STUDIA UBB CHEMIA, LVII, 3, 2012 (p. 157 – 166)
(RECOMMENDED CITATION)

THE EDGE WIENER INDEX OF ROOTED PRODUCT OF GRAPHS

ESMAEIL BABAEI[1], ALI IRANMANESH[1, *]

ABSTRACT. In a connected graph *G*, the sum of distances between all its vertex pairs is known as the Wiener index. The edge-Wiener index is conceived in an analogous manner as the sum of distances between all pairs of edges of the connected graph. In this paper, we compute the edge-Wiener index of the rooted product of graphs and some types of dendrimers.

Keywords: *graph, distance sum, edge-Wiener index*

INTRODUCTION

Let G be a connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively. Throughout this paper, we suppose that G is connected. The Wiener index is defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v \mid G)$, where $d(u,v \mid G)$ denotes the distance between vertices u and v.

This index was introduced by the chemist Harold Wiener [1] within the study of relations between the structure of organic compounds and their thermodynamic properties. It found many applications in chemistry, pharmaceutics etc [2- 9].

The edge-Wiener index version was defined in ref [10] as $W_{ei}(G) = \sum_{\{e,f\}\subseteq E(G)} d_i(e,f \mid G), 0 \le i \le 4.$ For $i = 0$, $d_0(e,f \mid G) = d(e,f \mid L(G))$, where, $L(G)$ is the line graph of G, i.e. a graph of which vertices are the edges of G, with two vertices connected in $L(G)$ whenever the corresponding edges of G are adjacent.

Also $d_3(e,f \mid G) = \begin{cases} d_1(e,f \mid G) & e \ne f \\ 0 & e = f \end{cases}$,

where $d_1(e,f \mid G) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$, such that $e = xy$ and $f = uv$. Similarly, $d_4(e,f \mid G) = \begin{cases} d_2(e,f \mid G) & e \ne f \\ 0 & e = f \end{cases}$,

[1] *Department of Mathematics, Tarbiat Modares University, P.O. Box: 14115-137, Tehran, Iran*
* *iranmanesh@modares.ac.ir*

where, $d_2(e,f\,|\,G)=\max\{d(x,u),d(x,v),d(y,u),d(y,v)\}$, such that $e=xy$ and $f=uv$. Next, d_1,d_2 are not distances and $d_0(e,f\,|G)=d_3(e,f\,|G)$ for all $\{e,f\}\subseteq E(G)$ [10]. Thus for the first edge-Wiener index we have

$$W_{e0}(G)=W_{e3}(G)=\sum_{\{e,f\}\subseteq E(G)} d_0(e,f\,|G)=\sum_{\{e,f\}\subseteq E(G)} d_3(e,f\,|G).$$

And for the second edge-Wiener index: $W_{e4}(G)=\sum_{\{e,f\}\subseteq E(G)} d_4(e,f\,|G)$.

The rooted product of graph G and rooted graph H, GoH, is obtained by taking one copy of G and $|V(G)|$ copies of H, and by joining the root vertex of the ith copy of H to the ith vertex of G for $i=1,2,...,|V(G)|$.

Let H be a labeled graph on n vertices, G be a sequence of n rooted graphs $G_1,...,G_n$, then $H(G)$ denotes the graph obtained by identifying the root of G_i with the ith vertex of H, which is called the rooted product of H by G. Thus, $GoH=G(\underbrace{H,...,H}_{|V(G)|})$ [11].

In this paper, we compute the edge-Wiener index of the rooted product of graphs and also obtain this index for some dendrimers.

Computation of the edge Wiener index of rooted product of graphs

Lemma 1 [10]**.** Let m be the number of edges of the graph G, then $W_{e0}(G)=W_{e1}(G)+\dfrac{m(m-1)}{2}$ and $W_{e4}(G)=W_{e2}(G)-m$.

