On the Wiener index of rooted product of graphs

Abbas Heydari [a, *], Bijan Taeri [a, †]
[a] *Department of Mathematical Sciences*
Isfahan University of Technology
Isfahan 84156-83111, Iran

Abstract. Let H be a simple graph with n vertices and G be a sequence of n rooted graphs G_1, G_2, ..., G_n. Godsil and McKay (Bull. Austral. Math. Soc. 18 (1978) 21-28) defined the rooted product $H(G)$, of H by G by identifying the root of G_i with the ith vertex of H. In this paper we calculate the Wiener index, that is the sum of distances between all pairs of vertices of a (connected) graph, of $H(G)$ in terms of Wiener indices of the graphs G_i, $i = 1, 2, \ldots, k$. As an application of our method we find a recursive relation to compute the Wiener index of Generalized Bethe trees.

Keywords: Wiener index, Rooted product, Generalized Bethe tree.

1 Introduction.

Let G be a finite, undirected and connected graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$. For vertices u and v, the standard distance of G, that is the number of edges on a shortest path connecting these vertices in G, is denoted by $d(u,v)$. The Wiener index is a graph invariant based on distances in a graph. It is denoted by $W(G)$ and is defined as the sum of distances between all pairs of vertices in G:

$$W(G) = \sum_{\{u,v\} \subset V(G)} d(u,v).$$

The name Wiener index for the quantity defined in above equation is usual in chemical literature, since Harold Wiener [5], in 1947, seemed to be the first to consider it.

* E-mail Address: a-heydari@math.iut.ac.ir
† E-mail Address: b.taeri@cc.iut.ac.ir (Corresponding author)

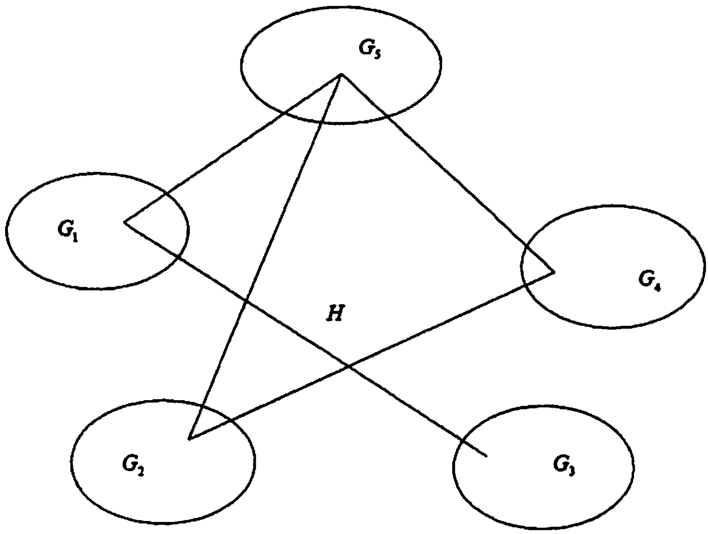

Figure 1: $H(G_1, G_2, G_3, G_4, G_5)$

One of the problems regarding to the Wiener index is finding methods so that the Wiener index of various graphs can be efficiently calculated. Finding simple conditions that provide the coincidence of the Wiener index for non isomorphic graphs is of interest both in theoretical investigations and in applications.

In this paper we consider an operation on simple graphs introduced by C. Godsil and B. Mckay [1], namely rooted product. Suppose that H is a labelled graph on k vertices and G is a sequence of k rooted graphs $G_1, G_2, \ldots, G_k$. The graph obtained by identifying the root of G_i with the ith vertex of H is called the rooted product of H by G and is denoted by $H(G)$. To represent an application of this operation, we consider some special cases for the graphs G_i and H, and calculate Wiener index of $H(G_1, G_2, \ldots, G_k)$ in terms of Wiener indices of G_i, $i = 1, 2, \ldots, k$.

