Chapter 13
The Edge-Wiener Index and Its Computation for Some Nanostructures

Ali Iranmanesh

Abstract The first and the second edge versions of Wiener index, which were based on the distance between two edges in a connected graph G, were introduced by Iranmanesh et al. in (MATCH Commun Math Comput Chem 61:663, 2009).

In this chapter, at first we obtain the explicit relation between different versions of Wiener number and due to this relation, the edge-Wiener numbers of some graph have been computed. Then we find the first edge-Wiener index of the composition and sum of graphs. As an application of our results, we find the first and the second edge-Wiener indices of some nanostructures.

13.1 Introduction

Topological indices are numerical descriptors derived from the associate graphs of chemical compounds. Some indices based on the distances in graph are widely used in establishing relationships between the structure of molecules and their physico-chemical properties. Usage of topological indices in chemistry began in 1947 when the chemist Harold Wiener introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs (Wiener 1947). Wiener originally defined his index (W) on trees and studied its use for correlations of physicochemical properties of alkanes, alcohols, amines and analogous compounds (Khadikar and Karmarkar 2002). Starting from the middle of the 1970s, the Wiener index gained much popularity and, since then, new results related to it are constantly being reported. For a review, historical details and further bibliography on the chemical applications of the Wiener index see, Gutman et al. (1993, 1997) and Nikoli'c et al. (1995).

A. Iranmanesh (✉)
Department of Mathematics, Tarbiat Modares University, P.O. Box: 14115-137, Tehran, Iran
e-mail: iranmanesh@modares.ac.ir

A.R. Ashrafi et al. (eds.), *Topological Modelling of Nanostructures and Extended Systems*, Carbon Materials: Chemistry and Physics 7, DOI 10.1007/978-94-007-6413-2_13,

Let G be a connected graph. The vertex set and edge set of G denoted by $V(G)$ and $E(G)$, respectively. The distance between the vertices u and v, $d(u, v)$, in a graph is the number of edges in a shortest path connecting them. Two graph vertices are adjacent if they are joined by a graph edge. The degree of a vertex $i \in V(G)$ is the number of vertices joining to i and denoted by δ_i.

The Wiener index of G is

$$W(G) = W_v(G) = \sum_{\{x,y\} \subseteq V(G)} d(x, y) \tag{13.1}$$

The edge versions of Wiener index which were based on the distance between edges introduced by Iranmanesh et al. (2009). These versions have been introduced for a connected graph G as the first and second edge-Wiener, that is, the first edge-Wiener number was introduced as follows:

$$W_{e0}(G) = \sum_{\{e,f\} \subseteq E(G)} d_0(e, f) \tag{13.2}$$

where $d_0(e, f) = \begin{cases} d_1(e, f) + 1 & e \neq f \\ 0 & e = f \end{cases}$ and $d_1(e, f) = \min\{d(x, u), d(x, v), d(y, u), d(y, v)\}$ such that $e = xy$ and $f = uv$. This version satisfies in $W_{e0}(G) = W_v(L(G))$.

The second edge-Wiener index was introduced as follows:

$$W_{e4}(G) = \sum_{\{e,f\} \subseteq E(G)} d_4(e, f) \tag{13.3}$$

where $d_4(e, f) = \begin{cases} d_2(e, f) & e \neq f \\ 0 & e = f \end{cases}$ and $d_2(e, f) = \max\{d(x, u), d(x, v), d(y, u), d(y, v)\}$ such that $e = xy$ and $f = uv$.

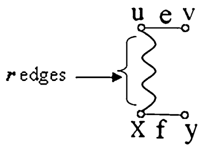
In this chapter, at first we obtain the explicit relation between different versions of Wiener number and due to this relation, the edge-Wiener numbers of some graph have been computed and then we compute the first and the second edge-Wiener indices of zigzag nanotube and TUC_4C_8(R) and TUC_4C_8(S) nanotubes.

In Sects. 13.3 and 13.4, we find the first edge-Wiener index of the composition and sum of graphs, respectively. As an application of our results, we find the first and the second edge-Wiener indices of C_4-nanotubes and C_4-nanotori.

13.2 Explicit Relation Between Vertex and Edge-Wiener Numbers

In this section, we restate some definitions and then we give an explicit relation between vertex and edge-Wiener indices. All of the results in the first part of this section have been published in Iranmanesh and Khormali (2011).

Fig. 13.1 The edges of *e* and *f* are not adjacent



We recall the conditions of the distances. d is the distance on set X if it satisfies in the following conditions:

(a) $\forall u, v \in X; \quad d(u,v) \geq 0$
(b) $\forall u, v \in X; \quad u = v \Leftrightarrow d(u,v) = 0$
(c) $\forall u, v \in X; \quad d(u,v) = d(v,u)$
(d) $\forall u, v, w \in X; \quad d(u,v) + d(v,w) \geq d(u,w)$

At first, we restate the first edge-Wiener number according to the distances between vertices.

Definition 13.2.1 Let $e = uv$, $f = xy$ be the edges of connected graph G. Then, we define $d'(e,f) = \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$ and $d''(e,f) = \begin{cases} \lceil d'(e,f) \rceil, & \{e,f\} \notin C \\ d'(e,f)+1, & \{e,f\} \in C \end{cases}$, where $C = \{\{e,f\} \subseteq E(G) \mid$ if $e = uv$ and $f = xy$; $\{d(u,x) = d(u,y) = d(v,x) = d(v,x)\}$ and $d_3(e,f) = \begin{cases} d''(e,f) & e \neq f \\ 0 & e = f \end{cases}$. Also, d' and d'' do not satisfy the condition (b), hence, they are not a distance and are like distance.

Claim $d_3 = d_0$.

Proof We have to show for any $e, f \in E(G)$, $d_3(e,f) = d_0(e,f)$.

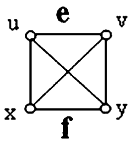
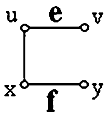
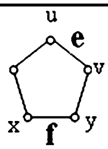
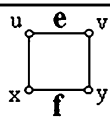
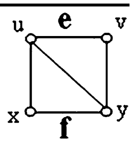
(i) If $e = f \in E(G)$, then $d_3(e,f) = d_0(e,f) = 0$.
(ii) If $e, f \in E(G)$ are adjacent edges, then,

$$d_0(e,f) = d_1(e,f) + 1 = 0 + 1 = 1 \text{ and } d_3(e,f) = d_2(e,f)$$
$$= \left\lceil \frac{1+1+2}{4} \right\rceil = 1. \text{ Therfore, } d_3(e,f) = d_0(e,f).$$

(iii) If $e, f \in E(G)$ are not adjacent such as Fig. 13.1, then:

1. If $\{e,f\} \notin C$, then $d_0(e,f) = d_1(e,f) + 1 = r + 1$ and $d_3(e,f) = d''(e,f) = \left\lceil \frac{r+(r+1)+(r+1)+(r+2)}{4} \right\rceil = r+1$. Therefore, $d_3(e,f) = d_0(e,f)$.
2. If $\{e,f\} \in C$, then $d_0(e,f) = d_1(e,f) + 1 = r + 1$ and $d_3(e,f) = d''(e,f) = \frac{r+r+r+r}{4} + 1 = r + 1$. Therefore, $d_3(e,f) = d_0(e,f)$. ∎

Table 13.1 Examples for sets which have been defined above

Set	C	A_1	A_2	A_3	A_4
Example					
d'	1	2	$\frac{7}{4}$	$\frac{6}{4}$	$\frac{5}{4}$
$d_3 = d_0$	2	2	2	2	2

Corollary 13.2.2

$$W_{e0}(G) = \sum_{\{e,f\}\subseteq E(G)} d_3(e, f).$$

Proof Since $d_3 = d_0$, we obtain the desired result. ∎

Before stating the explicit relations, we define several sets due to the distance d_3 as follow:

$$A_1 = \big\{\{e, f\} \subseteq E(G) \,\big|\, d_3(e, f) = d'(e, f)\big\},$$

$$A_2 = \left\{\{e, f\} \subseteq E(G) \,\middle|\, d_3(e, f) = d'(e, f) + \frac{1}{4}\right\},$$

$$A_3 = \left\{\{e, f\} \subseteq E(G) \,\middle|\, d_3(e, f) = d'(e, f) + \frac{2}{4}\right\},$$

$$A_4 = \left\{\{e, f\} \subseteq E(G) \,\middle|\, d_3(e, f) = d'(e, f) + \frac{3}{4}\right\}.$$

We denote all of the two element subsets of $E(G)$ with S and therefore $|S| = \binom{|E(G)|}{2}$. Also, we have: $S = A_1 \cup A_2 \cup A_3 \cup A_4 \cup C$ (Table 13.1).

Due to Definition 13.2.1 and Corollary 13.2.2, the relation between vertex and first edge versions of Wiener index has been defined.

Theorem 13.2.3 *Suppose G is a graph with m edges and* A_1, A_2, A_3, A_4 and C *are the sets which have been defined as above. Then, the first version of edge-Wiener number according to the distance between vertices of graph G is*

$$W_{e0}(G) = \frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)} \deg(x)\times\deg(y)\times d(x,y) - \frac{m}{4}+$$
$$\sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right) + \sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right) + \sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right) + |C|. \tag{13.4}$$

Proof By Definition 13.2.1 and Corollary 13.2.2, we have

$$\begin{aligned}
W_{e0}(G) &= \sum_{\{e,f\}\subseteq E(G)} d_3(e,f)\\
&= \sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv, f=xy}} \left\lceil \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\right\rceil\\
&= \sum_{\substack{\{e,f\}\in A_1\\ if\ e=uv, f=xy}} \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\\
&\quad + \sum_{\substack{\{e,f\}\in A_3\\ if\ e=uv, f=xy}} \left(\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}+\frac{1}{2}\right)\\
&\quad + \sum_{\substack{\{e,f\}\in A_2\\ if\ e=uv, f=xy}} \left(\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}+\frac{1}{4}\right)\\
&\quad + \sum_{\substack{\{e,f\}\in A4\\ if\ e=uv, f=xy}} \left(\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}+\frac{3}{4}\right)\\
&\quad + \sum_{\substack{\{e,f\}\in C\\ if\ e=uv, f=xy}} \left(\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}+1\right)\\
&= \sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv, f=xy}} \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\\
&\quad + \sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right) + \sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right) + \sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right) + |C|
\end{aligned}$$

For each pair of vertices $u, x \in V(G)$ such that $u \neq x$ which are not adjacent, the distance $d(u,x)$ in like distance d' is repeated $\deg(u)\times\deg(x)$ times. And if every pair of vertices $u, x \in V(G)$, $u \neq x$, is adjacent, distance $d(u,x)$ is repeated $\deg(u)\times\deg(x) - 1$ times. Therefore,

$$W_{e0}(G) = \frac{1}{8} \sum_{x \in V(G)} \sum_{y \in V(G)} \deg(x) \times \deg(y) \times d(x, y) - \frac{m}{4} +$$

$$\sum_{\{e,f\} \in A_3} \left(\frac{1}{2}\right) + \sum_{\{e,f\} \in A_2} \left(\frac{1}{4}\right) + \sum_{\{e,f\} \in A_4} \left(\frac{3}{4}\right) + |C|.$$

∎

Now, because of the fact that the first edge-Wiener number has been written by distances between vertices, we repeat this trend for second edge version with definition of new distance.

Definition 13.2.4 If $e, f \in E(G)$, we define

$$d'''(e, f) = \begin{cases} \lceil d'(e, f) \rceil & , \{e, f\} \notin A_1 \\ d'(e, f) + 1 & , \{e, f\} \in A_1 \end{cases} \text{ and } d_5(e, f) = \begin{cases} d'''(e, f) & e \neq f \\ 0 & e = f \end{cases}.$$

The mathematical quantity d''' is not distance because it does not satisfy the condition (b). Then, we say d''' is likedistance.

Claim $d_5 = d_4$.

Proof We have to show for any $e, f \in E(G)$, $d_5(e, f) = d_4(e, f)$.

(i) If $e = f \in E(G)$, then $d_5(e, f) = d_4(e, f) = 0$.
(ii) If $e, f \in E(G)$ are adjacent edges, then:
$d_4(e, f) = d_2(e, f) = 2$ and since $\{e, f\} \in A_1$, $d_5(e, f) = d_3(e, f) + 1 = \frac{1+1+2}{4} + 1 = 2$. Therefore, $d_5(e, f) = d_4(e, f)$ ..
(iii) If $e, f \in E(G)$ are not adjacent, then we have two sub-cases:

1. If $\{e, f\} \in A_1$ such as Fig. 13.1, then
$d_4(e, f) = d_2(e, f) = r + 2$ and $d_5(e, f) = d_3(e, f) + 1 = \frac{r+(r+1)+(r+1)+(r+2)}{4} + 1 = r + 2$. Therefore, $d_5(e, f) = d_4(e, f)$.
2. If $\{e, f\} \notin A_1$, then
If $d_4(e, f) = d_2(e, f) = r$, then $\max\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ is r and r is repeated at least two times in $d(u, x) + d(u, y) + d(v, x) + d(v, y)$ for d'. Hence,
$d(i, j)$, $i = u, v$ and $j = x, y$, takes r or $(r - 1)$, then $d_5(e, f) = d_3(e, f) = \left\lceil \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4} \right\rceil = r$. Therefore, $d_5(e, f) = d_4(e, f)$.

∎

Corollary 13.2.5 $W_{e4}(G) = \sum_{\{e,f\} \subseteq E(G)} d_5(e, f)$.

Theorem 13.2.6 *Suppose G is a graph with m edges and* A_1, A_2, A_3, A_4 and C *are the sets which have been defined in Definition* 13.2.1 *and Corollary* 13.2.2. *Then, we can repeat the second version of edge-Wiener number according to the distance between vertices of graph G as follows*:

$$W_{e4}(G) = \frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)} \deg(x)\times\deg(y)\times d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right) + \sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right) + \sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right) + |A_1|. \tag{13.5}$$

Proof Due to the definition of $W_{e4}(G)$ and Definition 13.2.4 and Corollary 13.2.5, we have

$$W_{e4}(G) = \sum_{\{e,f\}\subseteq E(G)} d_5(e,f) = \sum_{\{e,f\}\subseteq E(G)} d'''(e,f) = \sum_{\{e,f\}\subseteq E(G)} d'(e,f) + \sum_{\{e,f\}\in A_2}\frac{1}{4} + \sum_{\{e,f\}\in A_3}\frac{2}{4} + \sum_{\{e,f\}\in A_4}\frac{3}{4} + |A_1|\,.$$

For each pair of vertices u and x such that $u \neq x$ which is not adjacent, the distance $d(u,x)$ in like-distance d' is repeated $\deg(u)\times\deg(x)$ times. And if every pair of vertices u and x, $u \neq x$, which is adjacent, distance $d(u,x)$ is repeated $\deg(u)\times\deg(x) - 1$ times. Therefore,

$$W_{e4}(G) = \frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)} \deg(x)\times\deg(y)\times d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_2}\frac{1}{4} + \sum_{\{e,f\}\in A_3}\frac{2}{4} + \sum_{\{e,f\}\in A_4}\frac{3}{4} + |A_1|\,.$$

∎

Corollary 13.2.7 *The explicit relation between edge versions of Wiener index is*

$$W_{e4}(G) = W_{e0}(G) + |A_1| - |C|\,. \tag{13.6}$$

Proof According to the relations 13.4 and 13.5, we can get above relation easily. ∎

In the following table, we bring some examples for relation 13.6 (Table 13.2):

Now, we compute the first edge-Wiener number of cycles according to our relation as follows:

Corollary 13.2.8 *The first edge-Wiener index and its vertex version are equal for cycles.*

Table 13.2 Some examples due to relation 13.6

Graph (G)	$W_{e0}(G)$	$\|A_1\|$	$\|C\|$	$W_{e4}(G)$
P_n	$\frac{1}{6}n(n-1)(n-2)$	$\binom{n-1}{2}=\frac{(n-1)(n-2)}{2}$	0	$\frac{1}{6}(n-1)(n-2)(n+3)$
S_n	$\frac{1}{2}(n-1)(n-2)$	$\binom{n-1}{2}=\frac{(n-1)(n-2)}{2}$	0	$(n-1)(n-2)$
C_n, n is odd	$\frac{1}{8}n\left(n^2-1\right)$	$\binom{n}{2}-n=\frac{n(n-3)}{2}$	0	$\frac{1}{8}n\left(n^2+4n-13\right)$
C_n, n is even	$\frac{1}{8}n^3$	$\binom{n}{2}-\frac{n}{2}=\frac{n(n-2)}{2}$	0	$\frac{1}{8}n\left(n^2+4n-8\right)$

Proof The relation 13.3 can be stated for cycles as follows:

$$W_{e0}(G)=\frac{1}{2}\sum_{x\in V(G)}\sum_{y\in V(G)}d(x,y)-\frac{m}{4}+\begin{cases}\sum\limits_{\substack{\{e,f\}\in A_3\\ if e=uv, f=xy}}\left(\frac{1}{2}\right), \text{ if } n \text{ is even}\\ \sum\limits_{\substack{\{e,f\}\in A_1\\ if e=uv, f=xy}}\left(\frac{1}{4}\right), \text{ if } n \text{ is odd}\end{cases}$$

$$=\begin{cases}W_v(G)-\frac{m}{4}+\sum\limits_{\substack{\{e,f\}\in A_3\\ if e=uv, f=xy}}\left(\frac{1}{2}\right), \text{ if } n \text{ is even}\\ W_v(G)-\frac{m}{4}+\sum\limits_{\substack{\{e,f\}\in A_1\\ if e=uv, f=xy}}\left(\frac{1}{4}\right), \text{ if } n \text{ is odd}\end{cases}$$

The numbers of elements of A_3 in even cycles is $\frac{m}{2}$ and in odd cycles is m. Then, the first edge-Wiener number is equal to its vertex version for cycles. ∎

Now, we say the explicit relation of zigzag nanotube in pursue.

