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The hyper-Wiener index of graph operations

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ABSTRACT

Let G be a graph. The distance $d(u, v)$ between the vertices u and v of the graph G is equal to the length of a shortest path that connects u and v. The Wiener index $W(G)$ is the sum of all distances between vertices of G, whereas the hyper-Wiener index $WW(G)$ is defined as $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u, v)^2$. In this paper the hyper-Wiener indices of the Cartesian product, composition, join and disjunction of graphs are computed. We apply some of our results to compute the hyper-Wiener index of C_4 nanotubes, C_4 nanotori and q-multi-walled polyhex nanotori.

1. Introduction

Throughout this paper we consider graphs means simple connected graphs, connected graphs without loops and multiple edges. Suppose G is a graph with vertex set $V(G)$. The distance between the vertices u and v of $V(G)$ 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 Wiener index is one of the most studied topological indices, both from a theoretical point of view and applications. It is equal to the sum of distances between all pairs of vertices of the respective graph, see for details [1–5].

The hyper-Wiener index of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al. [6], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. 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 $d^2(u, v) = d(u, v)^2$. We encourage the reader to consult [7–13] for the mathematical properties of hyper-Wiener index and its applications in chemistry.

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 $G_1, G_2, \ldots, G_n$ are graphs then we denote $G_1 \times \cdots \times G_n$ by $\bigotimes_{i=1}^n G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\bigotimes_{i=1}^n G_i$ by G^n. The Wiener index of the Cartesian product graphs was studied in [14,15]. In [16], Klavzar, Rajapakse and Gutman computed the Szeged index of the Cartesian product graphs and the present authors computed some exact formulae for the vertex PI, edge PI, first Zagreb, second Zagreb and edge Szeged indices of product graphs, [17–20].

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. If $G = \underbrace{H + \cdots + H}_{n\ times}$ then we denote G by nH.

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V_1 \times V_2$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or ($u_1 = u_2$ and v_1 is adjacent with v_2), see [21, p. 22].

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The disjunction $G \vee H$ of graphs G and 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 symmetric difference $G \oplus H$ of two graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $E(G \oplus H) = \{(u_1, u_2)(v_1, v_2) \mid u_1v_1 \in E(G)$ or $u_2v_2 \in E(H)$ but not both$\}$. In [15], Sagan et al. computed some exact formulae for the Wiener polynomial of various graph operations containing Cartesian product, composition, join, disjunction and symmetric difference of graphs. In [22], the present authors computed the vertex PI and Szeged indices of the join and composition of graphs and in [19] the same calculations for the first and second Zagreb indices are done. The aim of this paper is to continue this program for computing the hyper-Wiener index of these operations on graphs.

Let G be a graph and $e = uv$ an edge of G. $m_u(e)$ denotes the number of edges lying closer to the vertex u than the vertex v, and $m_v(e)$ is the number of edges lying closer to the vertex v than the vertex u. The Padmakar–Ivan (PI) index of a graph G is defined as $PI(G) = \sum_{e \in E(G)}[m_u(e) + m_v(e)]$, see for details [23,24]. A vertex version of this index introduced by the present authors in [17]. In exact phrase, the vertex PI index of G, $PI_v(G)$, is the sum of $[n_u(e) + n_v(e)]$ over all edges of G, where $n_u(e)$ is the number of vertices lying closer to the vertex u than the vertex v and $n_v(e)$ is the number of vertices lying closer to the vertex v than the vertex u.

Throughout this paper our notation is standard and taken mainly from [25,26]. K_n denotes a complete graph on n vertices. IF H and G are graphs in which $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ then we call H to be a subgraph of G and write $H \leq G$. H is called a spanning subgraph of G, if $V(H) = V(G)$. A graph G is called to be a quasi multi-walled nanotorus (q-multi-walled nanotorus for short), if G is isomorphic to the direct product of a path P_n and an arbitrary nanotorus T, see [27].

2. Main results

In this section, some exact formulae for the hyper-Wiener index of the Cartesian product, composition, join, disjunction and symmetric difference of graphs are computed. We begin by computing the hyper-Wiener index of the Cartesian product of graphs. To do this, we need the following well-known theorem related to distance properties of the Cartesian product graphs. We encourage the reader to consult the book of Imrich and Klavzar [21], for more details.