Recall that a tree is a connected acyclic graph. In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degree. We agree that the root vertex is at level 1 and that T has k levels. In [4] Rojo and Robbiano, called such a tree generalized Bethe tree. They denoted the class of generalized Bethe trees of k levels by $\mathcal{B}_k$. Let H be the star graph of order $n+1$, P_1 be the graph of order 1 and β_{k-1} be the generalized Bethe tree of $k-1$ levels. By our notation $\beta_k = S_{n+1}(P_1, \underbrace{\beta_{k-1}, \beta_{k-1}, \ldots, \beta_{k-1}}_{n})$

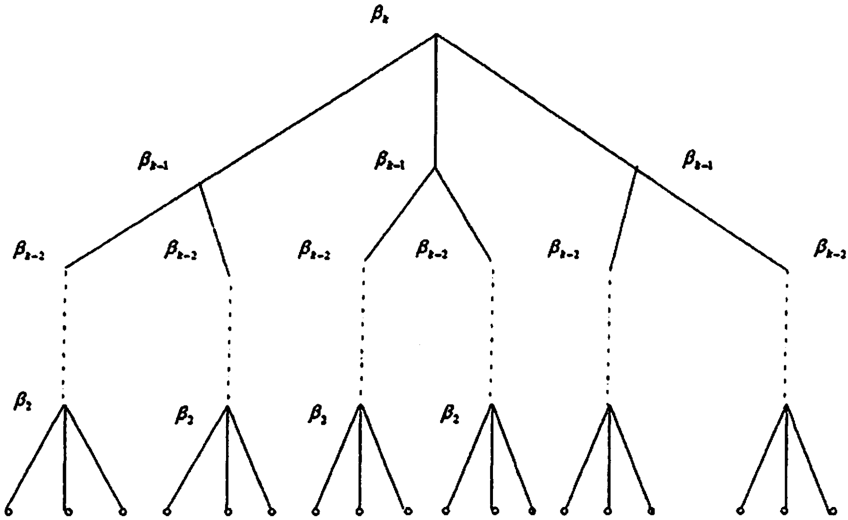

Figure 2: A generalized Bethe tree of k levels $\beta_k = H(P_1, \beta_{k-1}, \beta_{k-1}, \beta_{k-1})$, where H is the star of order 4

is a generalized Bethe tree of k levels, β_k such that degree of root vertex is n. Therefore the class of generalized Bethe trees of its k levels lies in the class defined above. Gutman and coauthors in [2, 3] calculated the Wiener indices of balanced trees in which the vertex degrees in all of levels of tree are equal (Bethe trees) as molecular graph of dendrimers. As a corollary of our results we calculate Wiener index of generalized Bethe trees.

2 Main results

In this section first we obtain Wiener index of $H(G_1, G_2, \ldots, G_k)$ in term Wiener indices of G_i, $i = 1, 2, \ldots, k$. Let $x_i \in G_i$, $1 \le i \le k$, be the root vertex of G_i and $V(H) = \{x_1, x_2, \ldots, x_k\}$. Throughout the paper n_i denotes the number of vertices of G_i, $\bar{n}_i = \sum_{j=1, j\neq i}^{k} n_j$, $d_i = \sum_{u\in V(G_i)} d(x_i, u)$ and $d_H(x_i, x_j)$ denotes the distance between vertices x_i and x_j in the graph H. In the following Theorem we compute the Wiener index of $H(G_1, G_2, \ldots, G_k)$.

Theorem 1. With the above notation we have

$$W(H(G)) = \sum_{i=1}^{k} W(G_i) + \sum_{i=1}^{k} \left(\bar{n}_i d_i + \frac{n_i}{2} \sum_{j=1, j\neq i}^{k} n_j d_H(x_i, x_j) \right).$$

Proof: Let $u_i \in G_i$ and $u_j \in G_j$, $1 \le i,j \le k$. Since we have

$$d(u_i,u_j) = d(u_i,x_i) + d_H(x_i,x_j) + d(x_j,u_j),$$

the summation of distance between vertices of G_i and $u_j \in G_j$ is

$$\begin{aligned}\sum_{i=1}^{n_i} d(u_i,u_j) &= \sum_{i=1}^{n_i}\Big(d(u_i,x_i) + d_H(x_i,x_j) + d(x_j,u_j)\Big) \\ &= d_i + n_i d_H(x_i,x_j) + n_i d(x_j,u_j).\end{aligned}$$

Thus if $d(G_i,G_j)$ is the summation of distances between all of the vertices of G_i and G_j, then

$$\begin{aligned}d(G_i,G_j) &= \sum_{j=1}^{n_j}\Big(d_i + n_i d_H(x_i,x_j) + n_i d(x_j,u_j)\Big) \\ &= n_j d_i + n_i n_j d_H(x_i,x_j) + n_i d_j.\end{aligned}$$