Theorem 13.2.9 *The explicit relation between vertex Wiener number and the first edge-Wiener number for zigzag nanotubes which have been consisted of vertices with degrees* 3 *and* 2 *is*

$$W_{e0}(G)=\frac{9}{4}W_v(G)+\frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d\,(x,y)$$
$$-\frac{5}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d\,(x,y)-\frac{m}{4}+\sum_{\{e,f\}\in A_3}\frac{1}{2}. \qquad (13.7)$$

Proof We can get this result with replacing the degree of vertices in relation 13.4 and the fact that the sets A_2, A_4 and C are empty. ∎

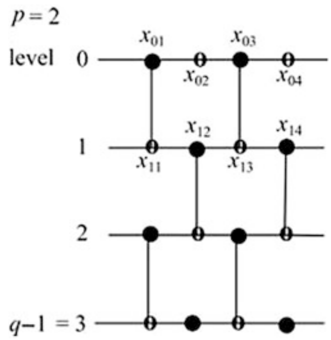


Fig. 13.2 $(n, 0)$ zigzag polyhex SWNTs

The vertex version of Wiener number of zigzag nanotube is computed in John and Diudea (2004). They have focused on $(n, 0)$ zigzag polyhex SWNTs which have p hexagons in a row and q hexagons in column. Because of their computation and relation (13.7), we state the first edge-Wiener number of zigzag nanotube such that p is even integer and q is odd integer.

They have colored the vertices with two colors white and black as shown in Fig. 13.2.

The white vertices in level 0 denote the vertices with degree 2 and the black vertices in last level denote the vertices with degree 2.

Lemma 13.2.10 (John and Diudea 2004) *The sum of distances of one white vertex of level* 0 *to all vertices of level* k, *for* $k = 0, 1, \ldots, q-1$, *is given as*:

$$w_k = \sum_{r=1}^{2p} d\left(x_{02}, x_{kr}\right) = \sum_{r=1}^{2p} d\left(x_{04}, x_{kr}\right) = \begin{cases} (p+k)^2 + k & o \le k < p \\ p\,(4k+1) & p \le k \end{cases}.$$

Lemma 13.2.11 $\sum\limits_{\substack{x \in V(G) \\ \deg(x)=2}} \sum\limits_{\substack{y \in V(G) \\ \deg(y)=2}} d(x, y) =$

$$\begin{cases} 2p\left(2\sum\limits_{i=1}^{\frac{p}{2}} 2i - p + 2\sum\limits_{i=1}^{\frac{q-1}{2}} (2q+1) + 2\sum\limits_{i=1}^{\frac{p}{2}-\frac{q-3}{2}} (2q+2i-1)\right), q < p \\ 2p\left(2\sum\limits_{i=1}^{\frac{p}{2}} 2i - p + 2\sum\limits_{i=1}^{\frac{p}{2}} (2q+1)\right), & p \le q \end{cases}.$$

Proof Due to Fig. 13.2, we can get this result easily. ∎

Lemma 13.2.12 $\sum\limits_{\substack{x \in V(G) \\ \deg(x)=2}} \sum\limits_{\substack{y \in V(G) \\ \deg(y)=3}} d(x, y)$ *is equal to*

$$2p \times \begin{cases} \sum_{k=1}^{q-1} w_k + 2\sum_{i=1}^{\frac{p}{2}} (2i-1) - 2\sum_{i=1}^{\frac{q-1}{2}} (2q+1) - 2\sum_{i=1}^{\frac{p}{2}-\frac{q+1}{2}} (2q+i), & q < p \\ \sum_{k=1}^{q-1} w_k + 2\sum_{i=1}^{\frac{p}{2}} (2i-1) - 2\sum_{i=1}^{\frac{p}{2}} (2q+1), & p \leq q \end{cases}.$$

Proof $\sum_{k=1}^{q-1} w_k$ is the sum of distances between x_{o2} and all of vertices in levels $k = 1, \ldots, q-1$. Then, we must reduce the distance between x_{o2} and vertices in last level with degree 2 and add the distances between vertex x_{o2} and vertices in level 0 with degree 3. Then, we can obtain the above relation. ∎

Theorem 13.2.13 (John and Diudea 2004) *The vertex-Wiener number of zigzag nanotubeG which has p hexagons in a row and q hexagons in column such that p is even integer and q is odd integer is*

$$W_v(G) = \begin{cases} \frac{pq}{2}\left[6p^2q + (4p+q)\left(q^2-1\right)\right], & 0 < q \leq p \\ \frac{p^2}{2}\left[p^2(4q+p) + q\left(8q^2-6\right) + p\right], & p \leq q \end{cases}.$$

Theorem 13.2.14 *The edge-Wiener number of zigzag nanotube G which has p hexagons in a row and q hexagons in column such that p is even integer and q is odd integer is*

$$W_{e0}(G)$$
$$= \begin{cases} pq\left(\frac{9}{4}qp^2+\frac{3}{4}q^2p-\frac{35}{8}p+\frac{3}{8}q^3-\frac{11}{16}q+\frac{3}{4}p^2+\frac{3}{4}pq+\frac{1}{4}q^2-\frac{1}{4}\right)- \\ p\left(\frac{29}{16}p^2-\frac{15}{4}p-\frac{55}{16}\right), & q < p \\ pq\left(\frac{3}{2}p^3+3pq^2-\frac{27}{4}p+\frac{3}{2}pq+\frac{q}{2}+\frac{1}{4}\right)-p\left(\frac{3}{8}p^4-\frac{1}{8}p^2+\frac{11}{4}p\right), & p \leq q \end{cases}$$

Proof In molecular graph of zigzag nanotube, we have two types of edges. The first type is the oblique edges and the second type is vertical edges. The number of pair oblique edges which belongs to A_3 is $2p\binom{q+1}{2}$, and the number of vertical edges which belongs to A_3 is $q\binom{p}{2}$. Therefore, according to relation 13.7, Lemmas 13.3.4 and 13.3.5, Theorem 13.3.6, and the number of elements of A_1, the above relations are computed easily. ∎

The explicit relation between first edge version and vertex version of Wiener number of nanotubes with vertex of degrees 3 and 2 has been declared in Theorem 13.2.9.

Corollary 13.2.15 *According to the relations*13.6 *and* 13.7, *the explicit relation between vertex and the second edge-Wiener number for zigzag nanotubes which consists of vertices with degrees* 3 *and* 2 *is obtained directly*:

$$W_{e4}(G) = \frac{9}{4}W_v(G) + \frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{y\in V(G)} d(x,y) - \sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_3}\frac{1}{2} + |A_1|. \tag{13.8}$$

Theorem 13.2.16 *The second edge-Wiener number of zigzag nanotubeG which has p hexagons in a row and q hexagons in column such that p is even integer and q is odd integer is*

$$W_{e4}(G) = \begin{cases} pq\left(\frac{9}{4}qp^2 + \frac{3}{4}q^2p - \frac{35}{8}p + \frac{3}{8}q^3 - \frac{11}{16}q + \frac{3}{4}p^2 + \frac{3}{4}pq + \frac{1}{4}q^2 - \frac{1}{4}\right) - \\ p\left(\frac{29}{16}p^2 - \frac{15}{4}p - \frac{55}{16}\right) + \binom{3pq+2p}{2} - \frac{2pq^2+qp^2+pq}{2}, & q < p \\ pq\left(\frac{3}{2}p^3 + 3pq^2 - \frac{27}{4}p + \frac{3}{2}pq + \frac{q}{2} + \frac{1}{4}\right) - p\left(\frac{3}{8}p^4 - \frac{1}{8}p^2 + \frac{11}{4}p\right) + \\ \binom{3pq+2p}{2} - \frac{2pq^2+qp^2+pq}{2}, & p \le q \end{cases}$$

Proof The number of edges of zigzag nanotube with p hexagons in a row and q hexagons in column is $3pq + 2p$. In molecular graph of this nanotube, we have $E(G) = A_1 \cup A_3$, and $|A_3| = \frac{2pq^2+qp^2+pq}{2}$. Therefore, according to $|A_1| = \binom{3pq+2p}{2} - \frac{2pq^2+qp^2+pq}{2}$, $W_{e4}(G)$ is computed easily by relation 13.6. ∎

In this part, as the application of the above results, we compute the first edge-Wiener indices of TUC_4C_8(R) nanotube which has been published in Mahmiani, et al. (2010a).

Corollary 13.2.17 *Since there are not any odd cycles in* $TUC_4C_8(R)$ *nanotube*, A_2 *is empty. Hence for* $TUC_4C_8(R)$ *nanotube, we have*

$$W_{e0}(G) = \frac{9}{4}W_v(G) + \frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{y\in V(G)} d(x,y) - \sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_3}\frac{1}{2} \tag{13.9}$$

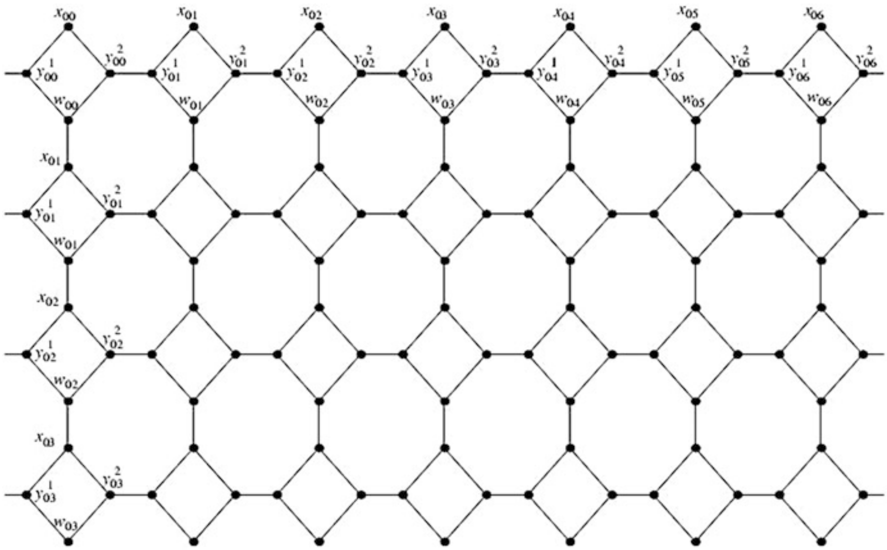


Fig. 13.3 A $T(p,q)$ lattice with $p = 7$ and $q = 4$

Abbas Heydari and Bijan Taeri in (2007a) computed the vertex-Wiener index $W_v(G)$ and $\sum_{\substack{x\in V(G)\\ \deg(x)=2}} \sum_{y\in V(G)} d(x,y)$.

We mention only the quantity of them in this part and omit details.

We denote TUC_4C_8(R) nanotube with $T(p,q)$ where p is the number of squares in a row and q is the number of squares in a column. Also, we assumed $P_1 = \left[\frac{p+1}{2}\right]$ and opted below coordinate label for vertices of $T(p,q)$ as shown in Fig. 13.3.

Lemma 13.2.18 (Heydari and Taeri 2007a) $\sum_{\substack{x\in V(G)\\ \deg(x)=2}} \sum_{y\in V(G)} d(x,y) = 2pS_x(q-1)$,

where

$$S_x(l) = \sum_{k=0}^{l} T_x(k) = \begin{cases} \frac{8}{3}l^3 + (2p+8)\,l^2 + \left(3p^2 + 2p\right) l + \\ \left(\frac{19}{3} + \frac{1+(-1)^p}{2}\right) l + 3p^2 + 1 + \frac{1+(-1)^p}{2}, & l < P_1 \\ 6pl^2 + \left(p^2 + 10p - \frac{1-(-1)^p}{2}\right) l + \\ \frac{1}{3}p^3 + p^2 + \frac{11}{3}p - + \frac{1-(-1)^p}{2}, & l \geq P_1 \end{cases}$$

$$and\ T_x(k) = \begin{cases} 3p^2 + 4kp + 8k^2 + 8k - 1 + \\ 3\dfrac{1+(-1)^p}{2}, & 0 \le k < P_1 \\ p^2 + 12kp + 4p - 1 + \\ \dfrac{1+(-1)^p}{2}, & k \ge P_1 \end{cases}.$$

Theorem 13.2.19 (Heydari and Taeri 2007a) *The Wiener index of T(p,q) is given by the following equation*:

$$W_v(p,q) = \begin{cases} \dfrac{pq}{3}\left(8q^3 + 8pq^2 + \left(18p^2 - 5 + 3\frac{1+(-1)^p}{2}\right)q - 8p\right), & q < P_1 \\ \dfrac{p}{6}\left(-p^4 + 8qp^3 + \left(12q^2 + 1 - \dfrac{1-(-1)^p}{2}\right)p^2\right) + \\ \dfrac{p^2}{6}\left(48q^3 - (14 + 3(1+(-1)^p))q\right) + \\ \left(1 - \dfrac{1+(-1)^p}{2}\right)\left(\dfrac{3}{2} - 12q^2\right), & q \ge P_1 \end{cases}$$

Lemma 13.2.20 *Summation* $\sum_{\substack{x\in V(G)\\ \deg(x)=2}} \sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)$ *is equal to in T(p,q)*:

If p is even:

$$\sum_{\substack{x\in V(G)\\ \deg(x)=2}} \sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y) = \begin{cases} 7q^2 - 7q + 4pq + p^2 - 2p + 1, & q < P_1 \\ 3pq + p^2 - 2p - 3q + 1, & q \ge P_1 \end{cases}$$

If p is odd:

$$\sum_{\substack{x\in V(G)\\ \deg(x)=2}} \sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y) = \begin{cases} 7q^2 + q + 4pq + p^2 - p - 2, & q < P_1 \\ 3pq + p^2 - p + 3q - 2, & q \ge P_1 \end{cases}$$

Proof There exist two types of vertices with degree 2. One of them is in the first row and another is in the last row (Fig. 13.3).

Since the situation of all vertices with degree 2 is the same, we can suppose a fix vertex x in first row. Then, we have for the first type

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the first row}\\ \deg(y)=2}} d(x,y) = \begin{cases} 2\sum_{i=1}^{\frac{p}{2}} 3i - \frac{3p}{2}, & p \text{ is even} \\ 2\sum_{i=1}^{\frac{p-1}{2}} 3i, & p \text{ is odd} \end{cases}$$

And we have for the second type:

(a) p is even:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the last row}\\ \deg(y)=2}} d(x,y)=\begin{cases} 2\sum_{i=0}^{q-1}(3q-1+i)+2\sum_{i=0}^{\frac{p}{2}-1}(4q-1+i)- \\ \left(4q+\frac{p}{2}-1\right), & q<P_1\\ 2\sum_{i=0}^{\frac{p}{2}-1}(3q-1+i)-\left(3q+\frac{p}{2}-1\right), & q\geq P_1\end{cases}$$

(b) p is odd:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the last row}\\ \deg(y)=2}} d(x,y)=\begin{cases} 2\sum_{i=0}^{q-1}(3q-1+i)+2\sum_{i=0}^{\frac{p+1}{2}-1}(4q-1+i), & q<P_1\\ 2\sum_{i=0}^{\frac{p+1}{2}-1}(3q-1+i), & q\geq P_1\end{cases}$$

Therefore, we can obtain the desired results.

