left( 4 e_{k+1} \sum_{i \neq j, i, j \in A_k} e_i e_j \prod_{p \in A_k - \{i, j\}} v_p \right) \]

\[ + \left( 2 e_{k+1} \sum_{i=1}^k d_i \prod_{j=1, j \neq i}^k v_j + 4 v_{k+1} \sum_{i, j \in A_k, i < j < l} (e_i e_j e_l \prod_{p \in A_k - \{i, j, l\}} v_p) \right) \]

\[ = \sum_{i=1}^{k+1} (w_i \prod_{j=1, j \neq i}^k v_j) + 2 \sum_{i \neq j, i, j \in A_k} (e_i d_j \prod_{l \in A_k - \{i, j\}} v_l) \\
+ 4 \sum_{(i, j, l \in A_k, i < j < l)} (e_i e_j e_l \prod_{p \in A_k - \{i, j, l\}} v_p) \]
This completes the proof. \hfill $\square$

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

$$W_p(Q_n) = W_p(\prod_{i=1}^{n} K_2) = 4 \sum_{(i,j) \in A_n, i < j \leq l} (e_i e_j e_l) \prod_{p \in A_n - \{i,j,l\}} v_p$$

$$= 4 \sum_{(i,j) \in A_n, i < j < l} (2^{n-3}) = 4 \binom{n}{3} \times 2^{n-3} = \frac{n^3}{3} \times 2^{n-1}.$$ 

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

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

$$W_p(G \circ H) = W_p(G). \left\{ |V(H)| + |E(H)| + \sum_{i=1}^{\left\lfloor \frac{|H|}{2} \right\rfloor} \frac{(d_i)}{2} \right\}$$

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

**Proof.** We first notice that the following equality holds:

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

see [26] for details. Next we assume that $d_{G \circ H}((a, b), (c, d)) = 3$. 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 $G \circ H$ by distance 3 is equal to $W_p(H).|V(G)|$.
2. Let $d_H(b, d) = 3, a \in E(G)$. In this case the number of pairs in $G \circ H$ 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 $G \circ H$ at distance 3 is equal to $W_p(H).|\sum_{i=1}^{\left\lfloor \frac{|G|}{2} \right\rfloor} \binom{(d_i)}{2}|$.
4. Let $d_G(a, c) = 3, b = d$. In this case the number of pairs in $G \circ H$ 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 $G \circ H$ 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 $G \circ H$ at distance 3 is equal to $W_p(G).|\sum_{i=1}^{\left\lfloor \frac{|H|}{2} \right\rfloor} \binom{(d_i)}{2}|$.
7. Let $d_G(a, c) = 3, d_H(b, d) = 3$. In this case the number of pairs in $G \circ H$ at distance 3 is equal to $W_p(G).W_p(H)$. 


Let \( \mathcal{E} \) with \( W \) edges are equal to 3 · \( W \) equal to \( G \) triangular graph. Then the Wiener polarity index of tensor product

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

This completes the proof. \( \square \)

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 \( G \odot H \) is equal to \( W_p(G) |V(H)|^2 + [|E(G)| - 3t_G](|V(H)|^2 - |E(H)|) \).

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

\[
d_{G \odot H}((a, b), (c, d)) = \begin{cases} 
2 & \left[ (ac \in E(G)) , (bd \notin E(H)) , (ac \notin \text{Tri}(G)) \right] \\
3 & \left[ (ac \notin E(G)) , (bd \notin E(H)) , (ac \notin \text{Tri}(G)) \right] \\
& \left[ (ac \in E(G)) , (bd \in E(H)) , (ac \notin \text{Tri}(G)) \right] \\
& \text{or} \left[ (ac \in E(G)) , (bd \notin E(H)) , (ac \notin \text{Tri}(G)) \right] \\
& \text{or} \left[ (ac \in E(G)) , (bd = d) , (ac \notin \text{Tri}(G)) \right] \\
& \text{or} \left[ (ac \in E(G)) , (bd = d) , (ac \notin \text{Tri}(G)) \right] \\
\end{cases}
\]

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

**Case 1:** Suppose \( d_{G \odot H}((a, b), (c, d)) = 3 \). Then \( [(ac \in E(G)) , (bd \notin E(H)) , (ac \notin \text{Tri}(G))] \) or \( [(ac \notin E(G)) , (bd \notin E(H)) , (ac \notin \text{Tri}(G))] \). Let \( t_G \) be the number of triangles in \( G \). If \( ac \notin \text{Tri}(G) \) then the number of such edges are equal to 3 · \( t_G \). 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 \( W_p(G \odot H) = 3 \) is \( [|E(G)| - 3t_G]|(|V(H)|^2 - |E(H)|) \).

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

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 \( t_i = |\bigcup_{v \in N(v_i)} (N(b) - N(v_i))| - 1 \).
Proof. We note that $d_{GoH}(a, b)$ is computed as follows:

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

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, $W_p(GoH) = W_p(G) + \sum_{i=1}^{[G]} t_i + |E(G)|.|V(G)|^2$. \hfill \qed

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.](image)

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
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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.

References


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