So the summation of distances between vertices of G_i and vertices of G_j, $j = 1,2,\ldots,i-1,i+1,\ldots,k$, can be computed as follows

$$\begin{aligned}\sum_{j=1,j\neq i}^{k} d(G_i,G_j) &= \sum_{j=1,j\neq i}^{k}\Big(n_j d_i + n_i n_j d_H(x_i,x_j) + n_i d_j\Big) \\ &= \bar{n}_i d_i + n_i \sum_{j=1,j\neq i}^{k} n_j d_H(x_i,x_j) + n_i \sum_{j=1,j\neq i}^{k} d_j.\end{aligned}$$

Therefore the summation of distances between vertices of G_i, $i = 1,2,\ldots,k$, and vertices of G_j, $j = 1,2,\ldots,i-1,i+1,\ldots,k$, can be computed as

$$\sum_{i=1}^{k}\Big(\bar{n}_i d_i + n_i \sum_{j=1,j\neq i}^{k} n_j d_H(x_i,x_j) + n_i \sum_{j=1,j\neq i}^{k} d_j\Big) = \sum_{i=1}^{k}\Big(2\bar{n}_i d_i + n_i \sum_{j=1,j\neq i}^{k} n_j d_H(x_i,x_j)\Big).$$

Now we can compute the Wiener index of K using its definition:

$$\begin{aligned}W(H(G)) &= \sum_{\{u,v\}\subset V(H(G))} d(u,v) \\ &= \sum_{i=1}^{k}\Big(\sum_{\{u,v\}\subset V(G_i)} d(u,v) + \frac{1}{2}\sum_{j=1,j\neq i}^{k} d(G_i,G_j)\Big) \\ &= \sum_{i=1}^{k} W(G_i) + \sum_{i=1}^{k}\Big(\bar{n}_i d_i + \frac{n_i}{2}\sum_{j=1,j\neq i}^{k} n_j d_H(x_i,x_j)\Big).\end{aligned}$$

This proves the Theorem. ■

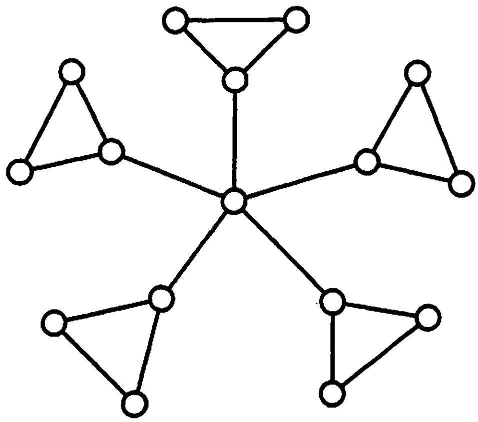

Figure 3: $S_6(P_1, C_3, C_3, C_3, C_3, C_3)$

Now we consider particular cases for G_i and H to obtain well known graphs and calculate Wiener indices of $H(G_1, G_2, \ldots, G_k)$ in terms of Wiener indices of G_i, $i = 1, 2, \ldots, k$.

Example 1. Let H be the star graph of order $k+1$, G_1 be the graph of order 1 and G_i, $i = 2, 3, \ldots, k+1$, be the cycle of order n . We will find the Wiener index of $K := S_{k+1}(P_1, \underbrace{C_n, C_n, \ldots, C_n}_{k})$ (see Figure 3) in terms of n and k. We have $W(P_1) = d_1 = 0$, $d_i = \frac{2}{n}W(C_n)$, $d_H(x_1, x_j) = 1$ and $d_H(x_i, x_j) = 2$, $i, j = 2, 3, \ldots, k+1$. Using Theorem 1, we can calculate Wiener index of this graph as follows

$$
\begin{aligned}
W(K) &= \sum_{i=1}^{k+1} W(G_i) + \sum_{i=1}^{k+1}\left(\bar{n}_i d_i + \frac{n_i}{2}\sum_{j=1, j\neq i}^{k} n_j d_H(x_i, x_j)\right) \\
&= kW(C_n) + \sum_{i=1}^{1}\frac{1}{2}\sum_{j=1, j\neq i}^{k+1} n \qquad (1) \\
&\quad + \sum_{i=2}^{k+1}\left((1+(k-1)n)\frac{2}{n}W(C_n) + \frac{n}{2}\sum_{j=1, j\neq i}^{k+1} n_j d_H(x_i, x_j)\right) \\
&= kW(C_n) + \frac{kn}{2} + k(1+(k-1)n)\frac{2}{n}W(C_n) + \frac{kn}{2}\sum_{j=1, j\neq i}^{k+1}(1+2(k-1)n) \\
&= k(k+\frac{1}{n})W(C_n) + k(k-1)n^2 + kn \qquad (2)
\end{aligned}
$$