Observation 13.2.21 The number of elements of A_1 is equal to: $(q-1)\binom{p}{2}+p\binom{q}{2}+2p\binom{2q}{2}$.

By the above lemmas, Theorem 13.2.19, Observation 13.2.21 and the fact that the number of edges in $T(p,q)$ are $6pq-p$, the following theorem can be proved:

Theorem 13.2.22 *The first version of edge-Wiener index of $T(p,q)$ is equal to*:

1. *If p is even*:

$$W_{e0}(T(p,q))=\begin{cases} -\frac{39}{2}p+2pq^3+6p^2q^4+\frac{9}{8}pq^2(-1)^p+ \\ \frac{3}{8}pq(-1)^p+\frac{27}{2}p^3q^2+6pq^5+ \\ \frac{81}{8}pq+\frac{15}{4}p^2-\frac{115}{8}pq^2-\frac{37}{4}p^2q+ \\ \frac{9}{4}p^3q-2p^3+\frac{3}{2}p^2q^2, & q<P_1\\ -\frac{3}{2}p-\frac{27}{2}q^2+\frac{3}{8}pq(-1)^p+\frac{9}{2}p^3q^2+ \\ \frac{21}{8}pq+\frac{7}{2}p^2+\frac{9}{8}p^2q(-1)^{p+1}+ \\ \frac{27}{16}(-1)^{p+1}+\frac{27}{16}-\frac{3}{8}p^5+\frac{1}{4}p^4+\frac{9}{4}pq^2- \\ \frac{85}{8}p^2q+\frac{3}{4}p^3q-\frac{29}{16}p^3+\frac{3}{16}p^3(-1)^p+ \\ 18p^2q^3+27q^2(-1)^p+\frac{9}{2}p^2q^2, & q\geq P_1\end{cases}$$

2. *If p is odd*:

$$W_{e0}\left(T(p,q)\right)=\begin{cases} -\frac{27}{2}p+2pq^3+6p^2q^4+\frac{9}{8}pq^2(-1)^p+\\ \frac{3}{8}pq(-1)^p+\frac{27}{2}p^3q^2+6pq^5-\\ \frac{47}{8}pq+\frac{7}{4}p^2-\frac{115}{8}pq^2-\frac{37}{4}p^2q+\\ \frac{9}{4}p^3q-2p^3+\frac{3}{2}p^2q^2, & q<P_1\\ \frac{9}{2}p-\frac{27}{2}q^2+\frac{3}{8}pq(-1)^p+\frac{9}{2}p^3q^2-\\ \frac{75}{8}pq+\frac{3}{2}p^2+\frac{9}{8}p^2q(-1)^{p+1}+\\ \frac{27}{16}(-1)^{p+1}+\frac{27}{16}-\frac{3}{8}p^5+\frac{1}{4}p^4+\\ \frac{9}{4}pq^2-\frac{85}{8}p^2q+\frac{3}{4}p^3q-\frac{29}{16}p^3+\\ \frac{3}{16}p^3(-1)^p+18p^2q^3+27q^2(-1)^p+\\ \frac{9}{2}p^2q^2, & q\geq P_1 \end{cases}.$$

Now, we computed the first and the second edge-Wiener indices of $TUC_4C_8(S)$ nanotube.

All of the following results have been published in Mahmiani, et al. (2010b).

Due to the fact that, there are no odd cycles in $TUC_4C_8(S)$ nanotube, A_2 is empty. Then, we have for $TUC_4C_8(S)$ nanotube, the relation 13.9.

Corollary 13.2.23 *According to the relations* 13.6 *and* 13.7, *the explicit relation between vertex and first edge-Wiener number for* $TUC_4C_8(S)$ *nanotubes which consists of vertices with degrees* 3 *and* 2 *is*

$$W_{e4}(G)=\frac{9}{4}W_v(G)+\frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{y\in V(G)}d(x,y)$$
$$-\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{m}{4}+\sum_{\{e,f\}\in A_3}\frac{1}{2}+|A_1|. \tag{13.10}$$

The explicit relation between edge versions of Wiener index is:

$$W_{e4}(G)=W_{e0}(G)+|A_1|-|C| \tag{13.11}$$

In $TUC_4C_8(S)$ nanotube, p is the number of square in a row and q is the number of rows which is shown in Fig. 13.4.

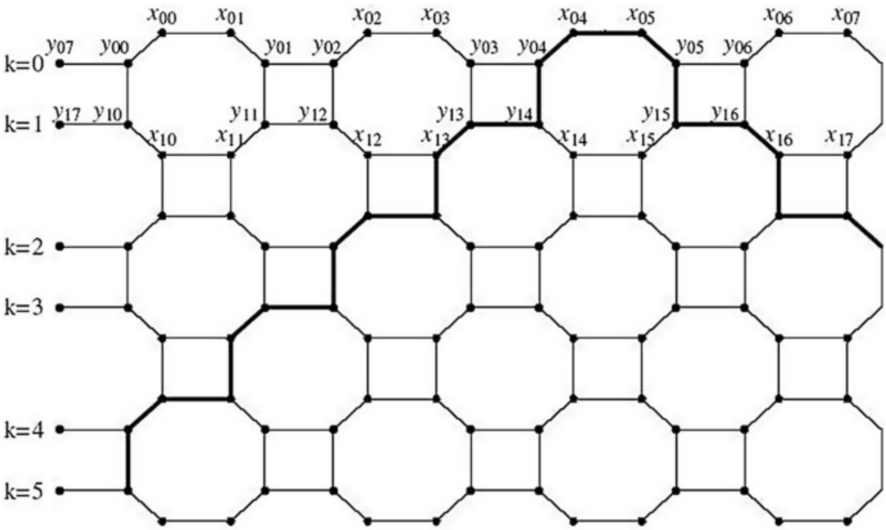


Fig. 13.4 A $TUC_4C_8(S)$ lattice with $p = 4$ and $q = 6$

In Heydari and Taeri (2007b), some notations are defined as follows. For all $0 \le r < q$ and $0 \le t < 2p$, let $a_{rt} \in \{x_{rt}, y_{rt}\}$ and let $d_{a_{rt}}(k)$ denote the sum of distances between a_{rt} and vertices on k-th row of the graph. By symmetry of the graph for all $0 \le t < 2p$, $d_{x_{rt}}(k)$ equal. So we may compute this summation for x_{0p} in the 0th row of the graph, which is denoted by $d_x(k)$.

Lemma 13.2.24 (Heydari and Taeri 2007b) *Let* $0 \le k < q$, *then* $d_x(k) = \begin{cases} 4p^2 + 4kp + 2\left(k^2 + k\right), & k \le p \\ 2p^2 + 8kp + 2p, & k > p \end{cases}$.

Therefore, according to the Lemma 13.2.24, we can obtain $\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x, y)$.

Lemma 13.2.25

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x, y) =$$

$$\begin{cases} \frac{8}{3} pq \left(6p^2 + 3pq - 3p + q^2 - 1\right), & q \le p \\ 8p^2 q \left(p + 2q - 1\right), & q > p \end{cases}.$$

Proof Due to the Lemma 13.2.24, $d_{x_{0p}}(k)$ denotes the sum of distances between x_{0p} and vertices on k-th row of the graph. There are *4p* vertices such as x_{0p} in the first row. Therefore,

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x, y) = 4p \sum_{k=0}^{q-1} d_x(k) =$$

$$\begin{cases} \frac{8}{3} pq \left(6p^2 + 3pq - 3p + q^2 - 1\right), & q \leq p \\ 8p^2 q\,(p + 2q - 1), & q > p \end{cases}.$$

∎

The vertex-Wiener index of $TUC_4C_8(S)$ is computed in Heydari and Taeri (2007b). We state only the main result as a theorem asfollows:

Theorem 13.2.26 (Heydari and Taeri 2007b) *The Wiener index of* $TUC_4C_8(S) = G$ *is given by the following equation*:

$$W_v(G) =$$

$$\begin{cases} \frac{pq}{3} \left(2q^3 + 8pq\,(3p + q) - 2q - 8p\right), & q \leq p \\ \frac{p^2}{3} \left(-2p^3 + 8qp^2 + \left(12q^2 + 2\right) p + 16q^3 - 12q\right) +, & q > p \end{cases}$$

Lemma 13.2.27 *Let*$TUC_4C_8(S) = G$. *Then*,

If p is even:

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x, y) =$$

$$\begin{cases} q^2 + 2q + 2pq + 4p^2 - p - 2 - 2\left[\frac{2p - 2q + 1}{4}\right], & q \leq p \\ 4pq + 3p^2 - 2p - 1, & q > p \end{cases}$$

If p is odd:

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x, y) =$$

$$\begin{cases} q^2 + q + 2pq + 2p^2 - 3p + 8\left[\frac{p}{2}\right] + 8\left[\frac{p}{2}\right]^2 - 2\left[\frac{2p - 2q + 1}{4}\right], & q \leq p \\ 4pq + p^2 - 2p + 8\left[\frac{p}{2}\right] + 8\left[\frac{p}{2}\right]^2, & q > p \end{cases}$$

Proof There exist two groups of vertices which have degree 2. One group is vertices in the first row and another is the vertices in the last row.

Due to the fact that the situation of all vertices with degree 2 is the same, we suppose the fix vertex x is in first row. Then, we have for the first group:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in first row}\\ \deg(y)=2}} d(x,y) =$$

$$\begin{cases} \left(\sum_{k=0}^{\frac{p-2}{2}} (16k+16)\right) - (4p+1)\,, & p \text{ is even} \\ \sum_{k=0}^{\left[\frac{p-2}{2}\right]} (16k+16), & p \text{ is odd} \end{cases}.$$

And we have for the second group:

(a) p is even:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in last row}\\ \deg(y)=2}} d(x,y) =$$

$$\begin{cases} \sum_{i=2q}^{3q-1}(2i) + \sum_{i=3q-1}^{2p+q-1}(i) - 2\left(\left[\frac{2p-2q-3}{4}\right]+1\right) - q, & q \le p \\ \sum_{i=2q}^{2q+p-1}(2i) - p, & q > p \end{cases}$$

(b) p is odd:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in last row}\\ \deg(y)=2}} d(x,y) =$$

$$\begin{cases} \sum_{i=2q}^{3q-1}(2i) + \sum_{i=3q-1}^{2p+q-1}(i) - 2\left[\frac{2p-2q-4}{4}\right] - 2p - 2q - 3, & q \le p \\ \sum_{i=2q}^{2q+p-1}(2i) - p, & q > p \end{cases}$$

Therefore, we can get results with the above summations. ∎

Observation 13.2.28 The number of elements of A_3 is equal to: $4p\binom{q}{2} + (q-1)\binom{2p}{2}$.

Due to the fact that the number of edges in $TUC_4C_8(S)$ is $6pq - 2p$, we state the first edge-Wiener index of $TUC_4C_8(S)$.

Theorem 13.2.29 *The first version of edge-Wiener index of* $TUC_4C_8(S) = G$ *is equal to*:

1. *If p is even*:

$$W_{e0}(T(p,q)) = \begin{cases} \frac{3}{2}pq^4 + 18p^3q^2 + 6p^2q^3 - \frac{pq^2}{2} - 8p^2q + 6p^3q + 3p^2q^2 - 6pq + pq^3 - \\ q^2 - 2q - 5p^2 + 2p + 2 + 2\left[\frac{2p-2q+1}{4}\right], & q \le p \\ \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 11p^2q + 3p^3q + 6p^2q^2 - 7pq - 4p^2 + \\ 3p + pq^2 + 1, & q > p \end{cases}$$

2. *If p is odd*:

$$W_{e0}(T(p,q)) = \begin{cases} \frac{3}{2}pq^4 + 18p^3q^2 + 6p^2q^3 - \frac{pq^2}{2} - 8p^2q + 6p^3q + 3p^2q^2 - 6pq + pq^3 - \\ q^2 - q - 3p^2 + 2\left[\frac{2p-2q+1}{4}\right] - 8\left[\frac{p}{2}\right] - 8\left[\frac{p}{2}\right]^2, & q \le p \\ \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 11p^2q + 3p^3q + 6p^2q^2 - 7pq - 2p^2 + \\ 3p + pq^2 - 8\left[\frac{p}{2}\right] - 8\left[\frac{p}{2}\right]^2, & q > p \end{cases}$$

Proof According to Lemmas 13.2.25 and 13.2.27, Theorem 13.2.26 and observation 13.2.28, we can conclude these results easily. ∎

Now, In this part, we compute the second edge-Wiener index of $TUC_4C_8(S)$.

Theorem 13.2.30 *The second version of edge-Wiener index of* $TUC_4C_8(S) = G$ *where p is the number of squares in a row and q is the number of rows is equal to*:

1. *If p is even, then*

$$W_{e0}(\mathrm{T}(p,q)) = \begin{cases} \frac{3}{2}pq^4 + 18p^3q^2 + 6p^2q^3 - \frac{pq^2}{2} - 22p^2q + 6p^3q + 21p^2q^2 - 6pq + pq^3 - \\ 2pq^2 - q^2 - 2q - p^2 + 2p + 2 + 2\left[\frac{2p-2q+1}{4}\right], & q \le p \\ \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 25p^2q + 3p^3q + 24p^2q^2 - 7pq + \\ 3p - pq^2 + 1, & q > p \end{cases}$$

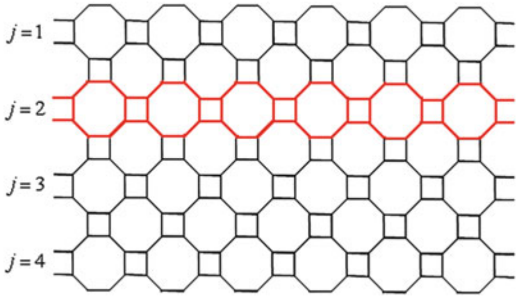


Fig. 13.5 $T\,(6,4)$ nanotube with $1 \le j \le 4$ periods

2. *If p is odd, then*

$$W_{e0}\,(\mathrm{T}(p,q)) = \begin{cases} \frac{3}{2}pq^4 + 18p^3q^2 + 6p^2q^3 - \frac{pq^2}{2} - 22p^2q + 6p^3q + 21p^2q^2 - 6pq + pq^3 - \\ 2pq^2 - q^2 - q + p^2 + 2\left[\frac{2p-2q+1}{4}\right] - 8\left[\frac{p}{2}\right] - 8\left[\frac{p}{2}\right]^2, & q \le p \\ \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 25p^2q + 3p^3q + 24p^2q^2 - 7pq + 2p^2 + \\ 3p - pq^2 - 8\left[\frac{p}{2}\right] - 8\left[\frac{p}{2}\right]^2, & q > p \end{cases}$$

Proof The number of edges of TUC_4C_8(S) nanotube with p squares in a row and q rows is $6pq - 2p$. In molecular graph of this nanotube, we have $E(G) = A_1 \cup A_3$ and

$$|A_3| = 4p\binom{q}{2} + (q-1)\binom{2p}{2}.$$

Therefore, according to reference Heydari and Taeri (2007a, b) and $|A_1| = 18p^2q^2 - 14p^2q + 4p^2 - 2pq^2$, $W_{e4}(G)$ is computed easily. ∎

In the above, we computed the first edge-Wiener index of TUC_4C_8 (S) nanotube by the result obtained in Iranmanesh and Khormali (2011). But, in Iranmanesh and Kafrani (2009), we computed this index with a different method. The base of this method is according to the definition of eight sets as follows:

Let $T\,(p,q) = TUC_4C_8$ (S) where p is denoted the number of octagonal in rows and q is the number of octagons in columns. We consider j periods, where $1 \le j \le q$, for this nanotube that each period has an upper row and a lower row. For example in Fig. 13.5, we show $T\,(6,4)$ nanotube.