Now, let H be a labeled graph on n vertices and m edges, G be a sequence of n rooted graphs; $G_1,...,G_n$ such that G_i has n_i vertices and m_i edges and $H(G)$ be the rooted product of H by G, then $H(G)$ will have $M=m+\sum_{i=1}^{n} m_i$ edges. We define

$$d_{ki}(G_i)=\sum_{e\in E(G_i)} d_k(e,x_i) \text{ and } d_{ki}(H)=\sum_{e\in E(H)} d_k(e,x_i), k=1,2,$$

where x_i is the root of G_i, also we define

$$d_1(e,x)=\min\{d(x,u),d(x,v)\}, d_2(e,x)=\max\{d(x,u),d(x,v)\}$$

such that $x\in V(G)$, $u\in E(G)$ and $e=uv$.

Proposition 1. Let H be a labeled graph on n vertices and m edges, G be a sequence of n rooted graphs: $G_1,...,G_n$ such that G_i has n_i vertices and m_i edges. Let $H(G)$ be the rooted product of H by G, then

$$W_{ek}(H(G))=\sum_{i=1}^{n}W_{ek}(G_i)+W_{ek}(H)+m\sum_{i=1}^{n}d_{ki}(G_i)+\sum_{i=1}^{n}m_i d_{ki}(H)$$
$$+\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}m_j d_{ki}(H)+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}m_i m_j d_H(x_i,x_j),k=1,2$$

Proof. Let $e_\lambda;\lambda=1,...,m_i$, be an edge of G_i, $e_\gamma;\gamma=1,...,m_j$ be an edge of G_j, $i\neq j$, then,

$$d_k(e_\lambda,e_\gamma)=d_k(e_\lambda,x_i)+d_H(x_i,x_j)+d_k(e_\gamma,x_j),k=1,2.$$

Hence

$$d_k(e_\lambda,G_j)=\sum_{\gamma=1}^{m_j}d_k(e_\lambda,e_\gamma)=\sum_{\gamma=1}^{m_j}[d_k(e_\lambda,x_i)+d_H(x_i,x_j)+d_k(e_\gamma,x_j)]$$
$$=m_j d_k(e_\lambda,x_i)+m_j d_H(x_i,x_j)+d_{kj}(G_j),$$

$$d_k(G_i,G_j)=\sum_{\lambda=1}^{m_i}d_k(e_\lambda,G_j)=\sum_{\lambda=1}^{m_i}[m_j d_k(e_\lambda,x_i)+m_j d_H(x_i,x_j)+d_{kj}(G_j)]$$
$$=m_j d_{ki}(G_i)+m_i m_j d_H(x_i,x_j)+m_i d_{kj}(G_j),$$

$$\sum_{j=1,j\neq i}^{n}d_k(G_i,G_j)=\sum_{j=1,j\neq i}^{n}[m_j d_{ki}(G_i)+m_i m_j d_H(x_i,x_j)+m_i d_{kj}(G_j)],$$

$$\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}d_k(G_i,G_j)=\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}[m_j d_{ki}(G_i)+m_i m_j d_H(x_i,x_j)+m_i d_{kj}(G_j)]$$
$$=2\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}m_j d_{ki}(G_i)+\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}m_i m_j d_H(x_i,x_j)$$

Now, let e be an edge of H, then,

$$d_k(e,G_j)=\sum_{\gamma=1}^{m_j}d_k(e,e_\gamma)=\sum_{\gamma=1}^{m_j}[d_k(e,x_j)+d_k(x_j,e_\gamma)]=m_j d_k(e,x_j)+d_{kj}(G_j)$$

$$d_k(H,G_j)=\sum_{i=1}^{m}d_k(e_i,G_j)=\sum_{i=1}^{m}[m_j d_k(e_i,x_j)+d_{kj}(G_j)]=m_j d_{kj}(H)+md_{kj}(G_j)$$

$$\sum_{j=1}^{n}d_k(H,G_j)=\sum_{j=1}^{n}[m_j d_{kj}(H)+md_{kj}(G_j)]=\sum_{j=1}^{n}m_j d_{kj}(H)+m\sum_{j=1}^{n}d_{kj}(G_j)$$