Thus, since

$$W(C_n) = \begin{cases} \dfrac{n^3}{8} & \text{if } n \text{ is even} \\[2ex] \dfrac{n(n^2-1)}{8} & \text{if } n \text{ is odd,} \end{cases}$$

from equation (2) we have

$$W(K) = \begin{cases} \dfrac{k}{8}\Big((2k-1)n^3 + (8k-6)n^2 + 8n\Big) & \text{if } n \text{ is even} \\[2ex] \dfrac{k}{8}\Big((2k-1)n^3 + (8k-6)n^2 - (2k-9)n - 2\Big) & \text{if } n \text{ is odd.} \end{cases}$$

3 Wiener index of generalized Bethe tree

Suppose β_k is the generalized Bethe tree with k levels and m_k vertices. Suppose d_{k-i+1} is the degree of vertices in level i, $i = 1, 2, \ldots, k$. If

$$e_i = \begin{cases} d_i & \text{if } i = k \\ d_i - 1 & \text{if } i \neq k, \end{cases}$$

then

$$m_k = 1 + e_k + e_k e_{k-1} + \cdots + e_k e_{k-1} \cdots e_2 = 1 + \sum_{i=2}^{k} \prod_{j=i}^{k} e_j.$$

Now if d_k denotes the summation of distances between root vertex in β_k and all vertices in the tree, then

$$d_k = e_k + 2e_k e_{k-1} + 3e_k e_{k-1} e_{k-2} + \cdots + (k-1)e_k e_{k-1} \cdots e_2 = \sum_{i=2}^{k} (k-j+1) \prod_{j=i}^{k} e_j.$$

Using above notation we can calculate the Wiener index of β_k. For this purpose β_k must be considered as a rooted product of some graphs.

Corollary 1. Let β_k be the generalized Bethe tree with k levels. Then

$$W(\beta_k) = e_k\Big(W(\beta_{k-1}) + (m_k - m_{k-1})d_{k-1} - m_{k-1}^2\Big) + m_k(m_k - 1).$$

Proof: Suppose H is the star graph of order $e_k + 1$, $G_1 = P_1$ and for $i = 2, 3, \ldots, e_k + 1$, G_i is equal to β_{k-1}, and one of the rooted subtree of β_k such that it's root vertex is a vertex in level $k-1$ of β_k. Then $\beta_k = H(P_1, \underbrace{\beta_{k-1}, \beta_{k-1}, \ldots, \beta_{k-1}}_{e_k+1})$. With the notations of Theorem 1, $W(G_1) =$

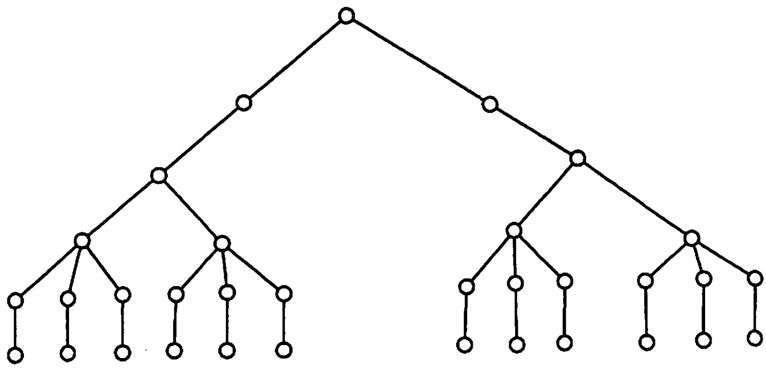

Figure 4: A generalized Bethe tree with 6 level.