Suppose $e \in E(G)$. Set

$$A_u = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an edge over octagones in upper row of } j-\text{th period}\}$$

$$A_d = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an edge over squares in lower row of } j-\text{th period}\}$$

$$B_u = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an edge under octagones in upper row of } j-\text{th period}\}$$

$$B_d = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an edge under squares in lower row of } j-\text{th period}\}$$

$$C_u = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an oblique edge in upper row of } j-\text{th period}\}$$

$$C_d = \bigcup_{j=1}^{q} \{e \in E(G) \mid e \text{ is an oblique edge in lower row of } j-\text{th period}\}$$

$$D = \bigcup_{j=1}^{q} \{e \in E(G)\ e \text{ is a vertical edge that located between upper and lower rows}\}$$

$$E = \bigcup_{j=1}^{q-1} \{e \in E(G) | e \text{ is vertical edge that located between } j-\text{th period and } j+1-\text{th period}\}$$

So we have

$$W_{e0}(G) = W_{e0}(A_u, G) + W_{e0}(A_d, G) + W_{e0}(B_u, G) + W_{e0}(B_d, G) + W_{e0}(C_u, G) + W_{e0}(C_d, G) + W_{e0}(D, G) + W_{e0}(E, G)$$

For compute the first edge index of $TUC_4C_8(S)$ nanotube, we obtained this index in three cases: $q \prec \left[\frac{p}{2}\right] + 1$, $q = \left[\frac{p}{2}\right] + 1$, and $q \succ \left[\frac{p}{2}\right] + 1$ any by six theorems we could obtain the first edge-Wiener index of $TUC_4C_8(S)$ nanotube.

13.3 Computation of the First Edge-Wiener Index of the Composition of Graphs

In this section, we find the first edge-Wiener index of the composition of graphs. All of the results in this section have been published in Azari et al. (2010).

We denote by $[u, v]$ the edge connecting the vertices u, v of G, and the degree of a vertex u is the number of edges incident to u and denoted by $\deg(u|G)$.

The Zagreb indices have been defined more than 30 years ago by Gutman and Trinajestic (1972):

Definition 13.3.1 The first Zagreb index of G is defined as $M_1(G) = \sum_{u \in V(G)} \deg(u|G)^2$.

Let us recall the definition of the composition of two graphs.

Definition 13.3.2 Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two connected graphs. We denote the composition of G_1 and G_2 by $G_1[G_2]$, that is a graph with the vertex set $V(G_1[G_2]) = V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) of $G_1[G_2]$ are adjacent if and only if: $[u_1 = v_1$ and $[u_2, v_2] \in E(G_2)]$ or $[u_1, v_1] \in E(G_1)$.

By definition of the composition, the distance between every pair of distinct vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1[G_2]$ is equal to

$$d(u, v|G_1[G_2]) = \begin{cases} d(u_1, v_1|G_1) & \text{if } u_1 \neq v_1 \\ 1 & \text{if } u_1 = v_1,\ [u_2, v_2] \in E(G_2) \\ 2 & \text{if } u_1 = v_1,\ v_2 \text{ is not adjacent to } u_2 \text{ in } G_2 \end{cases}$$

Consider the sets E_1 and E_2 as follows:

$$E_1 = \{[(u_1, u_2), (u_1, v_2)] \in E(G_1[G_2]) : u_1 \in V(G_1),\ [u_2, v_2] \in E(G_2)\}$$

$$E_2 = \{[(u_1, u_2), (v_1, v_2)] \in E(G_1[G_2]) : [u_1, v_1] \in E(G_1),\ u_2, v_2 \in V(G_2)\}$$

By definition of the composition, $E_1 \cup E_2 = E(G_1[G_2])$ and obviously, $E_1 \cap E_2 = \varphi$, $|E_1| = |V(G_1)||E(G_2)|$ and $|E_2| = |V(G_2)|^2 |E(G_1)|$.

Set

$$A = \{\{e, f\} \subseteq E(G_1[G_2]) : e \neq f,\ e, f \in E_1\}$$

$$B = \{\{e, f\} \subseteq E(G_1[G_2]) : e \neq f,\ e, f \in E_2\}$$

$$C = \{\{e, f\} \subseteq E(G_1[G_2]) : e \in E_1,\ f \in E_2\}$$

It is easy to see that each pair of the above sets is disjoint and the union of them is the set of all two element subsets of $E(G_1[G_2])$. Also we have $|A| = \binom{|E_1|}{2} = \binom{|V(G_1)|\ |E(G_2)|}{2}$, $|B| = \binom{|E_2|}{2} = \binom{|V(G_2)|^2 |E(G_1)|}{2}$, $|C| = |E_1|\ |E_2| = |V(G_1)|\ |V(G_2)|^2 |E(G_1)|\ |E(G_2)|$

Consider four subsets A_1, A_2, A_3 and A_4 of the set A as follows:

$$A_1 = \{\{e, f\} \in A : e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, u_2), (u_1, z_2)], \; u_1 \in V(G_1), \\ u_2, v_2, z_2 \in V(G_2)\}$$

$$A_2 = \{\{e, f\} \in A : e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, z_2), (u_1, t_2)], \; u_1 \in V(G_1), \\ u_2, v_2, z_2, t_2 \in V(G_2), \text{ both } z_2 \text{ and } t_2 \text{ are adjacent neither to } u_2 \text{ nor to } v_2 \\ \text{in } G_2\}$$

$$A_3 = \{\{e, f\} \in A : e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, z_2), (u_1, t_2)], \; u_1 \in V(G_1), \\ u_2, v_2 \in V(G_2), \; z_2, t_2 \in V(G_2) - \{u_2, v_2\}\} - A_2$$

$$A_4 = \{\{e, f\} \in A : e = [(u_1, u_2), (u_1, v_2)], f = [(v_1, z_2), (v_1, t_2)], \; u_1, v_1 \in V(G_1), \\ v_1 \neq u_1, \; u_2, v_2, z_2, t_2 \in V(G_2)\}$$

It is clear that every pair of the above sets is disjoint and $A = \bigcup_{i=1}^{4} A_i$.

In the next proposition, we characterize $d_0(e, f \,|G_1[G_2])$ for all $\{e, f\} \in A$.

Proposition 13.3.3 *Let* $\{e, f\} \in A$.

(i) *If* $\{e, f\} \in A_1$, *then* $d_0(e, f \,|G_1[G_2]) = 1$
(ii) *If* $\{e, f\} \in A_2$, *then* $d_0(e, f \,|G_1[G_2]) = 3$
(iii) *If* $\{e, f\} \in A_3$, *then* $d_0(e, f \,|G_1[G_2]) = 2$
(iv) *If* $\{e, f\} \in A_4$, *then* $d_0(e, f \,|G_1[G_2]) = 1 + d(u_1, v_1 \,|G_1)$,

where $e = [(u_1, u_2), (u_1, v_2)]$, $f = [(v_1, z_2), (v_1, t_2)]$

Proof

(i) Let $\{e, f\} \in A_1$ and $e = [(u_1, u_2), (u_1, v_2)]$, $f = [(u_1, u_2), (u_1, z_2)]$. Due to the distance between two vertices in $G_1[G_2]$ and by definition of $d_0(e, f)$, we have

$$\begin{aligned} d_0(e, f \,|G_1[G_2]) &= 1 + \min\{d((u_1, u_2), (u_1, u_2) \,|G_1[G_2]), \\ &\quad d((u_1, u_2), (u_1, z_2) \,|G_1[G_2]), \\ &\quad d((u_1, v_2), (u_1, u_2) \,|G_1[G_2]), d((u_1, v_2), (u_1, z_2) \,|G_1[G_2])\} \\ &= 1 + \min\{0, 1, 1, d(v_2, z_2 \,|G_2)\} = 1 + 0 = 1. \end{aligned}$$

(ii) Let $\{e, f\} \in A_2$ and $e = [(u_1, u_2), (u_1, v_2)]$, $f = [(u_1, z_2), (u_1, t_2)]$. By definition of the set A_2, z_2 is adjacent neither to u_2 nor to v_2 in G_2 and this is also true for t_2. Therefore,

$$d_0(e,f|G_1[G_2]) = 1+\min\{d((u_1,u_2),(u_1,z_2)|G_1[G_2]),$$
$$d((u_1,u_2),(u_1,t_2)|G_1[G_2]),$$
$$d((u_1,v_2),(u_1,z_2)|G_1[G_2]), d((u_1,v_2),(u_1,t_2)|G_1[G_2])\}$$
$$= 1+\min\{2,2,2,2\} = 3.$$

(iii) Let $\{e,f\} \in A_3$ and $e = [(u_1,u_2),(u_1,v_2)], f = [(u_1,z_2),(u_1,t_2)]$. By definition of the set A_3, $z_2 \notin \{u_2,v_2\}$, $t_2 \notin \{u_2,v_2\}$. On the other hand $\{e,f\} \notin A_2$, so at least one of the following situations occurs:

$$[u_2,z_2] \in E(G_2),\ [u_2,t_2] \in E(G_2),\ [v_2,z_2] \in E(G_2) \text{ or } [v_2,t_2] \in E(G_2).$$

This means that at least one of the distances $d((u_1,u_2),(u_1,z_2)|G_1[G_2])$, $d((u_1,u_2),(u_1,t_2)|G_1[G_2])$, $d((u_1,v_2),(u_1,z_2)|G_1[G_2])$ or $d((u_1,v_2),(u_1,t_2)|G_1[G_2])$ is equal to 1. Therefore,

$$d_0(e,f|G_1[G_2]) = 1+\min\{d((u_1,u_2),(u_1,z_2)|G_1[G_2]),$$
$$d((u_1,u_2),(u_1,t_2)|G_1[G_2]),$$
$$d((u_1,v_2),(u_1,z_2)|G_1[G_2]), d((u_1,v_2),(u_1,t_2)|G_1[G_2])\} = 1+1 = 2.$$

(iv) Let $\{e,f\} \in A_4$ and $e = [(u_1,u_2),(u_1,v_2)], f = [(v_1,z_2),(v_1,t_2)]$. Thus $v_1 \neq u_1$ and

$$d_0(e,f|G_1[G_2]) = 1+\min\{d((u_1,u_2),(v_1,z_2)|G_1[G_2]),$$
$$d((u_1,u_2),(v_1,t_2)|G_1[G_2]),$$
$$d((u_1,v_2),(v_1,z_2)|G_1[G_2]), d((u_1,v_2),(v_1,t_2)|G_1[G_2])\} =$$
$$1+\min\{d(u_1,v_1|G_1), d(u_1,v_1|G_1), d(u_1,v_1|G_1),$$
$$d(u_1,v_1|G_1)\} = 1+d(u_1,v_1|G_1),$$

so the proof is completed. ∎

In the following, we define five subsets B_1, B_2, B_3, B_4 and B_5 of the set B.

$$B_1 = \{\{e,f\} \in B : e = [(u_1,u_2),(v_1,v_2)], f = [(u_1,u_2),(v_1,z_2)],$$
$$u_1,v_1 \in V(G_1), u_2,v_2,z_2 \in V(G_2)\}$$
$$B_2 = \{\{e,f\} \in B : e = [(u_1,u_2),(v_1,v_2)], f = [(u_1,z_2),(v_1,t_2)],$$
$$u_1,v_1 \in V(G_1), u_2,v_2,z_2,t_2 \in V(G_2),\ z_2 \neq u_2,\ t_2 \neq v_2\}$$
$$B_3 = \{\{e,f\} \in B : e = [(u_1,u_2),(v_1,v_2)], f = [(u_1,u_2),(z_1,z_2)],$$
$$u_1,v_1,z_1 \in V(G_1), u_2,v_2,z_2 \in V(G_2),\ z_1 \neq v_1\}$$

$$B_4 = \{\{e, f\} \in B : e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, t_2), (z_1, z_2)],$$
$$u_1, v_1, z_1 \in V(G_1), u_2, v_2, t_2, z_2 \in V(G_2),\ z_1 \neq v_1,\ t_2 \neq u_2\}$$
$$B_5 = \{\{e, f\} \in B : e = [(u_1, u_2), (v_1, v_2)], f = [(z_1, z_2), (t_1, t_2)],$$
$$u_1, v_1 \in V(G_1), z_1, t_1 \in V(G_1) - \{u_1, v_1\},\ u_2, v_2, z_2, t_2 \in V(G_2)\}$$

It is clear that each pair of the above sets is disjoint and $B = \bigcup_{i=1}^{5} B_i$.

The next proposition characterizes $d_0(e, f\, |G_1[G_2])$ for all $\{e, f\} \in B$.

Proposition 13.3.4 *Let* $\{e, f\} \in B$.

(i) *If* $\{e, f\} \in B_1$, then $d_0(e, f\, |G_1[G_2]) = 1$
(ii) *If* $\{e, f\} \in B_2$, *then* $d_0(e, f\, |G_1[G_2]) = 2$
(iii) *If* $\{e, f\} \in B_3$, *then* $d_0(e, f\, |G_1[G_2]) = d_0([u_1, v_1], [u_1, z_1]\, |G_1)$, *where* $e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, u_2), (z_1, z_2)]$
(iv) *If* $\{e, f\} \in B_4$, *then* $d_0(e, f\, |G_1[G_2]) = d_0([u_1, v_1], [u_1, z_1]\, |G_1) + 1$, *where* $e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, t_2), (z_1, z_2)]$
(v) *If* $\{e, f\} \in B_5$, *then* $d_0(e, f\, |G_1[G_2]) = d_0([u_1, v_1], [z_1, t_1]\, |G_1)$, *where* $e = [(u_1, u_2), (v_1, v_2)], f = [(z_1, z_2), (t_1, t_2)]$

Proof

(i) Let $\{e, f\} \in B_1$ and $e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, u_2), (v_1, z_2)]$. Using the definition of $d_0(e, f)$, we have:

$$d_0(e, f\, |G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, u_2)\, |G_1[G_2]),$$
$$d((u_1, u_2), (v_1, z_2)\, |G_1[G_2]),$$
$$d((v_1, v_2), (u_1, u_2)\, |G_1[G_2]), d((v_1, v_2), (v_1, z_2)\, |G_1[G_2])\}$$
$$= 1 + \min\{0, 1, 1, d((v_1, v_2), (v_1, z_2)\, |G_1[G_2])\} = 1 + 0 = 1.$$

(ii) Let $\{e, f\} \in B_2$ and $e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, z_2), (v_1, t_2)]$. By definition of B_2, $z_2 \neq u_2$, $t_2 \neq v_2$. So due to the distance between two vertices in $G_1[G_2]$, the distances $d((u_1, u_2), (u_1, z_2)\, |G_1[G_2])$ and $d((v_1, v_2), (v_1, t_2)\, |G_1[G_2])$ are either 1 or 2. Therefore,

$$d_0(e, f\, |G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, z_2)\, |G_1[G_2]),$$
$$d((u_1, u_2), (v_1, t_2)\, |G_1[G_2]),$$
$$d((v_1, v_2), (u_1, z_2)\, |G_1[G_2]), d((v_1, v_2), (v_1, t_2)\, |G_1[G_2])\} =$$
$$1 + \min\{d((u_1, u_2), (u_1, z_2)\, |G_1[G_2]), 1, 1, d((v_1, v_2), (v_1, t_2)\, |G_1[G_2])\}$$
$$= 1 + 1 = 2.$$

(iii) Let $\{e, f\} \in B_3$ and $e = [(u_1, u_2), (v_1, v_2)], f = ((u_1, u_2), (z_1, z_2))$. By definition of B_3, $z_1 \neq v_1$. Hence,

$$d_0(e, f|G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, u_2)|G_1[G_2]),$$
$$d((u_1, u_2), (z_1, z_2)|G_1[G_2]),$$
$$d((v_1, v_2), (u_1, u_2)|G_1[G_2]), d((v_1, v_2), (z_1, z_2)|G_1[G_2])\} =$$
$$1 + \min\{d(u_1, u_1|G_1)\, d(u_1, z_1|G_1), d(v_1, u_1|G_1), d(v_1, z_1|G_1)\}$$
$$= d_0([u_1, v_1], [u_1, z_1]|G_1)$$

(iv) Let $\{e, f\} \in B_4$ and $e = [(u_1, u_2), (v_1, v_2)], f = [(u_1, t_2), (z_1, z_2)]$. By definition of B_4, $z_1 \neq v_1$, and $t_2 \neq u_2$. So $d(v_1, z_1|G_1) \geq 1$ and $d((u_1, u_2), (u_1, t_2)|G_1[G_2]) \geq 1$. Therefore,

$$d_0(e, f|G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, t_2)|G_1[G_2]),$$
$$d((u_1, u_2), (z_1, z_2)|G_1[G_2]),$$
$$d((v_1, v_2), (u_1, t_2)|G_1[G_2]), d((v_1, v_2), (z_1, z_2)|G_1[G_2])\} =$$
$$1 + \min\{d((u_1, u_2), (u_1, t_2)|G_1[G_2]), 1, 1, d(v_1, z_1|G_1)\}$$
$$= 1 + 1 = d_0([u_1, v_1], [u_1, z_1]|G_1) + 1.$$

(v) Let $\{e, f\} \in B_5$ and $e = [(u_1, u_2), (v_1, v_2)], f = [(z_1, z_2), (t_1, t_2)]$. By definition of B_5, $z_1 \neq u_1$, $z_1 \neq v_1$, $t_1 \neq u_1$, and $t_1 \neq v_1$. So the edges $[u_1, v_1]$ and $[z_1, t_1]$ of G_1 are distinct. Therefore,

$$d_0(e, f|G_1[G_2]) = 1 + \min\{d((u_1, u_2), (z_1, z_2)|G_1[G_2]),$$
$$d((u_1, u_2), (t_1, t_2)|G_1[G_2]),$$
$$d((v_1, v_2), (z_1, z_2)|G_1[G_2]), d((v_1, v_2), (t_1, t_2)|G_1[G_2])\} =$$
$$1 + \min\{d(u_1, z_1|G_1), d(u_1, t_1|G_1), d(v_1, z_1|G_1), d(v_1, t_1|G_1)\}$$
$$= d_0([u_1, v_1], [z_1, t_1]|G_1),$$

and the proof is completed. ∎

Now, we consider three subsets C_1, C_2 and C_3 of the set C as follows:

$$C_1 = \{\{e, f\} \in C : e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, u_2), (z_1, z_2)],$$
$$u_1, z_1 \in V(G_1), u_2, v_2, z_2 \in V(G_2)\}$$

$$C_2 = \{\{e, f\} \in C : e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, t_2), (z_1, z_2)], \\ u_1, z_1 \in V(G_1), u_2, v_2, t_2, z_2 \in V(G_2), \ t_2 \neq u_2, \ t_2 \neq v_2\}$$

$$C_3 = \{\{e, f\} \in C : e = [(u_1, u_2), (u_1, t_2)], f = [(v_1, v_2), (z_1, z_2)], \\ u_1, v_1, z_1 \in V(G_1), u_2, t_2, v_2, z_2 \in V(G_2), \ v_1 \neq u_1, \ z_1 \neq u_1\}$$

Clearly, every pair of the above sets is disjoint and $C = \bigcup_{i=1}^{3} C_i$.