Therefore,

$$W_{ek}(H(G)) = \sum_{\{e,f\}\subseteq E(H(G))} d_k(e,f \mid H(G))$$

$$= \sum_{i=1}^{n} \sum_{\{e,f\}\subseteq E(G_i)} d_k(e,f \mid G_i) = \frac{1}{2}\sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} d_k(G_i, G_j)$$

$$+ \sum_{i=1}^{n} d_k(H, G_i) + \sum_{\{e,f\}\subseteq E(H)} d_k(e,f \mid H)$$

Thus,

$$W_{ek}(H(G)) = \sum_{i=1}^{n} W_{ek}(G_i) + W_{ek}(H) + m\sum_{i=1}^{n} d_{ki}(G_i) + \sum_{i=1}^{n} m_i d_{ki}(H)$$

$$+ \sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} m_j d_{ki}(H) + \frac{1}{2}\sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} m_i m_j d_H(x_i, x_j), k = 1, 2.$$

Corollary 1. By the above assumption, we have

$$W_{e0}(H(G)) = W_{e1}(H(G)) + \frac{M(M-1)}{2}$$

and $W_{e4}(G) = W_{e2}(H(G)) - M$.

where $M = m + \sum_{i=1}^{n} m_i$.

Proof. This follows from Lemma 1.

Corollary 2. Let G be a connected graph with n_1 vertices and m_1 edges, H be a rooted graph with n_2 vertices and m_1 edges, then,

$$W_{ek}(GoH) = n_1 W_{ek}(H) + W_{ek}(G) + m_1 n_1^2 d_{k1}(H)$$

$$+ m_2 \sum_{j=1}^{n_1} d_{kj}(G) + \frac{1}{2}\sum_{i=1}^{n_1} \sum_{j=1, j\neq i}^{n_1} m_2^2 d_G(i, j), k = 1, 2.$$

Proof. Hence, $GoH = G(\underbrace{H, ..., H}_{n_1})$. Therefore, the result follows from proposition 1.

Lemma 2. Let K_n, P_n, C_n and S_n denote the complete graph, path, cycle and star on n vertices, respectively. Also let $K_{a,b}$ be the complete bipartite graph on the parts A and B of the sizes $|A|=a$ and $|B|=b$. Put $d_{ki}(G)=\sum_{e\in E(H)} d_k(e,i), k=1,2.$ where i is i[th] vertex of G. Then,

(i) $d_{1i}(K_{a,b})=\begin{cases} ab-b & i\in A \\ ab-a & i\in B \end{cases}$, $d_{2i}(K_{a,b})=\begin{cases} 2ab-b & i\in A \\ 2ab-a & i\in B \end{cases}$,

(ii) $d_{1i}(S_n)=d_{1i}(K_{1,n-1})=\begin{cases} 0 & i\in A \\ n-2 & i\in B \end{cases}$,

(iii) $d_{2i}(S_n)=d_{2i}(K_{1,n-1})=\begin{cases} n-1 & i\in A \\ 2n-3 & i\in B \end{cases}$,

(iv) $d_{1i}(K_n)=\dfrac{(n-1)(n-2)}{2}$, $d_{2i}(K_n)=(n-1)^2$

(v) $d_{1i}(C_n)=\begin{cases} \sum_{j=1}^{k-1} 2j & n=2k \\ \sum_{j=1}^{k-1} 2j+k & n=2k+1 \end{cases}$,

(vi) $d_{2i}(C_n)=\begin{cases} \sum_{j=1}^{k-1} 2j & n=2k \\ \sum_{j=1}^{k-1} 2j+k+1 & n=2k+1 \end{cases}$,

(vii) $d_{1i}(P_n)=\sum_{j=1}^{n-1-i} j+\sum_{j=1}^{i-1}(j-1)$, $d_{2i}(P_n)=\sum_{j=1}^{n-i} j+\sum_{j=1}^{i-1} j$.

Proof. Straight forward.