0, $d_H(x_i, x_j) = 2$, for $i, j = 2, 3, \dots, e_k + 1$ and $\bar{n}_i = (m_i - m_{i-1})$. So by Theorem 1

$$\begin{aligned}
W(\beta_k) &= \sum_{i=1}^{k} W(G_i) + \sum_{i=1}^{k}\left(\bar{n}_i d_i + \frac{n_i}{2}\sum_{j=1, j\neq i}^{k} n_j d_H(x_i, x_j)\right) \\
&= \sum_{i=2}^{e_k+1} W(G_i) + \sum_{i=2}^{e_k+1}(m_k - m_{k-1})d_{k-1} + \sum_{i=1}^{1}\sum_{j=1, j\neq i}^{e_k+1} m_{k-1} + \\
&\qquad \sum_{i=2}^{e_k+1}\left(\frac{m_{k-1}}{2}\sum_{j=1, j\neq i}^{e_k+1} 2n_j\right) \\
&= e_k\Big(W(\beta_{k-1}) + (m_k - m_{k-1})d_{k-1}\Big) + e_k m_{k-1} + \\
&\qquad m_{k-1}\sum_{i=2}^{e_k+1}\Big(1 + (e_k - 1)m_{k-1}\Big) \\
&= e_k\Big(W(\beta_{k-1}) + (m_k - m_{k-1})d_{k-1}\Big) + e_k m_{k-1} + e_k(e_k - 1)m_{k-1}^2 \\
&= e_k\Big(W(\beta_{k-1}) + (m_k - m_{k-1})d_{k-1} - m_{k-1}^2\Big) + m_k(m_k - 1).
\end{aligned}$$

Example 2. Let G be a tree of type β_6 as shown in Figure 4. For this tree we have $e_2 = 1, e_3 = 3, e_4 = 2, e_5 = 1, e_6 = 2$. So by (1) we have

$$\begin{aligned}
m_2 &= 1 + e_2 = 2 \\
m_3 &= 1 + e_3 + e_3 e_2 = 7 \\
m_4 &= 1 + e_4 + e_4 e_3 + e_4 e_3 e_2 = 15
\end{aligned}$$

$$m_5 = 1 + e_5 + e_5e_4 + e_5e_4e_3 + e_5e_4e_3e_2 = 16$$
$$m_6 = 1 + e_6 + e_6e_5 + e_6e_5e_4 + e_6e_5e_4e_3 + e_6e_5e_4e_3e_2 = 33.$$

Also by (2) we have

$$d_2 = e_2 = 1$$
$$d_3 = e_3 + 2e_3e_2 = 9$$
$$d_4 = e_4 + 2e_4e_3 + 3e_4e_3e_2 = 32$$
$$d_5 = e_5 + 2e_5e_4 + 3e_5e_4e_3 + 4e_5e_4e_3e_2 = 47.$$

Now let $W_i = W(\beta_i)$, by using of Corollary 1 we can calculate Wiener index of β_6.

$$W_1 = 0$$
$$W_2 = 1(0 + (2 - 1) - 1) + 2^2 - 2 = 1$$
$$W_3 = 3(1 + (7 - 2)1 - 4) + 7^2 - 7 = 48$$
$$W_4 = 2(48 + (15 - 7)9 - 49) + 15^2 - 15 = 352$$
$$W_5 = 1(352 + (16 - 15)32 - 15^2) + 16^2 - 16 = 399$$
$$W_6 = W(\beta_6) = 2(399 + (33 - 16)47 - 16^2) + 33^2 - 33 = 2940.$$

Using this recursive process we can compute the Wiener index of generalized Bethe trees of arbitrary levels.

Acknowledgement: The second author was partially supported by Center of Excellence of Mathematics of Isfahan University of Technology (CEAMA).

References

[1] C. D. Godsil and B. D. Mckay, A new graph product and its spectrum, Bull. Austral. Math. Soc. Vol. 18 (1978), 21-28.

[2] I. Gutman, Y. N. Yeh, S. L. Lee and Y. L. Luo, Some recent results in the theory of the Wiener number, Indian J. Chem. 32A (1993), 651-661.

[3] I. Gutman, Y. N. Yeh, S. L. Lee and J. C. Chen, Wiener numbers of dendrimers, Comm. Math. Chem. (MATCH) 30 (1994), 103-115.

[4] O. Rojo and M. Robbiano, An explicit formula for eigenvalues of Bethe trees and upper bounds on the largest eigenvalue of any tree, Linear Algebra Appl. 427 (2007) 138-150.

[5] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947), 17-20.