In the following proposition, we find $d_0(e, f|G_1[G_2])$ for all $\{e, f\} \in C$.

Proposition 13.3.5 *Let* $\{e, f\} \in C$.

(i) *If* $\{e, f\} \in C_1$, *then* $d_0(e, f|G_1[G_2]) = 1$
(ii) *If* $\{e, f\} \in C_2$, *then* $d_0(e, f|G_1[G_2]) = 2$
(iii) *If* $\{e, f\} \in C_3$, *then* $d_0(e, f|G_1[G_2]) = 1 + \min\{d(u_1, v_1|G_1), d(u_1, z_1|G_1)\}$, *where* $e = [(u_1, u_2), (u_1, t_2)], f = [(v_1, v_2), (z_1, z_2)]$

Proof

(i) Let $\{e, f\} \in C_1$ and $e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, u_2), (z_1, z_2)]$.
By definition of $d_0(e, f)$, we have

$$d_0(e, f|G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, u_2)|G_1[G_2]), \\ d((u_1, u_2), (z_1, z_2)|G_1[G_2]), \\ d((u_1, v_2), (u_1, u_2)|G_1[G_2]), d((u_1, v_2), (z_1, z_2)|G_1[G_2])\} \\ = 1 + \min\{0, 1, 1, 1\} = 1 + 0 = 1.$$

(ii) Let $\{e, f\} \in C_2$ and $e = [(u_1, u_2), (u_1, v_2)], f = [(u_1, t_2), (z_1, z_2)]$. By definition of C_2, $t_2 \neq u_2, \ t_2 \neq v_2$. Thus, due to the distance between two vertices in $G_1[G_2]$, the distances $d((u_1, u_2), (u_1, t_2)|G_1[G_2])$ and $d((u_1, v_2), (u_1, t_2)|G_1[G_2])$ are either 1 or 2. So

$$d_0(e, f|G_1[G_2]) = 1 + \min\{d((u_1, u_2), (u_1, t_2)|G_1[G_2]), \\ d((u_1, u_2), (z_1, z_2)|G_1[G_2]), \\ d((u_1, v_2), (u_1, t_2)|G_1[G_2]), d((u_1, v_2), (z_1, z_2)|G_1[G_2])\} = \\ 1 + \min\{d((u_1, u_2), (u_1, t_2)|G_1[G_2]), 1, d((u_1, v_2), (u_1, t_2)|G_1[G_2]), 1\} \\ = 1 + 1 = 2.$$

(iii) Let $\{e, f\} \in C_3$ and $e = [(u_1, u_2), (u_1, t_2)], f = [(v_1, v_2), (z_1, z_2)]$. By definition of C_3, $v_1 \neq u_1, \ z_1 \neq u_1$. Therefore,

$$d_0(e,f\,|G_1[G_2]) = 1+\min\{d((u_1,u_2),(v_1,v_2)\,|G_1[G_2]),$$
$$d((u_1,u_2),(z_1,z_2)\,|G_1[G_2]),$$
$$d((u_1,t_2),(v_1,v_2)\,|G_1[G_2]),d((u_1,t_2),(z_1,z_2)\,|G_1[G_2])\} =$$
$$1+\min\{d(u_1,v_1\,|G_1),d(u_1,z_1\,|G_1),d(u_1,v_1\,|G_1),d(u_1,z_1\,|G_1)\} =$$
$$1+\min\{d(u_1,v_1\,|G_1),d(u_1,z_1\,|G_1)\},$$

and the proof is completed. ∎

Definition 13.3.6 Let $G=(V(G),E(G))$ be a graph.

(i) Let $u\in V(G)$. Set $\Delta_u=\{z\in V(G):[z,u]\in E(G)\}$. In fact, Δ_u is the set of all vertices of G, which are adjacent to u. Suppose that δ_u is the number of all vertices of G, which are adjacent to u. Clearly, $\delta_u=|\Delta_u|=\deg(u\,|G)$.

(ii) For each pair of distinct vertices $u,v\in V(G)$, let $\delta_{(u,v)}$ be the number of all vertices of G, which are adjacent both to u and v. Obviously, $\delta_{(u,v)}=|\Delta_u\cap\Delta_v|$.

(iii) Let u, v, and z be three vertices of G, which every pair of them is distinct.
Assume that $\delta_{(u,v,z)}$ denotes the number of all vertices of G which are adjacent to vertices u, v and z. It is easy to see that $\delta_{(u,v,z)}=|\Delta_u\cap\Delta_v\cap\Delta_z|$.

(iv) Suppose that u, v and z be three vertices of graph G, which every pair of them is distinct. Denote by $N_{(z,\tilde{u},\tilde{v})}$ the number of all vertices of G, which are adjacent to z, but neither to u nor to v. By the definition of $N_{(z,\tilde{u},\tilde{v})}$, we have

$$N_{(z,\tilde{u},\tilde{v})}=|\Delta_z-(\Delta_u\cup\Delta_v)|=|\Delta_z|-|\Delta_z\cap(\Delta_u\cup\Delta_v)|$$
$$=|\Delta_z|-|(\Delta_z\cap\Delta_u)\cup(\Delta_z\cap\Delta_v)|=$$
$$|\Delta_z|-(|\Delta_z\cap\Delta_u|+|\Delta_z\cap\Delta_v|-|\Delta_z\cap\Delta_u\cap\Delta_v|)$$
$$=\delta_z-\delta_{(z,u)}-\delta_{(z,v)}+\delta_{(z,u,v)}.$$

Lemma 13.3.7

$$\sum_{\{e,f\}\in A} d_0(e,f\,|G_1[G_2])=|E(G_2)|^2\left(\binom{|V(G_1)|+1}{2}+W(G_1)\right)$$
$$-\frac{1}{4}|V(G_1)|\;(2M_1(G_2)-N(G_2)),$$

where, $N(G_2)=\sum_{[u_2,v_2]\in E(G_2)}\;\sum_{z_2\in V(G_2)-(\Delta_{u_2}\cup\Delta_{v_2})} N_{(z_2,\tilde{u}_2,\tilde{v}_2)}.$

Proof At first, we need to find $|A_2|$ and $|A_2\cup A_3|$. It is easy to see that

$$|A_2| = \frac{1}{4}|V(G_1)| \sum_{[u_2,v_2]\in E(G_2)} \sum_{z_2\in V(G_2)-\left(\Delta_{u_2}\cup\Delta_{v_2}\right)} N_{(z_2,\tilde{u}_2,\tilde{v}_2)} = \frac{1}{4}|V(G_1)|\, N(G_2),$$

$$|A_2 \cup A_3| = \frac{1}{2}|V(G_1)| \sum_{[u_2,v_2]\in E(G_2)} \left(|E(G_2)| - (\delta_{u_2} + \delta_{v_2} - 1)\right) =$$

$$\frac{1}{2}|V(G_1)| \left(\sum_{[u_2,v_2]\in E(G_2)} |E(G_2)| - \sum_{[u_2,v_2]\in E(G_2)} (\delta_{u_2} + \delta_{v_2}) + \sum_{[u_2,v_2]\in E(G_2)} 1 \right) =$$

$$\frac{1}{2}|V(G_1)| \left(|E(G_2)|^2 + |E(G_2)| - M_1(G_2) \right),$$

Recall that, each pair of the sets A_i $(1 \le i \le 4)$ is disjoint and $A = \bigcup_{i=1}^{4} A_i$, then by
Proposition 13.3.3, we have

$$\sum_{\{e,f\}\in A} d_0(e,f\,|G_1[G_2]) = \sum_{i=1}^{4} \sum_{\{e,f\}\in A_i} d_0(e,f\,|G_1\,[G_2])$$

$$= |A_1| + 3|A_2| + 2|A_3| +$$

$$\sum \{1 + d(u_1, v_1\,|G_1) : \{e,f\} \in A_4, e = [(u_1,u_2),(u_1,v_2)],$$

$$f = [(v_1,z_2),(v_1,t_2)]\} = |A_1| + 3|A_2| + 2|A_3| + |A_4| +$$

$$\sum \{d(u_1, v_1\,|G_1) : \{e,f\} \in A_4, e = [(u_1,u_2),(u_1,v_2)], f = [(v_1,z_2),(v_1,t_2)]\} =$$

$$\sum_{i=1}^{4} |A_i| + (|A_2| + |A_3|) + |A_2| + |E(G_2)|^2 \sum_{\{u_1,v_1\}\subseteq V(G_1)} d(u_1, v_1\,|G_1) =$$

$$\left| \bigcup_{i=1}^{4} A_i \right| + |A_2 \cup A_3| + |A_2| + |E(G_2)|^2 W(G_1) = |A| + |A_2 \cup A_3| + |A_2|$$

$$+ |E(G_2)|^2 W(G_1) =$$

$$\binom{|V(G_1)|\ |E(G_2)|}{2} + \frac{1}{2}|V(G_1)|\ \left(|E(G_2)|^2 + |E(G_2)| - M_1(G_2) \right)$$

$$+ \frac{1}{4}|V(G_1)|\, N(G_2) + |E(G_2)|^2 W(G_1) =$$

$$\frac{1}{2}\Big(|V(G_1)|^2 |E(G_2)|^2 - |V(G_1)|\ |E(G_2)| + |V(G_1)|\ |E(G_2)|^2$$

$$+ |V(G_1)|\ |E(G_2)| \Big) -$$

$$\frac{1}{2}\left|V\left(G_1\right)\right| M_1\left(G_2\right)+\frac{1}{4}\left|V\left(G_1\right)\right| N\left(G_2\right)+\left|E\left(G_2\right)\right|^2 W\left(G_1\right)=$$

$$\left|E\left(G_2\right)\right|^2\left(\binom{\left|V\left(G_1\right)\right|+1}{2}+W\left(G_1\right)\right)-\frac{1}{4}\left|V\left(G_1\right)\right|\ \left(2 M_1\left(G_2\right)-N\left(G_2\right)\right).$$

∎

Lemma 13.3.8 $\sum_{\{e,f\}\in B} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right) = \left|V\left(G_2\right)\right|^2\binom{|V(G_2)|}{2} M_1\left(G_1\right) + \left|V\left(G_2\right)\right|^4 W_{e_0}\left(G_1\right)$

Proof For the proof of this lemma, we need to obtain $|B_1|$, $|B_2|$, and $|B_4|$. It is easy to see that:

$$\left|B_1\right|=2\left|E\left(G_1\right)\right|\left|V\left(G_2\right)\right|\binom{|V(G_2)|}{2},\ \left|B_2\right|=2\left|E\left(G_1\right)\right|\binom{|V(G_2)|}{2}^2,$$

$$\left|B_4\right|=\left|V\left(G_2\right)\right|^3\left(\left|V\left(G_2\right)\right|-1\right)\sum_{u_1\in V(G_1)}\binom{\delta_{u_1}}{2}=\left|V\left(G_2\right)\right|^2\binom{|V(G_2)|}{2}$$
$$\left(M_1\left(G_1\right)-2\left|E\left(G_1\right)\right|\right).$$

Afterwards, we find $\sum_{\{e,f\}\in B_3\cup B_4\cup B_5} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right)$. By Proposition 13.3.3, we have

$$\sum_{\{e,f\}\in B_3} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right)=\sum\left\{d_0\left(\left[u_1,v_1\right],\left[u_1,z_1\right]\left|G_1\right.\right):\right.$$
$$\left.\{e,f\}\in B_3, e=\left[\left(u_1,u_2\right),\left(v_1,v_2\right)\right], f=\left[\left(u_1,u_2\right),\left(z_1,z_2\right)\right]\right\}=\}$$
$$\left|V\left(G_2\right)\right|^3\sum_{u_1\in V(G_1)}\ \sum_{\{[u_1,v_1],[u_1,z_1]\}\subseteq E(G_1)} d_0\left(\left[u_1,v_1\right],\left[u_1,z_1\right]\left|G_1\right.\right)$$
$$=\frac{1}{2}\left|V\left(G_2\right)\right|^3\sum_{[u_1,v_1]\in E(G_1)}\ \sum_{\substack{z_1\in\{u_1,v_1\},\\ [z_1,t_1]\in E(G_1)}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right),$$

$$\sum_{\{e,f\}\in B_4} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right)=\sum\left\{d_0\left(\left[u_1,v_1\right],\left[u_1,z_1\right]\right|G_1\right)+1:\{e,f\}\in B_4,$$
$$\left.e=\left[\left(u_1,u_2\right),\left(v_1,v_2\right)\right], f=\left[\left(u_1,t_2\right),\left(z_1,z_2\right)\right]\right\}=$$
$$\left(\left|V\left(G_2\right)\right|^4-\left|V\left(G_2\right)\right|^3\right)\sum_{u_1\in V(G_1)}\ \sum_{\{[u_1,v_1],[u_1,z_1]\}\subseteq E(G_1)} d_0\left(\left[u_1,v_1\right],\left[u_1,z_1\right]\left|G_1\right.\right)+\left|B_4\right|=$$
$$\frac{1}{2}\left(\left|V\left(G_2\right)\right|^4-\left|V\left(G_2\right)\right|^3\right)\sum_{[u_1,v_1]\in E(G_1)}\ \sum_{\substack{z_1\in\{u_1,v_1\},\\ [z_1,t_1]\in E(G_1)}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right)+\left|B_4\right|,$$

$$\sum_{\{e,f\}\in B_5} d_0\left(e,f\left|G_1[G_2]\right.\right) = \sum\left\{d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right): \right.$$

$$\left.\{e,f\}\in B_5, e=\left[\left(u_1,u_2\right),\left(v_1,v_2\right)\right], f=\left[\left(z_1,z_2\right),\left(t_1,t_2\right)\right]\right\} =$$

$$\frac{1}{2}\left|V\left(G_2\right)\right|^4 \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{[z_1,t_1]\in E(G_1),\\ z_1,t_1\notin\{u_1,v_1\}}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right).$$