Lemma 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.*

Theorem 1. *Let G and H be graphs. Then* $WW(G \times H) = |V(H)|^2WW(G) + |V(G)|^2WW(H) + 2W(G)W(H)$.

Proof. Set $V(G) = \{u_1, \ldots, u_m\}$ and $V(H) = \{v_1, \ldots, v_n\}$. Applying Lemma 1, we have:

$$\begin{aligned}
WW(G \times H) &= \frac{1}{2} \sum_{\{u,v\}\subseteq V(G\times H)} [d^2_{G\times H}(u, v) + d_{G\times H}(u, v)] \\
&= \frac{1}{4} \sum_{(u_i,v_k)} \sum_{(u_j,v_l)} [d^2_{G\times H}((u_i, v_k), (u_j, v_l)) + d_{G\times H}((u_i, v_k), (u_j, v_l))] \\
&= \frac{1}{4} \sum_{k,l=1}^{n} \sum_{i,j=1}^{m} [d^2_G(u_i, u_j) + d_G(u_i, u_j)] + \frac{1}{4} \sum_{i,j=1}^{m} \sum_{k,l=1}^{n} [d^2_H(v_k, v_l) \\
&\quad + d_H(v_k, v_l)] + \frac{1}{2} \left[\sum_{k,l=1}^{n} d_H(v_k, v_l)\right] \times \left[\sum_{i,j=1}^{m} d_G(u_i, u_j)\right] \\
&= |V(H)|^2WW(G) + |V(G)|^2WW(H) + 2W(G)W(H). \quad \square
\end{aligned}$$

Graovac and Pisanski [14], computed an exact formula for the Wiener index of the Cartesian product of graphs. In what follows, we first apply a similar method as Theorem 1 which is simpler than earlier proof to find an exact expression for the Wiener index of the Cartesian product of graphs.

$$\begin{aligned}
W(G \times H) &= \sum_{\{u,v\}\subseteq V(G\times H)} d_{G\times H}(u, v) \\
&= \frac{1}{2} \sum_{(u_i,v_k)} \sum_{(u_j,v_l)} d_{G\times H}((u_i, v_k), (u_j, v_l)) \\
&= \frac{1}{2} \sum_{k,l=1}^{n} \sum_{i,j=1}^{m} d_G(u_i, u_j) + \frac{1}{2} \sum_{i,j=1}^{m} \sum_{k,l=1}^{n} d_H(v_k, v_l) \\
&= |V(H)|^2W(G) + |V(G)|^2W(H).
\end{aligned}$$

By an inductive argument, one can see that $W\left(\bigotimes_{i=1}^n G_i\right) = |V|^2 \sum_{i=1}^n \frac{W(G_i)}{|V_i|^2}$, where $V = V\left(\bigotimes_{i=1}^n G_i\right)$.

Corollary. *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$, $1 \le i \le n$, and $V = V(\bigotimes_{i=1}^{n} G_i)$. Then*

$$WW\left(\bigotimes_{i=1}^{n} G_i\right) = |V|^2 \left(\sum_{i=1}^{n} \frac{WW(G_i)}{|V_i|^2} + \left[\sum_{i=1}^{n} \frac{W(G_i)}{|V_i|^2}\right]^2 - \sum_{i=1}^{n} \frac{W^2(G_i)}{|V_i|^4}\right).$$

In particular, $WW(G^n) = n|V(G)|^{2n-4}(|V(G)|^2 WW(G) + (n-1)W^2(G))$.