Computation of the edge Wiener index of some dendrimers

Definition 1 (Generalized Bethe Tree)**.** Let B_k be a generalized Bethe tree of k levels (k>1) or a rooted tree in which vertices at the same level/ generation have the same degree [12]. For $j=1,2,...,k$, denote by d_{k-j+1} and

n_{k-j+1}, the degree of the vertices at the level j and their numbers, respectively. Thus, $d_1 = 1$ is the degree of the vertices at the level k and d_k is the degree of the rooted vertex. On the other hand, $n_k = 1$, pertaining to the single vertex at the first level, the root vertex. For example, B_4 is given in Figure 1.

Proposition 2. Let B_k be a generalized Bethe tree. Then we have

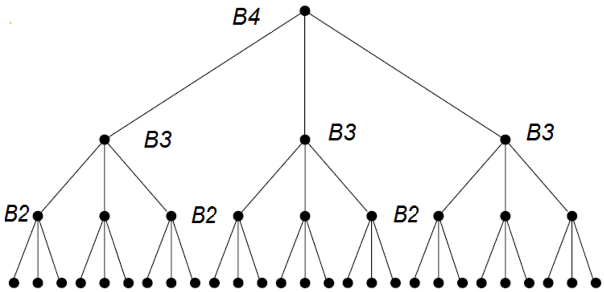

Figure 1. Generalaized Beth tree of 4 levels

$$W_{e1}(B_k) = d_k W_{e1}(B_{k-1}) + d_k^{2}(d_{1i}(B_{k-1}) + m_{k-1}d_{1i}(B_{k-1}) + m_{k-1}^{2}) - d_k(m_{k-1}d_{1i}(B_{k-1}) + m_{k-1}^{2}),$$
$$W_{e2}(B_k) = d_k W_{e2}(B_{k-1}) + d_k^{2}(1 + m_{k-1} + d_{2i}(B_{k-1}) + m_{k-1}d_{2i}(B_{k-1}) + m_{k-1}^{2}) - d_k(m_{k-1}d_{2i}(B_{k-1}) + m_{k-1}^{2}),$$

where, m_k is the number of edges of B_k. Therefore,

$$W_{e0}(B_k) = W_{e1}(B_k) + \frac{m_k(m_k - 1)}{2} \text{ and } W_{e4}(B_k) = W_{e2}(B_k) - m_k .$$

Proof: Suppose that B_k is a generalized Bethe tree with k levels, then a subtree B_{k-j+1} of B_k corresponding to j th level, is a tree with its root at level j. Now, we can define B_k by the rooted product of trees. Let B_i be a subtree corresponding to $k-i+1$-th level of B_k; in this case, B_i will be defined as

$$B_i = S_{d_{k-i+1}+1}(P_1, B_{i-1}, B_{i-1}, \ldots, B_{i-1})$$

where, S_{d+1} is a star on the $d+1$ vertices. Accordingly, B_k will be defined as

$$B_k = S_{d_k+1}(P_1, B_{k-1}, B_{k-1}, \ldots, B_{k-1})$$

The number of edges of B_k is obtained by

$$m_k = d_k + d_k d_{k-1} + d_k d_{k-1} .. d_2$$

Also we have

$$d_{1i}(B_k) = \sum_{e \in E(B_k)} d_1(e,i) = d_k d_{k-1} + 2d_k d_{k-1} d_{k-2} + ... + (k-1) d_k d_{k-1} .. d_2$$

$$d_{2i}(B_k) = \sum_{e \in E(B_k)} d_2(e,i) = d_k + 2d_k d_{k-1} + ... + k d_k d_{k-1} .. d_2$$

where, i is the root of B_k.