Based on the above computations and since each pair of $B_i (1 \le i \le 5)$ is disjoint, we have

$$\sum_{\{e,f\}\in B_3\cup B_4\cup B_5} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right) = \sum_{i=3}^{5}\sum_{\{e,f\}\in B_i} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right) =$$

$$\frac{1}{2}\left|V\left(G_2\right)\right|^3 \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{z_1\in\{u_1,v_1\},\\ [z_1,t_1]\in E(G_1)}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right)+$$

$$\frac{1}{2}\left(\left|V\left(G_2\right)\right|^4-\left|V\left(G_2\right)\right|^3\right) \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{z_1\in\{u_1,v_1\},\\ [z_1,t_1]\in E(G_1)}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right)+\left|B_4\right|+$$

$$\frac{1}{2}\left|V\left(G_2\right)\right|^4 \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{[z_1,t_1]\in E(G_1),\\ z_1,t_1\notin\{u_1,v_1\}}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right) =$$

$$\frac{1}{2}\left|V\left(G_2\right)\right|^4 \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{z_1\in\{u_1,v_1\},\\ [z_1,t_1]\in E(G_1)}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right)+\left|B_4\right|+$$

$$\frac{1}{2}\left|V\left(G_2\right)\right|^4 \sum_{[u_1,v_1]\in E(G_1)} \sum_{\substack{[z_1,t_1]\in E(G_1),\\ z_1,t_1\notin\{u_1,v_1\}}} d_0\left(\left[u_1,v_1\right],\left[z_1,t_1\right]\left|G_1\right.\right) =$$

$$\left|B_4\right|+\frac{1}{2}\left|V\left(G_2\right)\right|^4\left(2W_{e_0}\left(G_1\right)\right) = \left|B_4\right|+\left|V\left(G_2\right)\right|^4 W_{e_0}\left(G_1\right).$$

Now, since $B = \bigcup_{i=1}^{5} B_i$, we have

$$\sum_{\{e,f\}\in B} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right) = \sum_{\{e,f\}\in B_1} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right)+$$

$$\sum_{\{e,f\}\in B_2} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right)+\sum_{\{e,f\}\in B_3\cup B_4\cup B_5} d_0\left(e,f\left|G_1\left[G_2\right]\right.\right) =$$

$$|B_1| + 2|B_2| + |B_4| + |V(G_2)|^4 W_{e_0}(G_1)$$

$$= 2|E(G_1)| \binom{|V(G_2)|}{2} \left(|V(G_2)| + 2\binom{|V(G_2)|}{2} - |V(G_2)|^2 \right) +$$

$$|V(G_2)|^2 \binom{|V(G_2)|}{2} M_1(G_1) + |V(G_2)|^4 W_{e_0}(G_1)$$

$$= |V(G_2)|^2 \binom{|V(G_2)|}{2} M_1(G_1) + |V(G_2)|^4 W_{e_0}(G_1).$$

■

Lemma 13.3.9 $\sum_{\{e,f\}\in C} d_0(e, f\,|G_1[G_2]) = |E(G_1)|\ |E(G_2)|\,|V(G_2)|\,(|V(G_1)|$
$|V(G_2)| + 2|V(G_2)| - 4) + |E(G_2)|\,|V(G_2)|^2 \mathrm{Min}(G_1)$
where, $\mathrm{Min}(G_1) = \sum_{u_1\in V(G_1)} \sum_{[v_1,z_1]\in E(G_1)} \min\{d(u_1, v_1|G_1), d(u_1, z_1|G_1)\}$

Proof First, we find $|C_2|$ and $\sum_{\{e,f\}\in C_3} d_0(e, f\,|G_1[G_2])$. It is easy to see that

$$|C_2| = |V(G_2)|\,(|V(G_2)| - 2)\,|E(G_2)|$$
$$\times \sum_{u_1\in V(G_1)} \delta_{u_1} = 2|E(G_1)|\,|E(G_2)|\,|V(G_2)|\,(|V(G_2)| - 2),$$

and by Proposition 13.3.5, we have

$$\sum_{\{e,f\}\in C_3} d_0(e, f\,|G_1[G_2])$$
$$= \sum \{1 + \min\{d(u_1, v_1|G_1), d(u_1, z_1|G_1) :$$
$$\times\ \{e, f\} \in C_3, e = [(u_1, u_2), (u_1, t_2)], f = [(v_1, v_2), (z_1, z_2)]\}$$
$$= |C_3| + |E(G_2)|\,|V(G_2)|^2 \sum_{u_1\in V(G_1)} \sum_{\substack{[v_1,z_1]\in E(G_1)\\ v_1\neq z_1, z\neq_1 u_1}} \min\{d(u_1, v_1|G_1), d(u_1, z_1|G_1)\}$$
$$= |C_3| + |E(G_2)|\,|V(G_2)|^2 \sum_{u_1\in V(G_1)} \sum_{[v_1,z_1]\in E(G_1)} \min\{d(u_1, v_1|G_1), d(u_1, z_1|G_1)\}$$
$$= |C_3| + |E(G_2)|\,|V(G_2)|^2 \mathrm{Min}(G_1).$$

Since each pair of the sets C_i $(1 \le i \le 3)$ is disjoint and $C = \bigcup_{i=1}^{3} C_i$, we have

$$\sum_{\{e,f\}\in C} d_0(e,f\,|G_1[G_2]) = \sum_{\{e,f\}\in C_1\cup C_2} d_0(e,f\,|G_1[G_2])$$
$$+ \sum_{\{e,f\}\in C_3} d_0(e,f\,|G_1[G_2])$$
$$= |C_1| + 2|C_2| + |C_3| + |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1)$$
$$= \sum_{i=1}^{3}|C_i| + |C_2| + |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1)$$
$$= \left|\bigcup_{i=1}^{3} C_i\right| + |C_2| + |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1)$$
$$= |C| + |C_2| + |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1)$$
$$= |V(G_1)|\,|V(G_2)|^2\,|E(G_1)|\,|E(G_2)|$$
$$+ 2|E(G_1)|\,|E(G_2)|\,|V(G_2)|\,(|V(G_2)|-2)$$
$$+ |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1)$$
$$= |E(G_1)|\,|E(G_2)|\,|V(G_2)|\,(|V(G_1)|\,|V(G_2)| + 2|V(G_2)| - 4)$$
$$+ |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1).$$

∎

Now, as the main purpose of this section, we express Theorem 13.3.10, which characterizes the first edge Wiener index of the composition of two graphs.

Theorem 13.3.10 *Let* $G_1 = (V(G_1), E(G_1))$ *and* $G_2 = (V(G_2), E(G_2))$ *be two simple undirected connected finite graphs, then*

$$W_{e_0}(G_1[G_2]) = |E(G_2)|^2\binom{|V(G_1)|+1}{2}$$
$$+ |E(G_1)|\,|E(G_2)|\,|V(G_2)|\,(|V(G_1)|\,|V(G_2)| + 2|V(G_2)| - 4)$$
$$+ |E(G_2)|^2 W(G_1) + |V(G_2)|^4 W_{e_0}(G_1) + |V(G_2)|^2\binom{|V(G_2)|}{2}$$
$$M_1(G_1) + |E(G_2)|\,|V(G_2)|^2\mathrm{Min}(G_1) - \frac{1}{4}|V(G_1)|\,(2M_1(G_2) - N(G_2)),$$

where $\mathrm{Min}(G_1) = \sum_{u_1\in V(G_1)}\sum_{[v_1,z_1]\in E(G_1)} \min\{d(u_1,v_1|G_1), d(u_1,z_1|G_1)\}$ *and* $N(G_2) = \sum_{[u_2,v_2]\in E(G_2)}\sum_{z_2\in V(G_2)-(\Delta_{u_2}\cup\Delta_{v_2})} N_{(z_2,\tilde{u}_2,\tilde{v}_2)}$.

Proof Remember that each pair of the sets A, B, and C is disjoint, and union of them is the set of all two element subsets of $E(G_1[G_2])$. Now, using the definition of the first edge-Wiener index, we obtain that

$$W_{e_0}(G_1[G_2]) = \sum_{\{e,f\}\subseteq E(G_1[G_2])} d_0(e,f|G_1[G_2]) = \sum_{\{e,f\}\in A} d_0(e,f|G_1[G_2])$$
$$+\sum_{\{e,f\}\in B} d_0(e,f|G_1[G_2]) + \sum_{\{e,f\}\in C} d_0(e,f|G_1[G_2]).$$

Now, by the above lemmas, the proof is completed. ∎

13.4 Computation of the Edge Wiener Indices of the Sum of Graphs

In this section, we find the edge-Wiener indices of the sum of graphs. Then as an application of our results, we find the edge-Wiener indices of graphene, C_4 - nanotubes and C_4 – nanotori. All of the results in this section have been published in Azari and Iranmanesh (2011).

At first, we give the definition of sum of two graphs.

Definition 13.4.1 Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be connected graphs. The sum of G_1 and G_2 is denoted by $G_1 + G_2$, that is, a graph with the vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) of $G_1 + G_2$ are adjacent if and only if $[u_1 = v_1$ and $[u_2, v_2] \in E(G_2)]$ or $[u_2 = v_2$ and $[u_1, v_1] \in E(G_1)]$.

Theorem 13.4.2 (Stevanovic 2001) *Let* $G_1 = (V(G_1), E(G_1))$ *and* $G_2 = (V(G_2), E(G_2))$ *be two connected graphs. The distance between two vertices* (u_1, u_2) *and* (v_1, v_2) *of* $G_1 + G_2$ *is equal to* $d((u_1, u_2), (v_1, v_2)|G_1 + G_2) = d(u_1, v_1|G_1) + d(u_2, v_2|G_2)$.

In order to find the edge-Wiener indices of $G_1 + G_2$, first we define the sets A and B as follows:

$$A = \{[(u_1, u_2), (u_1, v_2)] \in E(G_1 + G_2) : u_1 \in V(G_1),\ [u_2, v_2] \in E(G_2)\}$$
$$B = \{[(u_1, u_2), (v_1, u_2)] \in E(G_1 + G_2) : u_2 \in V(G_2),\ [u_1, v_1] \in E(G_1)\}$$

It is easy to see that $A \cup B = E(G_1 + G_2)$, $A \cap B = \phi$, $|A| = |V(G_1)|\ |E(G_2)|$ and

$$|B| = |E(G_1)|\ |V(G_2)|.$$

Set

$$A_1 = \{\{e, f\} \subseteq A : e \neq f, e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, u_2), (a_1, v_2)], u_1, a_1 \in V(G_1), u_2, v_2 \in V(G_2)\}$$

$$A_2 = \{\{e, f\} \subseteq A : e \neq f, e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (a_1, b_2)], u_1, a_1 \in V(G_1), u_2, v_2, a_2, b_2 \in V(G_2), [u_2, v_2] \neq [a_2, b_2]\}$$

$$B_1 = \{\{e, f\} \subseteq B : e \neq f, e = [(u_1, u_2), (v_1, u_2)], f = [(u_1, a_2), (v_1, a_2)], u_1, v_1 \in V(G_1), u_2, a_2 \in V(G_2)\}$$

$$B_2 = \{\{e, f\} \subseteq B : e \neq f, e = [(u_1, u_2), (v_1, u_2)], f = [(a_1, a_2), (b_1, a_2)], u_2, a_2 \in V(G_2), u_1, v_1, a_1, b_1 \in V(G_1), [u_1, v_1] \neq [a_1, b_1]\}$$

Obviously, $A_1 \cap A_2 = B_1 \cap B_2 = \phi$ and $A_1 \cup A_2$, $B_1 \cup B_2$ are the sets of all two element subsets of A and B, respectively. Also,

$$|A_1| = \binom{|V(G_1)|}{2} |E(G_2)|, |B_1| = \binom{|V(G_2)|}{2} |E(G_1)|.$$

In the first proposition, we find $d_0(e, f | G_1 + G_2)$ and $d_4(e, f | G_1 + G_2)$ for all $\{e, f\} \subseteq A$.

Proposition 13.4.3 *Let $\{e, f\} \subseteq A$ and $e \neq f$.*

(i) *If $\{e, f\} \in A_1$ and $e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, u_2), (a_1, v_2)]$, then*

$$d_0(e, f | G_1 + G_2) = d_4(e, f | G_1 + G_2) = d(u_1, a_1 | G_1) + 1$$

(ii) *If $\{e, f\} \in A_2$ and $e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (a_1, b_2)]$, then for $i \in \{0, 4\}$, $d_i(e, f | G_1 + G_2) = d_i([u_2, v_2], [a_2, b_2] | G_2) + d(u_1, a_1 | G_1)$*

Proof

(i) Let $\{e, f\} \in A_1$ and $e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, u_2), (a_1, v_2)]$. Using the definition of $d_0(e, f)$, $d_4(e, f)$ and the formula of the distance between two vertices of $G_1 + G_2$, we have

$$\begin{aligned} d_0(e, f | G_1 + G_2) = 1 + \min\{&d((u_1, u_2), (a_1, u_2) | G_1 + G_2), \\ &\times d((u_1, u_2), (a_1, v_2) | G_1 + G_2) \\ &d((u_1, v_2)(a_1, u_2) | G_1 + G_2), d((u_1, v_2), (a_1, v_2) | G_1 + G_2)\} \\ &= 1 + \min\{d(u_1, a_1 | G_1) + \\ &d(u_2, u_2 | G_2), d(u_1, a_1 | G_1) + d(u_2, v_2 | G_2), d(u_1, a_1 | G_1) \\ &+ d(v_2, u_2 | G_2), d(u_1, a_1 | G_1) + \end{aligned}$$

$$d\left(v_2, v_2\left|G_2\right.\right)\} = 1 + \min\left\{d\left(u_2, u_2\left|G_2\right.\right), d\left(u_2, v_2\left|G_2\right.\right), d\left(v_2, u_2\left|G_2\right.\right),\right.$$
$$\times\ d\left(v_2, v_2\left|G_2\right.\right)\} +$$
$$d\left(u_1, a_1\left|G_1\right.\right) = 1 + \min\{0, 1, 1, 0\} + d\left(u_1, a_1\left|G_1\right.\right) = d\left(u_1, a_1\left|G_1\right.\right) + 1 \text{ and}$$
$$d_4\left(e, f\left|G_1 + G_2\right.\right) = \max\left\{d\left(\left(u_1, u_2\right), \left(a_1, u_2\right)\left|G_1 + G_2\right.\right),\right.$$
$$\times d\left(\left(u_1, u_2\right), \left(a_1, v_2\right)\left|G_1 + G_2\right.\right),$$
$$d\left(\left(u_1, v_2\right)\left(a_1, u_2\right)\left|G_1 + G_2\right.\right), d\left(\left(u_1, v_2\right), \left(a_1, v_2\right)\left|G_1 + G_2\right.\right)\}$$
$$= \max\left\{d\left(u_1, a_1\left|G_1\right.\right) +\right.$$
$$d\left(u_2, u_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right) + d\left(u_2, v_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right)$$
$$+ d\left(v_2, u_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right) +$$
$$d\left(v_1, v_2\left|G_2\right.\right)\} = \max\left\{d\left(u_2, u_2\left|G_2\right.\right), d\left(u_2, v_2\left|G_2\right.\right), d\left(v_2, u_2\left|G_2\right.\right)\right.$$
$$\times d\left(v_2, v_2\left|G_2\right.\right)\} +$$
$$d\left(u_1, a_1\left|G_1\right.\right) = \max\{0, 1, 1, 0\} + d\left(u_1, a_1\left|G_1\right.\right) = d\left(u_1, a_1\left|G_1\right.\right) + 1.$$

Therefore $d_0\left(e, f\left|G_1 + G_2\right.\right) = d_4\left(e, f\left|G_1 + G_2\right.\right) = d\left(u_1, a_1\left|G_1\right.\right) + 1$ and the equality in part (i) of Proposition 13.2.1 holds.