Proof. Applying an induction argument and Theorem 1, we have:

$$\begin{aligned} WW\left(\bigotimes_{i=1}^{n} G_i\right) &= WW\left(\bigotimes_{i=1}^{n-1} G_i \times G_n\right) \\ &= |V_n|^2 \left(\sum_{i=1}^{n-1} \frac{WW(G_i)}{|V_i|^2} + \left[\sum_{i=1}^{n-1} \frac{W(G_i)}{|V_i|^2}\right]^2 - \sum_{i=1}^{n-1} \frac{W^2(G_i)}{|V_i|^4}\right) \\ &\quad + WW(G_n)\frac{|V|^2}{|V_n|^2} + 2\frac{W(G_n)}{|V_n|^2}\sum_{i=1}^{n-1}\frac{W(G_i)}{|V_i|^2}|V|^2 \\ &= |V|^2 \left(\sum_{i=1}^{n} \frac{WW(G_i)}{|V_i|^2} + \left[\sum_{i=1}^{n} \frac{W(G_i)}{|V_i|^2}\right]^2 - \sum_{i=1}^{n} \frac{W^2(G_i)}{|V_i|^4}\right). \quad \square \end{aligned}$$

Example 1. Let P_n and C_n denote a path and cycle with n vertices, respectively. By [15], $W(P_n) = \frac{n(n^2-1)}{6}$ and $W(C_n) = \begin{cases} \frac{n^3}{8} & 2|n \\ \frac{n(n^2-1)}{8} & 2 \not| n \end{cases}$. By definition of hyper-Wiener index and a simple calculation with Maple 9.5, $WW(P_n) = \frac{1}{24}(n^4 + 2n^3 - n^2 - 2n)$ and $WW(C_n) = \begin{cases} \frac{n^2(n+1)(n+2)}{48} & 2|n \\ \frac{n(n^2-1)(n+3)}{48} & 2 \not| n \end{cases}$.

Consider a complete graph K_n. For arbitrary vertices $u, v \in V(K_n)$, $d(u, v) = 1$ and so between graphs with exactly n vertices, complete graph K_n has the minimum hyper-Wiener index. Hence for every n-vertex graph G, $WW(G) \ge WW(K_n) = \binom{n}{2}$. In [28], Ivan Gutman proved that the path P_n has the maximum value of the λ-th power of the distance for trees and it holds for all graphs as adding an edge the hyper-Wiener index will decrease. Therefore, for all n-vertex graph G, $WW(P_n) \ge WW(G)$.

Example 2. Yousefi-Azari et al. [20], computed the PI index of C_4 nanotubes and nanotori. In this example, we compute the hyper-Wiener index of these molecular graphs. Suppose R and S denote a C_4 nanotube and nanotorus, respectively. Then $R = P_n \times C_m$ and $S = C_k \times C_m$. In Example 1, the hyper-Wiener index of P_n and C_n are computed. Therefore, by Theorem 1,

$$WW(R) = \begin{cases} \frac{1}{48}(m^4n^2 + 2m^3n^3 + 2m^2n^4 + 3m^3n^2 + 4m^2n^3 - 2m^2n^2 - 2m^3n - 4m^2n + 2n^2) & 2|m \\ \frac{1}{48}(m^4n^2 + 2m^3n^3 + m^2n^4 + 3m^3n^2 + 2m^2n^3 - 2m^2n^2 \\ \quad - 2m^3n - 2mn^3 - 2m^2n - 3mn^2 + 2mn) & 2 \not| m \end{cases}$$

$$WW(S) = \begin{cases} \frac{1}{96}(2m^4n^2 + 3m^3n^3 + 6m^3n^2 + 8m^2n^2 + 6m^2n^3 + 2m^2n^4) & m\&n \text{ are even} \\ \frac{1}{96}(2m^4n^2 + 3m^3n^3 + 6m^3n^2 - 3m^3n + 2m^2n^4 + 6m^2n^3 + 2m^2n^2 - 6m^2n) & m+n \text{ is odd} \\ \frac{1}{96}(2m^4n^2 + 3m^3n^3 + 6m^3n^2 - 3m^3n - 4m^2n^2 + 2m^2n^4 \\ \quad + 6m^2n^3 - 6m^2n - 3mn^3 - 6mn^2 + 3mn) & m \,\&\, n \text{ are odd.} \end{cases}$$

Example 3. Consider the graph G whose vertices are the r-tuples $b_1b_2\cdots b_N$ with $b_i \in \{0, 1, \ldots, n_i - 1\}$, $n_i \ge 2$, and let two vertices be adjacent if the corresponding tuples differ in precisely one place. Such a graph is called a Hamming graph. It is well-known fact that a graph G is a Hamming graph if and only if it can be written in the form $G = \bigotimes_{i=1}^{N} K_{n_i}$. By the previous corollary, it is possible to compute the hyper-Wiener index of a Hamming graph, but we consider only the case that $b_1 = b_2 = \cdots = b_N = 2$. Such a graph is called a hypercube of dimension N and denoted by Q_N. Then, $WW(Q_N) = 2^{2N-4}(N^2 + 3N)$.