Therefore, by Proposition 1, we have:

$$W_{el}(B_k) = W_{el}(S_{d_k+1}(P_1, B_{k-1}, B_{k-1}, ..., B_{k-1}))$$

$$= \sum_{i=2}^{d_k+1} W_{el}(B_{k-1}) + W_{el}(S_{d_k+1}) + d_k \sum_{i=2}^{d_k+1} d_{li}(B_{k-1}) + \sum_{i=2}^{d_k+1} m_{k-1} d_{li}(S_{d_k+1})$$

$$+ \sum_{i=2}^{d_k+1} \sum_{j=2, j \neq i}^{d_k+1} m_{k-1} d_{li}(B_{k-1}) + \frac{1}{2} \sum_{i=2}^{d_k+1} \sum_{j=2, j \neq i}^{d_k+1} m_{k-1}{}^2 d_H(i_1, i_2), l = 1, 2,$$

where, i_1 and i_2 are the roots of two B_{k-1} in the level 2. We have $d_{S_{d_k+1}}(i_1, i_2) = 2$ and $W_{e1}(S_{d_k+1}) = 0; W_{e2}(S_{d_k+1}) = d_k{}^2$. Also by Lemma 2, we have $d_{1i}(S_{d_k+1}) = 0; d_{2i}(S_{d_k+1}) = d_k$. Therefore, the results are obtained.

Definition 2 (Dendrimer Graph)**.** A highly branched tree, $T_{k,d}$, is called a regular dendrimer graph, for $k \geq 0$ and $d \geq 3$, in particular, $T_{k,d}$ stands for the k[th] regular dendrimer graph of degree d [8,13]. Dendrimer graph is a kind of generalized Bethe tree for any $d \geq 3$. $T_{0,d}$ is the one-vertex graph and $T_{1,d}$ is the star with $d+1$ vertices. Then for $k = 2,3,...$ and $d \geq 3$ the tree is obtained by attaching $d-1$ new vertices of degree one to the vertices of degree one of $T_{k-1,d}$. Figure 2 presents the first four regular dendrimer graphs of degree four. An auxiliary tree $B_{k,d}$ is introduced below.

Each of the d branches attached to the central vertex of $T_{k,d}$ is isomorphic to $B_{k-1,d}$. It is immediately seen that $B_{0,d}$ is the one-vertex graph and $B_{1,d}$ is the star with d vertices. Further, for $k = 2,3,...$ and $d \geq 3$, the tree $B_{k,d}$, is obtained by attaching $d-1$ new vertices of degree one to the vertices of degree one of $B_{k-1,d}$. The tree of the type $B_{3,4}$ is given in Figure 3.

Proposition 3. Let $T_{k,d}$ be a dendrimer graph for which $k \geq 0$ and $d \geq 3$, then we have

$$W_{e1}(T_{k,d}) = dW_{e1}(B_{k,d}) + d^2(d_{1i}(B_{k,d}) + m_{k,d}d_{1i}(B_{k,d}) + m_{k,d}{}^2) - d(m_{k,d}d_{1i}(B_{k,d}) + m_{k,d}{}^2),$$

$$W_{e2}(T_{k,d}) = dW_{e2}(B_{k,d}) + d^2(1 + m_{k,d} + d_{2i}(B_{k,d}) + m_{k,d}d_{2i}(B_{k,d}) + m_{k,d}{}^2) - d(m_{k,d}d_{2i}(B_{k,d}) + m_{k,d}{}^2),$$

Therefore,

$$W_{e0}(T_{k,d}) = W_{e1}(T_{k,d}) + \frac{m(m-1)}{2} \text{ and } W_{e4}(T_{k,d}) = W_{e2}(T_{k,d}) - m$$

where m is the number of edges of $T_{k,d}$.

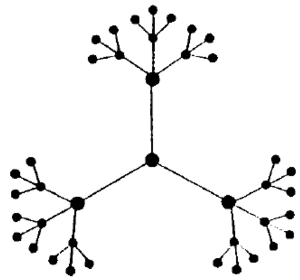

Figure 2. Example of regular dendrimer graphs

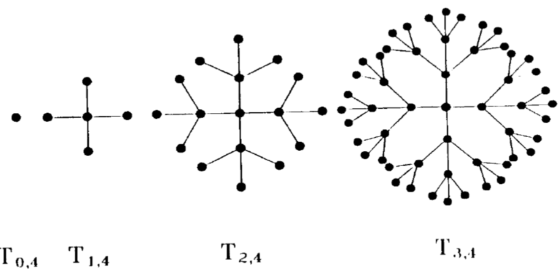

Figure 3. Tree of the type $B_{3,4}$

Proof. The number of edges of $T_{k,d}$ is obtained as:

$$m = |E(T_{k,d})| = d + d(d-1) + d(d-1)^2 + ... + d(d-1)^{k-1}$$

Also the number of edges of $B_{k,d}$ is obtained as:

$$m_{k,d} = |E(B_{k,d})| = (d-1) + (d-1)^2 + ... + (d-1)^k$$

Now we can define $B_{k,d}$ and $T_{k,d}$ by the rooted product of trees similar to Proposition 2

$$B_{k,d} = S_d(P_1, B_{k-1,d}, B_{k-1,d}, ..., B_{k-1,d})$$
$$T_{k,d} = S_{d+1}(P_1, B_{k,d}, B_{k,d}, ..., B_{k,d})$$

Also, we have

$$d_{1i}(B_k) = \sum_{e \in E(B_k)} d_1(e,i) = (d-1)^2 + 2(d-1)^3 + ... + (k-1)(d-1)^k ,$$
$$d_{2i}(B_k) = \sum_{e \in E(B_k)} d_2(e,i) = (d-1) + 2(d-1)^2 + ... + k(d-1)^k .$$

where i is the root of $B_{k,d}$. Then the result is obtained by Proposition 2.

As examples, we calculated the first and second type of edge-Wiener index of $T_{3,4}$. The results are listed in Tables 1 and 2.

Table 1. Edge-Wiener index of $T_{k,4}$.

k	1	2	3
$m_{k,4}$	3	12	39
$d_{1i}(B_{k,4})$	0	9	63
$d_{2i}(B_{k,4})$	3	21	102
$W_{e1}(B_{k,4})$	54	1755	29700
$W_{e1}(B_{k,4})$	171	3195	43857

Table 2. Edge-Wiener index of $T_{3,4}$.

$m = \| E(T_{3,4}) \|$	52
$W_{e1}(T_{3,4})$	167544
$W_{e0}(T_{3,4})$	168870
$W_{e2}(T_{3,4})$	243688
$W_{e4}(T_{3,4})$	243636

ACKNOWLEDGEMENTS

The authors would like to thank the referee for his careful reading and useful suggestions.

REFERENCES

[1] H. Wiener, *J. Am. Chem. Soc.*, **1947**, *69*, 17.

[2] F. Buckley, F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, CA, **1990**.

[3] F. Buckley, *Congr. Number*, **1981**, *32*, 153.

[4] A.A. Dobrynin, R. Entringer, I. Gutman, *Acta Apppl. Math.*, **2001**, *66*, 211.

[5] A.A. Dobrynin, I. Gutman, S. Klavzar, P. Zigert, *Acta Appl. Math.*, **2002**, *72*, 247.

[6] A.A. Dobrynin, L.S. Mel'nikov, *MATCH Commun. Math. Comput. Chem.*, **2005**, *53*, 209.

[7] I. Gutman, O. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, Germany, 1986.

[8] I. Gutman, Yeong-Nan Yeh, Shyi-Long Lee, Jiang-Cherng Chen, *MATCH Commun. Math. Comput. Chem.*, **1994**, *30*, 103.

[9] A. Gravac, T. Pisaski, *J. Math. Chem.*, **1991**, *8*, 53.

[10] A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, *MATCH Commun. Math. Comput. Chem.*, **2009**, *61*, 663.

[11] C.D. Godsil, B.D. Mckay, *Bull. Austral. Math. Soc.*, **1978**, *18*, 21.

[12] O. Rojo, *Lin. Algebra Appl.*, **2007**, *420*, 490.

[13] A. Heydari, On the topological indices of graph of nanotubes, Ph.D. Thesis, Isfahan University of Technology, Isfahan, Iran, **2008**.