(ii) Let $\{e, f\} \in A_2$ and $e = [(u_1, u_2), (u_1, v_2)]$, $f = [(a_1, a_2), (a_1, b_2)]$. In this case $[u_2, v_2] \neq [a_2, b_2]$ and we have

$$d_0\left(e, f\left|G_1 + G_2\right.\right) = 1 + \min\left\{d\left(\left(u_1, u_2\right), \left(a_1, a_2\right)\left|G_1 + G_2\right.\right),\right.$$
$$\times d\left(\left(u_1, u_2\right), \left(a_1, b_2\right)\left|G_1 + G_2\right.\right),$$
$$d\left(\left(u_1, v_2\right), \left(a_1, a_2\right)\left|G_1 + G_2\right.\right), d\left(\left(u_1, v_2\right), \left(a_1, b_2\right)\left|G_1 + G_2\right.\right)\}$$
$$\times = 1 + \min\left\{d\left(u_1, a_1\left|G_1\right.\right) +\right.$$
$$d\left(u_2, a_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right) + d\left(u_2, b_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right)$$
$$+ d\left(v_2, a_2\left|G_2\right.\right), d\left(u_1, a_1\left|G_1\right.\right) +$$
$$d\left(v_2, b_2\left|G_2\right.\right)\} = 1 + \min\left\{d\left(u_2, a_2\left|G_2\right.\right), d\left(u_2, b_2\left|G_2\right.\right), d\left(v_2, a_2\left|G_2\right.\right),\right.$$
$$\times d\left(v_2, b_2\left|G_2\right.\right)\} +$$
$$d\left(u_1, a_1\left|G_1\right.\right) = d_0\left(\left[u_2, v_2\right], \left[a_2, b_2\right]\left|G_2\right.\right) + d\left(u_1, a_1\left|G_1\right.\right) \text{ and}$$
$$d_4\left(e, f\left|G_1 + G_2\right.\right) = \max\left\{d\left(\left(u_1, u_2\right), \left(a_1, a_2\right)\left|G_1 + G_2\right.\right),\right.$$
$$\times d\left(\left(u_1, u_2\right), \left(a_1, b_2\right)\left|G_1 + G_2\right.\right),$$
$$d\left(\left(u_1, v_2\right), \left(a_1, a_2\right)\left|G_1 + G_2\right.\right), d\left(\left(u_1, v_2\right), \left(a_1, b_2\right)\left|G_1 + G_2\right.\right)\}$$
$$= \max\left\{d\left(u_1, a_1\left|G_1\right.\right) + d\left(v_2, b_2\left|G_2\right.\right)\right\} =$$

$$d\left(u_2,a_2\left|G_2\right.\right),d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_2,b_2\left|G_2\right.\right),d\left(u_1,a_1\left|G_1\right.\right)$$
$$+\,d\left(v_2,a_2\left|G_2\right.\right),d\left(u_1,a_1\left|G_1\right.\right)+$$
$$\max\left\{d\left(u_2,a_2\left|G_2\right.\right),d\left(u_2,b_2\left|G_2\right.\right),d\left(v_2,a_2\left|G_2\right.\right),d\left(v_2,b_2\left|G_2\right.\right)\right\}$$
$$+\,d\left(u_1,a_1\left|G_1\right.\right)=d_4\left(\left[u_2,v_2\right],\left[a_2,b_2\right]\left|G_2\right.\right)+d\left(u_1,a_1\left|G_1\right.\right).$$

Therefore, for $i \in \{0,4\}$, $d_i\left(e,f\left|G_1+G_2\right.\right)=d_i\left(\left[u_2,v_2\right],\left[a_2,b_2\right]\left|G_2\right.\right)+d\left(u_1,a_1\left|G_1\right.\right)$,
which completes the proof. ∎

In the next proposition, we find $d_0\left(e,f\left|G_1+G_2\right.\right)$ and $d_4\left(e,f\left|G_1+G_2\right.\right)$ for all $\{e,f\}\subseteq B$.

Proposition 13.4.4 *Let $\{e,f\}\subseteq B$ and $e\neq f$.*

(i) If $\{e,f\}\in B_1$ and $e=\left[\left(u_1,u_2\right),\left(v_1,u_2\right)\right], f=\left[\left(u_1,a_2\right),\left(v_1,a_2\right)\right]$, then

$$d_0\left(e,f\left|G_1+G_2\right.\right)=d_4\left(e,f\left|G_1+G_2\right.\right)=d\left(u_2,a_2\left|G_2\right.\right)+1$$

(ii) If $\{e,f\}\in B_2$ and $e=\left[\left(u_1,u_2\right),\left(v_1,u_2\right)\right], f=\left[\left(a_1,a_2\right),\left(b_1,a_2\right)\right]$, then for $i\in\{0,4\}$,

$$d_i\left(e,f\left|G_1+G_2\right.\right)=d_i\left(\left[u_1,v_1\right],\left[a_1,b_1\right]\left|G_1\right.\right)d\left(u_2,a_2\left|G_2\right.\right).$$

Proof The proof is similar to the proof of Proposition 13.4.3. ∎

In the next proposition, we find $d_0\left(e,f\left|G_1+G_2\right.\right)$ and $d_4\left(e,f\left|G_1+G_2\right.\right)$ for all $e\in A$, $f\in B$.

Proposition 13.4.5 *Let $e\in A$ and $f\in B$, such that $e=\left[\left(u_1,u_2\right),\left(u_1,v_2\right)\right]$ and $f=\left[\left(a_1,a_2\right),\left(b_1,a_2\right)\right]$, then*

(i)
$$d_0\left(e,f\left|G_1+G_2\right.\right)=1+\min\left\{d\left(u_1,a_1\left|G_1\right.\right),d\left(u_1,b_1\left|G_1\right.\right)\right\}+$$
$$\min\left\{d\left(u_2,a_2\left|G_2\right.\right),d\left(v_2,a_2\left|G_2\right.\right)\right\}$$

(ii)
$$d_4\left(e,f\left|G_1+G_2\right.\right)=\max\left\{d\left(u_1,a_1\left|G_1\right.\right),d\left(u_1,b_1\left|G_1\right.\right)\right\}+$$
$$\max\left\{d\left(u_2,a_2\left|G_2\right.\right),d\left(v_2,a_2\left|G_2\right.\right)\right\}$$

Proof Let $e\in A$ and $f\in B$, such that $e=\left[\left(u_1,u_2\right),\left(u_1,v_2\right)\right]$ and $f=\left[\left(a_1,a_2\right),\left(b_1,a_2\right)\right]$, then

(i)
$$d_0\left(e,f\left|G_1+G_2\right.\right)=1+\min\left\{d\left(\left(u_1,u_2\right),\left(a_1,a_2\right)\left|G_1+G_2\right.\right),\right.$$
$$\times d\left(\left(u_1,u_2\right),\left(b_1,a_2\right)\left|G_1+G_2\right.\right),\ d\left(\left(u_1,v_2\right),\left(a_1,a_2\right)\left|G_1+G_2\right.\right),$$

$$d\left((u_1,v_2),(b_1,a_2)\left|G_1+G_2\right.\right)\} = 1+\min\{d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_2,a_2\left|G_2\right.\right),$$
$$\times d\left(u_1,b_1\left|G_1\right.\right)+$$
$$d\left(u_2,a_2\left|G_2\right.\right), d\left(u_1,a_1\left|G_1\right.\right)+d\left(v_2,a_2\left|G_2\right.\right), d\left(u_1,b_1\left|G_1\right.\right)$$
$$+d\left(v_2,a_2\left|G_2\right.\right)\}$$
$$= 1+\min\{\min\{d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_1,b_1\left|G_1\right.\right)\}+d\left(u_2,a_2\left|G_2\right.\right),$$
$$\min\{d\left(u_1,a_1\left|G_1\right.\right)+\left(u_1,b_1\left|G_1\right.\right)\}+d\left(v_2,a_2\left|G_2\right.\right)\}$$
$$= 1+\min\{d\left(u_1,a_1\left|G_1\right.\right), d\left(u_1,b_1\left|G_1\right.\right)\}+$$
$$\min\{d\left(u_2,a_2\left|G_2\right.\right), d\left(v_2,a_2\left|G_2\right.\right)$$

and part (i) of Proposition 13.4.5, holds.

(ii)
$$d_4\left(e,f\left|G_1+G_2\right.\right) = \max\{d\left((u_1,u_2),(a_1,a_2)\left|G_1+G_2\right.\right),$$
$$d\left((u_1,u_2),(b_1,a_2)\left|G_1+G_2\right.\right), d\left((u_1,v_2),(a_1,a_2)\left|G_1+G_2\right.\right),$$
$$d((u_1,v_2),(b_1,a_2)\left|G_1+G_2\right.)\} = \max\{d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_1,a_2\left|G_2\right.\right),$$
$$d\left(u_1,b_1\left|G_1\right.\right)+d\left(u_2,a_2\left|G_2\right.\right), d\left(u_1,a_1\left|G_1\right.\right)$$
$$+d\left(v_2,a_2\left|G_2\right.\right),\ d\left(u_1,b_1\left|G_1\right.\right)+d\left(v_2,a_2\left|G_2\right.\right)\}$$
$$= \max\{\max\{d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_1,b_1\left|G_1\right.\right)\}+d\left(u_2,a_2\left|G_2\right.\right),$$
$$\max\{d\left(u_1,a_1\left|G_1\right.\right)+d\left(u_1,b_1\left|G_1\right.\right)\}+d\left(v_2,a_2\left|G_2\right.\right)\}$$
$$= \max\{d\left(u_1,a_1\left|G_1\right.\right), d\left(u_1,b_1\left|G_1\right.\right)\}$$
$$+\max\{d\left(u_2,a_2\left|G_2\right.\right), d\left(v_2,a_2\left|G_2\right.\right)\},$$

so part (ii) of Proposition 13.4.5 holds. ∎

Using Proposition 13.4.3, we conclude two following lemmas:

Lemma 13.4.6 $\sum_{\{e,f\}\in A_1} d_0\left(e,f\left|G_1+G_2\right.\right) = \sum_{\{e,f\}\in A_1} d_4\left(e,f\left|G_1+G_2\right.\right)$ $= \left|E\left(G_2\right)\right| W\left(G_1\right) + \binom{|V(G_1)|}{2}\left|E\left(G_2\right)\right|$

Proof By part (i) of Proposition 13.4.3, we have

$$\sum_{\{e,f\}\in A_1} d_0\left(e,f\left|G_1+G_2\right.\right) = \sum_{\{e,f\}\in A_1} d_4\left(e,f\left|G_1+G_2\right.\right)$$
$$= \sum\{d\left(u_1,a_1\left|G_1\right.\right)+1 : \{e,f\}\in A_1, e = \left[(u_1,u_2),(u_1,v_2)\right],$$
$$\times\ f = \left[(a_1,u_2),(a_1,v_2)\right]\}$$
$$= \sum\{d\left(u_1,a_1\left|G_1\right.\right) : \{e,f\}\in A_1,\ e = \left[(u_1,u_2),(u_1,v_2)\right],$$
$$f = \left[(a_1,u_2),(a_1,v_2)\right]\} + |A_1|$$

$$= |E(G_2)| \sum_{\{u_1,a_1\}\subseteq V(G_1)} d(u_1, a_1 | G_1) + \binom{|V(G_1)|}{2} |E(G_2)|$$

$$= |E(G_2)| W(G_1) + \binom{|V(G_1)|}{2} |E(G_2)|.$$

∎

Lemma 13.4.7 *For* $i \in \{0, 4\}$, *we have*: $\sum_{\{e,f\}\in A_2} d_i(e, f | G_1 + G_2)$ $= |V(G_1)|^2 W_{e_i}(G_2) + 2\binom{|E(G_2)|}{2} W(G_1)$.

Proof By part (ii) of Proposition 13.4.3, for $i \in \{0, 4\}$, we have

$$\sum_{\{e,f\}\in A_2} d_i(e, f | G_1 + G_2)$$

$$= \sum \{d_i([u_2, v_2], [a_2, b_2] | G_2) + d(u_1, a_1 | G_1) : \{e, f\} \in A_2,$$

$$\times e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (a_1, b_2)]\}$$

$$= \sum \{d_i([u_2, v_2], [a_2, b_2] | G_2) :$$

$$\{e, f\} \in A_2, e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (a_1, b_2)]\}$$

$$+ \sum \{d(u_1, a_1 | G_1) : \{e, f\} \in A_2,$$

$$e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (a_1, b_2)]\} = |V(G_1)|^2$$

$$\sum_{\{[u_2,v_2],[a_2,b_2]\}\subseteq E(G_2)} ([u_2, v_2], [a_2, b_2] | G_2) +$$

$$2\binom{|E(G_2)|}{2} \sum_{\{u_1,a_1\}\subseteq V(G_1)} d(u_1, a_1 | G_1) = |V(G_1)|^2 W_{e_i}(G_2)$$

$$+ 2\binom{|E(G_2)|}{2} W(G_1).$$

∎

By Lemmas 13.4.6 and 13.4.7, we have the following result:

Corollary 13.4.8 *For* $i \in \{0, 4\}$, *we have*

$$\sum_{\{e,f\}\subseteq A} d_i(e, f | G_1 + G_2) = |E(G_2)|^2 W(G_1) + |V(G_1)|^2 W_{e_i}(G_2)$$

$$+ \binom{|V(G_1)|}{2} |E(G_2)|$$

Proof Since d_0 and d_4 are distances, so for every $e \in E(G_1 + G_2)$, we have $d_0(e, e|G_1 + G_2) = d_4(e, e|G_1 + G_2) = 0$. Now by Lemmas 13.4.6 and 4.7, for $i \in \{0, 4\}$, we have

$$\sum_{\{e,f\}\subseteq A} d_i(e, f|G_1 + G_2) = \sum_{\{e,f\}\subseteq A, e\neq f} d_i(e, f|G_1 + G_2)$$

$$= \sum_{\{e,f\}\in A_1} d_i(e, f|G_1+G_2) + \sum_{\{e,f\}\in A_2} d_i(e, f|G_1+G_2) = |E(G_2)|\, W(G_1)$$

$$+ \binom{|V(G_1)|}{2} |E(G_2)| + |V(G_1)|^2 W_{e_i}(G_2) + 2\binom{|E(G_2)|}{2} W(G_1)$$

$$= |E(G_2)|^2 W(G_1) + |V(G_1)|^2 W_{e_i}(G_2) + \binom{|V(G_1)|}{2} |E(G_2)|.$$

∎

Using Proposition 13.4.4, we conclude two next lemmas.

Lemma 13.4.9

$$\sum_{\{e,f\}\in B_1} d_0(e, f|G_1 + G_2) = \sum_{\{e,f\}\in B_1} d_4(e, f|G_1 + G_2)$$

$$= |E(G_1)|\, W(G_2) + \binom{|V(G_2)|}{2} |E(G_1)|$$

Lemma 13.4.10 *For* $i \in \{0, 4\}$, *we have* $\sum_{\{e,f\}\in B_2} d_i(e, f|G_1 + G_2)$ $= |V(G_2)|^2 W_{e_i}(G_1) + 2\binom{|E(G_1)|}{2} W(G_2)$

Lemmas 13.4.9 and 13.4.10, indicate the following corollary:

Corollary 13.4.11 *For* $i \in \{0, 4\}$, *we have*

$$\sum_{\{e,f\}\subseteq B} d_i(e, f|G_1 + G_2) = |E(G_1)|^2 W(G_2) + |V(G_2)|^2 W_{e_i}(G_1)$$

$$+ \binom{|V(G_2)|}{2} |E(G_1)|$$

Proof Similar to the proof of Corollary 13.4.8, we can obtain the desired result. ∎

Here, we introduce two topological indices of a graph G as follows:

$$\mathrm{Min}(G) = \sum_{u\in V(G)} \sum_{[a,b]\in E(G)} \min\{d(u,a|G), d(u,b|G)\}$$

$$\mathrm{Max}(G) = \sum_{u\in V(G)} \sum_{[a,b]\in E(G)} \max\{d(u,a|G), d(u,b|G)\}$$

Using Proposition 13.4.5, we have the following lemma:

Lemma 13.4.12

(i)
$$\sum_{e\in A, f\in B} d_0(e,f|G_1+G_2) = |V(G_1)||V(G_2)||E(G_1)||E(G_2)| + |V(G_2)||E(G_2)|\,\mathrm{Min}(G_1) + |V(G_1)||E(G_1)|\,\mathrm{Min}(G_2),$$

(ii)
$$\sum_{e\in A, f\in B} d_4(e,f|G_1+G_2) = |V(G_2)||E(G_2)|\,\mathrm{Max}(G_1) + |V(G_1)| |E(G_1)|\,\mathrm{Max}(G_2)$$