Example 4. Yousefi and Ashrafi [29], computed an exact formula for computing the Wiener index of a polyhex nanotorus $T = T[p, q]$. Here p and q denote the number vertical zigzags and rows, respectively. They proved that:

$$W(T)=\begin{cases}\dfrac{pq^2}{24}(6p^2+q^2-4) & q<p\\ \dfrac{p^2q}{24}(3q^2+p^2+3pq-4) & q\geq p.\end{cases}$$

The present authors [30] computed the hyper-Wiener index of a polyhex nanotorus. We apply Theorem 1 to compute the hyper-Wiener index of q-multi-walled nanotube $R = P_n \times T$. Using a tedious calculation, we have:

$$WW(R)=\begin{cases}\dfrac{1}{576}[12p^2q^2n^4+(24p^3q^2+24p^2q^2+4pq^4-16pq^2)n^3+(36p^2q^2+18pq^5)n^2\\ \quad-(72pq^3+24p^3q^2+4pq^5+24p^2q^2-16pq^2)n] \quad q\leq p\\ \dfrac{1}{576}[12p^2q^2n^4+(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-16p^2q)n^3\\ \quad+(168p^3q+318p^5q+576p^4q+48pq^3-288p^3q^2+24p^2q^4\\ \quad+36p^3q^3-168p^4q^2+pq^5-12p^2q^2)n^2\\ \quad-(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-16p^2q)n] \quad p=\frac{q}{2}\\ \dfrac{1}{576}[12p^2q^2n^4+(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-36p^2q)n^3\\ \quad+(12p^2q^2-120p^2q+30p^5q+24p^2q^4+72p^2q^3+96p^2q^2+36p^3q^3+24p^4q^2)n^2\\ \quad-(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-36p^2q)n] \quad p<\frac{q}{2}\\ \dfrac{1}{576}[12p^2q^2n^4+(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-36p^2q)n^3\\ \quad+(-12p^2q^2-120p^3q-72pq^3+24p^4q^2+96p^2q^2+20p^5q+24p^2q^4+36p^3q^3)n^2\\ \quad-(24p^2q^2+12p^2q^3+12p^3q^2+4p^4q-36p^2q)n] \quad \frac{q}{2}<p<q.\end{cases}$$

In what follows we prove an elementary lemma which is crucial in computing the hyper-Wiener index of composition of graphs.

Lemma 2. *Let G_1 and G_2 be graphs. If G_1 is connected, $|V(G_1)| > 1$ and $G = G_1[G_2]$ then for every vertex $(u_1, v_1), (u_2, v_2) \in V(G)$ we have:*

$$d_G((u_1,v_1),(u_2,v_2))=\begin{cases}d_{G_1}(u_1,u_2) & u_1\neq u_2\\ 0 & u_1=u_2\ \&\ v_1=v_2\\ 1 & u_1=u_2\ \&\ v_1v_2\in E_2\\ 2 & u_1=u_2\ \&\ v_1v_2\notin E_2.\end{cases}$$

Proof. Suppose $u_1u_2 \in E_1$. Then for every vertex $v_1, v_2 \in V_2$, $d_G((u_1, v_1), (u_2, v_2)) = 1 = d_{G_1}(u_1, u_2)$. Therefore, for every u_1u_2 not in E_1, $d_G((u_1, v_1), (u_2, v_2)) <= d_{G_1}(u_1, u_2)$ and if $d_G((u_1, v_1), (u_2, v_2)) < d_{G_1}(u_1, u_2) = p$ then there is a path $(u_1, v_1)(a_1, b_1)\ldots(a_q, b_q)(u_2, v_2)$ in G such that $q + 1 < p$. But by definition $u_1a_1a_2\ldots a_qu_2$ is a path in G_1 and this means $q + 1 = p$. So $d_G((u_1, v_1), (u_2, v_2)) = d_{G_1}(u_1, u_2)$. Other cases are immediate consequences of the definition. □

Theorem 2. *Let G and H be graphs. Then $WW(G + H) = \frac{3}{2}|(V(G))|^2 + \frac{3}{2}|V(H)|^2 - 2|E(H)| - 2|(E(G))| - \frac{3}{2}|V(G)| - \frac{3}{2}|V(H)| + |V(G)||V(H)|$.*

Proof. By definition of the join of two graphs, one can see that,

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

Therefore, $WW(G+H) = \frac{1}{4}\sum_{\{u,v\}\subseteq V(G+H)}[d^2_{G+H}(u, v)+d_{G+H}(u, v)] = \frac{1}{4}\sum_{v\in V(G)}[2\deg_G(v)+6(|V(G)|-\deg_G(v)-1)+2|V(H)|]+\frac{1}{4}\sum_{v\in V(H)}[2\deg_H(v)+6(|V(H)|-\deg_H(v)-1)+2|V(G)|] = \frac{3}{2}|(V(G))|^2+\frac{3}{2}|V(H)|^2-2|E(H)|-2|(E(G))|-\frac{3}{2}|V(G)|-\frac{3}{2}|V(H)|+|V2(G)||V(H)|$, as desired. □

Corollary. *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$ and $E_i = E(G_i)$, $1 \leq i \leq n$. Then*

$$WW(G_1+\cdots+G_n)=\sum_{i=1}^{n}\left(3\binom{|V_i|}{2}-2|E_i|\right)+\frac{1}{2}\sum_{i\neq j,i,j=1}^{n}|V_i||V_j|.$$

In particular, $WW(nG) = \frac{1}{2}(n^2 + 2n)|V(G)|^2 - 2n|E(G)| - \frac{3n}{2}|V(G)|$.

Proof. Apply Theorem 2 and an inductive argument. □

Example 5. Consider a complete n-partite graph $G = K_{m_1,m_2,\ldots,m_n}$ containing $v = |V(G)|$ vertices. By definition of this graph, $V = V(G)$ can be partitioned into subsets $V_1, V_2, \ldots, V_n$ of V such that for every i, $1 \le i \le n$, there is no edge between the vertices of V_i. It is easy to see that $K_{m_1,m_2,\ldots,m_n}$ is the join of n empty graphs $G_1, \ldots, G_n$ with exactly $m_1, \ldots, m_n$ vertices, respectively. So by previous corollary $WW(K_{m_1,m_2,\ldots,m_n}) = 3\sum_{i=1}^{n}\binom{m_i}{2} + \frac{1}{2}\sum_{i\neq j,i,j=1}^{n} m_i m_j$.

Theorem 3. *Let G and H be graphs and G be connected. Then* $WW(G[H]) = |V(H)|^2 WW(G) + 3|V(G)|\binom{|V(H)|}{2} - 2|V(G)||E(H)| = |V(H)|^2 WW(G) + \frac{|V(G)|}{2}(WW(2H) - |V(H)|^2)$.

Proof. Set $V(G) = \{u_1, \ldots, u_m\}$ and $V(H) = \{v_1, \ldots, v_n\}$. Then by Lemma 2, we have:

$$\begin{aligned}
WW(G[H]) &= \frac{1}{2}\sum_{\{u,v\}\subseteq V(G[H])}[d^2_{G[H]}(u,v) + d_{G[H]}(u,v)] \\
&= \frac{1}{4}\sum_{(u_i,v_k)}\sum_{(u_j,v_l)}[d^2_{G[H]}((u_i,v_k),(u_j,v_l)) + d_{G[H]}((u_i,v_k),(u_j,v_l))] \\
&= \frac{1}{4}\sum_{p=1}^{m}\sum_{k,l=1}^{n}[d^2_{G[H]}((u_p,v_k),(u_p,v_l)) + d_{G[H]}((u_p,v_k),(u_p v_l))] \\
&\quad + \frac{1}{4}\sum_{k,l=1}^{n}\sum_{i\neq j,i,j=1}^{m}[d^2_{G[H]}((u_i,v_k),(u_j,v_l)) + d_{G[H]}((u_i,v_k),(u_j v_l))] \\
&= \frac{1}{4}\sum_{p=1}^{m}\sum_{i=1}^{n}[2\deg_H(v_i) + 6(|V(H)| - \deg_H(v_i) - 1)] + |V(H)|^2 WW(G) \\
&= |V(H)|^2 WW(G) + 3|V(G)|\binom{|V(H)|}{2} - 2|V(G)||E(H)|.
\end{aligned}$$