Proof

(i) By part (i) of Proposition 13.4.5, we have

$$\sum_{e\in A, f\in B} d_0(e,f|G_1+G_2) = \sum\{1+\min\{d(u_1,a_1|G_1), d(u_1,b_1|G_1)\} + \min\{d(u_2,a_2|G_2), d(v_2,a_2|G_2)\} : e\in A, f\in B, e=[(u_1,u_2),(u_1,v_2)], f=[(a_1,a_2),(b_1,a_2)]\} = |A||B| + \sum\{\min\{d(u_2,a_2|G_1), d(u_1,b_1|G_1)\} : e\in A, f\in B, e=[(u_1,u_2),(u_1,v_2)], f=[(a_1,a_2),(b_1,a_2)]\} + \sum\{\min\{d(u_2,a_2|G_2), d(v_2,a_2|G_2)\} : e\in A, f\in B, e=[(u_1,u_2),(u_1,v_2)], f=[(a_1,a_2),(b_1,a_2)]\} = |V(G_1)||V(G_2)| |E(G_1)||E(G_2)|$$

$$+ |V(G_2)| |E(G_2)| \sum_{u_1 \in V(G_1)} \sum_{[a_1,b_1] \in E(G_1)} \min\{d(u_1, a_1 | G_1), d(u_1, b_1 | G_1)\}$$

$$+ |V(G_1)| |E(G_1)| \sum_{a_2 \in V(G_2)} \sum_{[u_2,v_2] \in E(G_2)} \min\{d(u_2, a_2 | G_2), d(v_2, a_2 | G_2)\}$$

$$= |V(G_1)| |V(G_2)| |E(G_1)| |E(G_2)| + |V(G_2)| |E(G_2)| \operatorname{Min}(G_1)$$

$$+ |V(G_1)| |E(G_1)| \operatorname{Min}(G_2).$$

(ii) By part (ii) of Proposition 13.4.5, we have

$$\sum_{e \in A, f \in B} d_4(e, f | G_1 + G_2) = \sum \{\max\{d(u_1, a_1 | G_1), d(u_1, b_1 | G_1)\}$$

$$+ \max\{d(u_2, a_2 | G_2), d(v_2, a_2 | G_2)\} :$$

$$e \in A, f \in B, e = [(u_1, u_2), (u_1, v_2)], f = [(a_1, a_2), (b_1, a_2)]\}$$

$$= \sum \{\max\{d(u_1, a_1 | G_1), d(u_1, b_1 | G_1)\} :$$

$$e \in A, f \in B, e = [(u_1, u_2), (u_1, v_2)],$$

$$f = [(a_1, a_2), (b_1, a_2)]\} + \sum \{\max\{d(u_2, a_2 | G_2), d(v_2, a_2 | G_2)\} :$$

$$e \in A, f \in B, e = [(u_1, u_2), (u_1, v_2)],$$

$$f = [(a_1, a_2), (b_1, a_2)]\} = |V(G_2)| |E(G_2)|$$

$$\sum_{u_1 \in V(G_1)} \sum_{[a_1,b_1] \in E(G_1)} \max\{d(u_1, a_1 | G_1), d(u_1, b_1 | G_1)\} +$$

$$|V(G_1)| |E(G_1)| \sum_{a_2 \in V(G_2)} \sum_{[u_2,v_2] \in E(G_2)} \max\{d(u_2, a_2 | G_2), d(v_2, a_2 | G_2)\}$$

$$= |V(G_2)| |E(G_2)| \operatorname{Max}(G_1) + |V(G_1)| |E(G_1)| \operatorname{Max}(G_2).$$

∎

Finally, as the main purpose of this part, we express Theorem 13.4.13, which characterizes the edge Wiener indices of the sum of two graphs.

Theorem 13.4.13 *Let* $G_1 = (V(G_1), E(G_1))$ *and* $G_2 = (V(G_2), E(G_2))$ *be two simple undirected connected finite graphs, then*

(i) $$W_{e_0}(G_1 + G_2) = |E(G_2)|^2 W(G_1) + |E(G_1)|^2 W(G_2) + |V(G_2)|^2 W_{e_0}(G_1)$$

$$+ |V(G_1)|^2 W_{e_0}(G_2) + \binom{|V(G_1)|}{2} |E(G_2)| + \binom{|V(G_2)|}{2} |E(G_1)|$$

$$+ |V(G_1)| |V(G_2)| |E(G_1)| |E(G_2)| + |V(G_2)| |E(G_2)| \operatorname{Min}(G_1)$$

$$+ |V(G_1)| |E(G_1)| \operatorname{Min}(G_2)$$

(ii) $$W_{e_4}(G_1+G_2)=|E(G_2)|^2 W(G_1)+|E(G_1)|^2 W(G_2)+|V(G_2)|^2 W_{e_4}(G_1) + |V(G_1)|^2 W_{e_4}(G_2)+\binom{|V(G_1)|}{2}|E(G_2)|+\binom{|V(G_2)|}{2}|E(G_1)| + |V(G_2)|\,|E(G_2)|\,\mathrm{Max}(G_1)+|V(G_1)|\,|E(G_1)|\,\mathrm{Max}(G_2)$$

Proof Since $E(G_1+G_2)=A\cup B$, $A\cap B=\phi$, for $i\in\{0,4\}$, we have

$$W_{e_i}(G_1+G_2)=\sum_{\{e,f\}\subseteq E(G_1+G_2)} d_i(e,f\,|G_1+G_2)=\sum_{\{e,f\}\subseteq A} d_i(e,f\,|G_1+G_2)+ \sum_{\{e,f\}\subseteq B} d_i(e,f\,|G_1+G_2)+\sum_{e\in A,f\in B} d_i(e,f\,|G_1+G_2).$$

Now by Corollaries 13.4.8 and 13.4.11 and Lemma 13.4.12, the proof is clear. ∎

Corollary 13.4.14 *For every two simple undirected connected finite graphs* $G_1=(V(G_1),E(G_1))$ and $G_2=(V(G_2),E(G_2))$, we have

$$W_{e_4}(G_1+G_2)-W_{e_0}(G_1+G_2)=|V(G_2)|^2\left(W_{e_4}(G_1)-W_{e_0}(G_1)\right) + |V(G_1)|^2\left(W_{e_4}(G_2)-W_{e_0}(G_2)\right)+ |V(G_2)|\,|E(G_2)|\left(\mathrm{Max}(G_1)-\mathrm{Min}(G_1)\right)+|V(G_1)|\,|E(G_1)|\left(\mathrm{Max}(G_2) -\mathrm{Min}(G_2)\right)-|V(G_1)|\,|V(G_2)|\,|E(G_1)|\,|E(G_2)|$$

The Wiener index and edge-Wiener indices of these graphs have been computed previously (Iranmanesh et al. 2009; Sagan et al. 1996). So, we have the following tables (Tables 13.3 and 13.4):

Carbon nanotubes, carbon nanotori and graphene are three important types of carbon structures. See Figs. 13.6, 13.7 and 13.8, respectively. Carbon nanotubes (CNTs) are allotropes of carbon with molecular structures that are tubular in shape, having diameters on the order of a few nanometers and lengths that can be as much as several millimeters.

Nanotubes are categorized as single-walled (SWNTs) and multi-walled (MWNTs) nanotubes. If a nanotube is bent so that its ends meet, a nanotorus is produced. These types of carbon structures, form the strongest and stiffest materials yet discovered on Earth. Their novel properties make them potentially useful in many applications in materials science, nanotechnology, electronics, optics and architecture.

Graphene is a one-atom-thick planer sheet of carbon atoms that are densely packed in a two-dimensional (2D) honeycomb crystal lattice and is a basic building block for graphitic materials of all other dimensionalities. It can be wrapped up into 0D fullerenes, rolled into 1D nanotubes, or stacked into 3D graphite (Fig. 13.9). The term graphene was coined as a combination of graphite and the suffix -ene by Hannes-Peter Boehm, who described single-layer carbon foils in 1962.

Table 13.3 Some topological indices of P_n and C_n

Graph (G)	P_n	C_n n is odd	C_n n is even
$\lvert V(G)\rvert$	n	n	n
$\lvert E(G)\rvert$	$n-1$	n	n
$W(G)$	$\binom{n+1}{3}$	$\frac{n}{8}\left(n^2-1\right)$	$\frac{n^3}{8}$
$W_{e_0}(G)$	$\binom{n}{3}$	$\frac{n}{8}\left(n^2-1\right)$	$\frac{n^3}{8}$
$W_{e_4}(G)$	$\binom{n-1}{2}\frac{n+3}{3}$	$\frac{n}{8}\left(n^2+4n-13\right)$	$\frac{n}{8}\left(n^2+4n-8\right)$

Table 13.4 Some topological indices of S_n, K_n, and $K_{a,b}$

Graph (G)	S_n	K_n	$K_{a,b}$
$\lvert V(G)\rvert$	n	n	$a+b$
$\lvert E(G)\rvert$	$n-1$	$\binom{n}{2}$	ab
$W(G)$	$(n-1)^2$	$\binom{n}{2}$	$(a+b)^2-ab$ $-a-b$
$W_{e_0}(G)$	$\binom{n-1}{2}$	$\binom{n}{2}\binom{n-1}{2}$	$\frac{ab}{2}(2ab-a-b)$
$W_{e_4}(G)$	$2\binom{n-1}{2}$	$3\binom{n+1}{4}$	$ab(ab-1)$

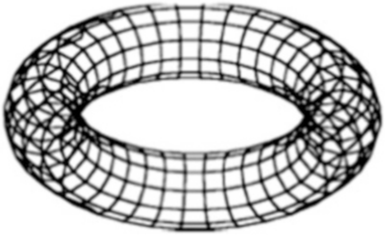


Fig. 13.6 A C_4-nanotori

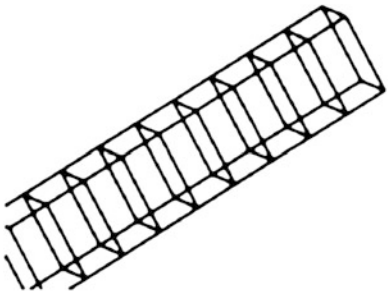


Fig. 13.7 A C_4-nanotube

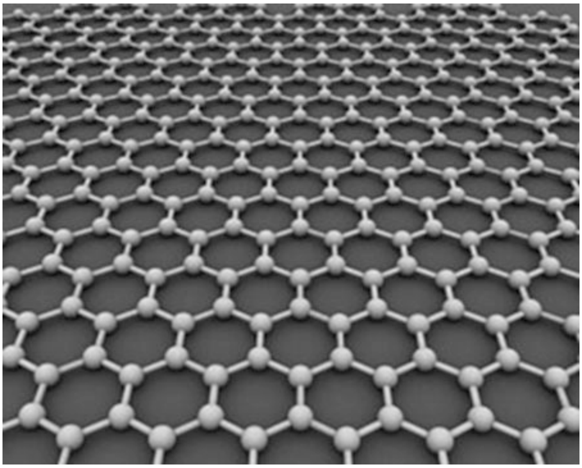


Fig. 13.8 Graphene

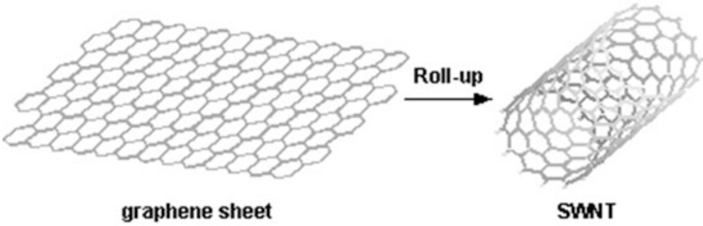


Fig. 13.9 Graphene sheet can be rolled in to a single walled nanotube

According to the tables, Theorem 13.4.13 and Corollary 13.4.14, we can easily obtain the edge-Wiener indices of the sum of each pair of the above-mentioned graphs. Specially, we can obtain the edge-Wiener indices of graphene, C_4-nanotubes, and C_4 -nanotori as $P_n + P_m$, $P_n + C_m$, and $C_n + C_m$, respectively.

Example 13.4.15 Suppose that $G = P_n + P_m$, where n and m are not necessarily equal. The edge Wiener indices of G, are as follows:

$$W_{e_0}(P_n + P_m) = \frac{m^3}{6}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 - 12n^2 + 8n - 3\right) - \frac{m}{3}\left(2n^3 - 4n^2 + 2n - 1\right) + \frac{n}{6}\left(n^2 - 3n + 2\right),$$

$$W_{e_4}(P_n + P_m) = \frac{m^3}{6}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 - 7n + 3\right) - \frac{m}{6}\left(4n^3 + 7n^2 - 2n - 2\right) + \frac{n}{6}\left(n^2 + 3n + 2\right)$$

Example 13.4.16 Suppose that $G = P_n + C_m$, where n and m are not necessarily equal, then $G = TUC_4[m, n]$ is a C_4-nanotube (John and Diudea 2004). The edge-Wiener indices of G are as follows:

Case 1. If m is odd, then

$$W_{e_0}(P_n + C_m) = \frac{m^3}{8}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 - 6n^2 + 5n - 3\right) + \frac{m}{8}\left(4n^2 - 8n + 3\right)$$

$$W_{e_4}(P_n + C_m) = \frac{m^3}{8}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 + 6n^2 - 10n + 3\right) - \frac{m}{8}\left(16n^2 - 3\right)$$

Case 2. If m is even, then

$$W_{e_0}(P_n + C_m) = \frac{m^3}{8}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 - 6n^2 + 5n - 3\right) + \frac{m}{2}(n-1)^2$$

$$W_{e_4}(P_n + C_m) = \frac{m^3}{8}(2n-1)^2 + \frac{m^2}{6}\left(4n^3 + 6n^2 - 10n + 3\right) - \frac{m}{2}\left(n^2 + 2n - 1\right)$$

Example 13.4.17 Suppose that $G = C_n + C_m$, where n and m are not necessarily equal, then $G = TC_4[m, n]$ is a C_4 -nanotorus (Diudea and John 2001). The first edge-Wiener index of G is equal to $W_{e_0}(C_n + C_m) = \frac{m^3}{2}n^2 + \frac{m^2}{2}n\left(n^2 + 1\right) + \frac{m}{2}n(n-2)$

The second edge-Wiener index of G is as follows:

Case 1. If m and n are odd, then

$$W_{e_4}(C_n + C_m) = \frac{m^3}{2}n^2 + \frac{m^2}{2}n\left(n^2 + 4n - 4\right) - mn(2n+1)$$

Case 2. If m and n are even, then

$$W_{e_4}(C_n + C_m) = \frac{m^3}{2}n^2 + \frac{m^2}{2}n\left(n^2 + 4n - 1\right) - \frac{m}{2}n(n+2)$$

Case 3. If n is odd and m is even, then

$$W_{e_4}(C_n + C_m) = \frac{m^3}{2}n^2 + \frac{m^2}{2}n\left(n^2 + 4n - 4\right) - \frac{m}{2}n(n+2)$$

Acknowledgment This work was partially supported by Center of Excellence of Algebraic Hyperstructures and its Applications of Tarbiat Modares University (CEAHA).

References

Azari M, Iranmanesh A (2011) Ars Combinatoria 100:113
Azari M, Iranmanesh A, Tehranian A (2010) Stud Univ Babes bolyai Chemia Liv 4:183
Diudea MV, John PE (2001) MATCH Commun Math Comput Chem 44:103
Gutman I, Potgieter JH (1997) J Serb Chem Soc 62:185
Gutman I, Trinajstic N (1972) Chem Phys Lett 17:535
Gutman I, Yeh YN, Lee SL, Luo L (1993) Indian J Chem 32A:651
Heydari A, Taeri B (2007a) J Comput Thoer NanoSci 4:158
Heydari A, Taeri B (2007b) MATCH Commun Math Comput Chem 57:665
Iranmanesh A, Kafrani AS (2009) MATCH Commun Math Comput Chem 62:311
Iranmanesh A, Khormali O (2011) J Comput Thoer NanoSci 8:133
Iranmanesh A, Gutman I, Khormali O, Mahmiani A (2009) MATCH Commun Math Comput Chem 61:663
John PE, Diudea MV (2004) Croat Chem Acta 77:127
Khadikar PV, Karmarkar S (2002) Acta Chim Slov 49:755
Mahmiani A, Khormali O, Iranmanesh A (2010a) Optoelectron Adv Mater Rapid Commun 4:252
Mahmiani A, Khormali O, Iranmanesh A, Ahmadi A (2010b) Optoelectron Adv Mater Rapid Commun 4:256
Nikoli’c S, Trinajsti’c N, Mihali’c Z (1995) Croat Chem Acta 68:105
Sagan BE, Yen YN, Zhang P (1996) Int J Quantum Chem 60:959
Stevanovic D (2001) Discrete Math 235:237
Wiener H (1947) J Am Chem Soc 69:17