The second equality is an immediate consequence of Theorem 2. □

Lemma 3. *Let G and H be connected graphs. Then*

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

Proof. The first two cases of the expression of $d_{G\vee H}((a,b),(c,d))$ are immediate consequences of the definition of disjunction. Suppose $(a,c) \neq (b,d)$, $ac \notin E(G)$ and $bd \notin E(H)$. Therefore, $d_{G\vee H}((a,b),(c,d)) > 1$. Since G and H are connected, there exist $x \in V(G)$ and $y \in V(H)$ such that $ax \in E(G)$ and $dy \in E(H)$. So $d_{G\vee H}((a,b),(x,y)) = d_{G\vee H}((c,d),(x,y)) = 1$, proving the lemma. □

Suppose G is a graph and $x \in V(G)$. Define $d(x,G) = \sum_{y\in G} d(x,y)$ and $d^2(x,G) = \sum_{y\in V(G)} d^2(x,y)$.

Theorem 4. *Let G and H be graphs. Then* $WW(G\vee H) = 3\binom{|V(G)||V(H)|}{2} + 4|E(G)||E(H)| - 2|V(H)|^2|E(G)| - 2|V(G)|^2|E(H)|$.

Proof. It is sufficient to count the number of vertices of unit distance from a fixed vertex (a,b). By definition and Lemma 3, $|\{v \in V(G\vee H) \mid d_{G\vee H}((a,b),v) = 1\}| = |\{(c,d) \mid ac \in E(G)\}| + |\{(c,d) \mid bd \in E(H)\}| - |\{(c,d) \mid ac \in E(G) \,\&\, bd \in E(H)\}| = \deg_G(a)|V(H)| + \deg_H(b)|V(G)| - \deg_G(a)\deg_H(b)$. Since $|V(G\vee H)| = |V(G)||V(H)|$, $d^2((a,b),G\vee H) + d((a,b),G\vee H) = 6|V(G)||V(H)| - 4\deg_G(a)|V(H)| - 4\deg_H(b)|V(G)| + 4\deg_G(a)\deg_H(b) - 6$. Therefore, $WW(G\vee H) = \frac{1}{4}\sum_{v\in V(H)}\sum_{u\in V(G)}[6|V(G)||V(H)| - 4\deg_G(u)|V(H)| - 4\deg_H(v)|V(G)| + 4\deg_G(u)\deg_H(v) - 6] = 3\binom{|V(G)||V(H)|}{2} + 4|E(G)||E(H)| - 2|V(H)|^2|E(G)| - 2|V(G)|^2|E(H)|$, as desired. □

Using similar arguments as Lemma 3 and Theorem 4, one can prove the following results:

Lemma 4. *Let G and H be connected graphs. Then*

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

Theorem 5. *Let G and H be connected graphs. Then* $WW(G\oplus H) = 3\binom{|V(G)||V(H)|}{2} + 8|E(G)||E(H)| - 2|V(H)|^2|E(G)| - 2|V(G)|^2|E(H)|$. □

We end the paper with the following simple but elegant lemma:

Lemma 5. *Let H be a spanning subgraph of G then $WW(H) \geq WW(G)$.*

Proof. The proof is straightforward and omitted. $\square$

Using Lemmas 1(d) and 5, one can see that for arbitrary connected graphs G and H, since $G \times H \leq G[H] \leq G \vee H$, $WW(G \times H) \geq WW(G[H]) \geq WW(G \vee H)$ and $WW(G \times H) \geq WW(H[G]) \geq WW(G \vee H)$. On the other hand, $G \times H \leq G \oplus H \leq G \vee H$ and so $WW(G \times H) \geq WW(G \oplus H) \geq WW(G \vee H)$.

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References

[1] A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.
[2] A.A. Dobrynin, I. Gutman, S. Klavzar, P. Zigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
[3] I. Gutman, S. Klavzar, B. Mohar (Eds.), Fifty years of the Wiener index, MATCH Commun. Math. Comput. Chem. 35 (1997), 1259.
[4] I. Gutman, S. Klavzar, B. Mohar (Eds.), Fiftieth anniversary of the Wiener index, Discrete Appl. Math. 80 (1) (1997), 1113.
[5] H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.
[6] D.J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, J. Chem. Inf. Comput. Sci. 35 (1995) 50–52.
[7] G.G. Cash, Relationship between the Hosoya polynomial and the Hyper-Wiener index, Appl. Math. Lett. 15 (2002) 893–895.
[8] G.G. Cash, Polynomial expressions for the hyper-Wiener index of extended hydrocarbon networks, Comput. Chem. 25 (2001) 577–582.
[9] I. Gutman, Relation between hyper-Wiener and Wiener index, Chem. Phys. Lett. 364 (2002) 352–356.
[10] S. Klavzar, P. Zigert, I. Gutman, An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons, Comput. Chem. 24 (2000) 229–233.
[11] S. Klavzar, I. Gutman, A theorem on Wiener-type invariants for isometric subgraphs of hypercubes, Appl. Math. Lett. 19 (2006) 1129–1133.
[12] X. Li, A.F. Jalbout, Bond order weighted hyper-Wiener index, J. Mol. Structure (Theochem) 634 (2003) 121–125.
[13] B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett. 394 (2004) 93–95.
[14] A. Graovac, T. Pisanski, On the Wiener index of a graph, J. Math. Chem. 8 (1991) 53–62.
[15] B.E. Sagan, Y.-N. Yeh, P. Zhang, The Wiener polynomial of a graph, Int. J. Quant. Chem. 60 (5) (1996) 959–969.
[16] S. Klavzar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, Appl. Math. Lett. 9 (1996) 45–49.
[17] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, Vertex and edge PI indices of cartesian product graphs, Discrete Appl. Math. (2007) doi:10.1016/j.dam.2007.08.041.
[18] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, I. Gutman, The Edge Szeged Index of Product Graphs, Croat. Chem Acta, 81 (2) (2008) (in press).
[19] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, The first and second zagreb indices of graph operations (in press).
[20] H. Yousefi-Azari, B. Manoochehrian, A.R. Ashrafi, The PI index of product graphs, Appl. Math. Lett. 21 (6) (2008) 624–627.
[21] W. Imrich, S. Klavzar, Product Graphs: Structure and Recognition, Wiley, New York, USA, 2000.
[22] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, A matrix method for computing szeged and vertex pi indices of join and composition of graphs, Linear Algebra Appl. (2008) doi:10.1016/j.laa.2008.01.015.
[23] P.V. Khadikar, On a novel structural descriptor PI, Nat. Acad. Sci. Lett. 23 (2000) 113–118.
[24] A.R. Ashrafi, A. Loghman, PI index of zig-zag polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 55 (2) (2006) 447–452.
[25] M.V. Diudea, I. Gutman, L. Jantschi, Molecular Topology, Huntington, NY, 2001.
[26] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.
[27] H. Yousefi-Azari, A.R. Ashrafi, Padmakar-Ivan Index of q-Multi-walled Carbon Nanotubes and Nanotori, J. Comput. Theor. Nanosci. (in press).
[28] I. Gutman, A property of the Wiener number and its modifications, Indian J. Chem. 36A (1997) 128–132.
[29] S. Yousefi, A.R. Ashrafi, An Exact expression for the wiener index of a polyhex nanotorus, MATCH Commun. Math. Comput. Chem. 56 (2006) 169–178.
[30] S. Yousefi, H. Yousefi-Azari, A.R. Ashrafi, M.H. Khalifeh, Computing Distance Matrix and Related Topological Indices of a Polyhex Nanotorus (submitted for publication).