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Research Article

Entire Wiener index of graphs

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Abstract: Topological indices are graph invariants computed usually by means of the distances or degrees of vertices of a graph. In chemical graph theory, a molecule can be modeled by a graph by replacing atoms by the vertices and bonds by the edges of this graph. Topological graph indices have been successfully used in determining the structural properties and in predicting certain physicochemical properties of chemical compounds. Wiener index is the oldest topological index which can be used for analyzing intrinsic properties of a molecular structure in chemistry. The Wiener index of a graph G is equal to the sum of distances between all pairs of vertices of G. Recently, the entire versions of several indices have been introduced and studied due to their applications. Here we introduce the entire Wiener index of a graph. Exact values of this index for trees and some graph families are obtained, some properties and bounds for the entire Wiener index are established. Exact values of this new index for subdivision and k-subdivision graphs and some graph operations are obtained.

Keywords: topological graph index, entire Wiener index

AMS Subject classification: 05C05, 05C07, 05C30, 05C38

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1. Significance of the work

The theory of graphs became more interesting day by day because it has a lot of applications in different areas long with some industrial applications. The topological indices is one of important topics of graph theory which has attention more than the others topics as it is very important to study the molecular graph in applied chemistry, physical sciences, medical sciences, etc. The Wiener index is one of the interested indices. Its calculation based on the distances inside the graph between the vertices and recently new version of the Wiener index based on the distances between edges is defined and studied. In this paper, we define new version called entire Wiener index of graphs this new index based on the distances between both vertices and edges in the graph because in some applied situations required to use all distances based on the vertices and edges.

2. Introduction

In this paper, we consider graphs which they are simple and connected and has no loops and no multiple edges. Let G be a connected graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The open and closed neighborhoods of a vertex u are denoted by $N(u) = \{v \in V : uv \in E\}$ and $N[u] = N(u) \cup \{u\}$, respectively. The degree of a vertex u in G is denoted by $deg_G(u)$ and is defined to be the number of edges incident with u. The line graph of a simple graph G is a graph denoted by $L(G)$ that represents the adjacencies between the edges of G. In other words, $L(G)$ is the graph of which the vertices are the edges of G. For more detailed information about the definitions and terminologies about graphs, see [15].
A topological index of a graph is a real number associated with the graph which is equal under the isomorphism of graphs, means it does not depend on the method of labeling or the representation of a graph. In applied chemistry, topological indices have many applications as tools for modeling chemical and other properties of molecules. One of the oldest and famous indices is the Wiener index. This index was the first topological index to be used in chemistry. The Wiener index of a graph $G = (V, E)$, denoted by $W(G)$, has been introduced in 1947 by chemist Harold Wiener [21] within the study of relations between the structure of organic compounds and their properties, as the sum of distances between all vertices of G,

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

Details about Wiener index and its chemical applications, can be found in some related surveys [5, 6, 8, 12, 14].
In analogy to the definition of the Wiener index of graph, the edge version of the

Wiener index has been considered as

$$W_e(G) = \sum_{\{e,f\}\subseteq E(G)} d(e,f),$$

where $d(e,f)$ is the distance between the two edges e and f in a graph G which defined as the distance between the e and f as vertices in the line graph $L(G)$ of the graph G, see [16].

The Zagreb indices of a graph G where introduced in [13]. They are denoted by $M_1(G)$ and $M_2(G)$ and were defined as

$$M_1(G) = \sum_{u\in V(G)} \left[d(u)\right]^2$$

and

$$M_2(G) = \sum_{uv\in E(G)} d(u)d(v),$$

respectively. In [17], it was shown that

$$M_1(G) = \sum_{u\in V(G)} \sum_{v\in N(u)} d(v) = \sum_{uv\in E(G)} \left[d(u)+d(v)\right],$$

and

$$M_2(G) = \frac{1}{2} \sum_{u\in V(G)} d(u) \sum_{v\in N(u)} d(v).$$

The Zagreb indices have been studied extensively. Many new reformulated versions of Zagreb indices are introduced, see [3, 11, 17, 19, 20, 24].

The huge applications of Wiener index and the reality that the intermolecular forces inside the molecular do not only exists between the atoms but also between the atoms and bonds, motivated and supported us to introduce and study the entire Wiener index of graph.

Definition 1. Let $G = (V,E)$ be a connected graph. The entire Wiener index of G is defined as,

$$W^{\mathcal{E}}(G) = \sum_{\{x,y\}\in B(G)} d(x,y),$$

where $d(x,y)$ is the distance between the elements x and y in G and $B(G)$ is the set of all $\{x,y\}$ such that $\{x,y\} \subseteq V(G)\cup E(G)$. The distance between the elements in $B(G)$ are defined as:

1. for any vertex u and any edge $e = wz$,

$$d(u,e) = min\{d(u,w), d(u,z)\},$$

2. for any two distinct edges $e = uv$ and $f = wz$,

$$d(e, f) = min\{d(u, w), d(v, w), d(u, z), d(v, z)\} + 1,$$

3. for any two vertices u and v, the distance between u and v is the length of the shortest path between them.

Example 1. 1. For any star S_n,

- $W(S_n) = (n-1)^2$.
- $W_e(S_n) = \frac{1}{2}(n-1)(n-2)$.
- $W^{\mathcal{E}}(S_n) = \frac{1}{2}(n-1)(5n-8)$.

2. For any complete graph K_n,

- $W(K_n) = \frac{1}{2}n(n-1)$.
- $W_e(K_n) = \frac{1}{4}n\big(n-1\big)^2(n-2)$.
- $W^{\mathcal{E}}(K_n) = \frac{1}{4}n^2(n-1)^2$.

3. For any cycle C_n with $n \geq 3$,

- $W(C_n) = W_e(C_n) = \begin{cases} \frac{1}{8}n^3, & \text{if } n \text{ is even;} \\ \frac{1}{8}n(n^2-1), & \text{if } n \text{ is odd.} \end{cases}$
- $W^{\mathcal{E}}(C_n) = \frac{1}{2}n^2(n-1)$.

4. For any path P_n with $n \geq 3$,

- $W(P_n) = \binom{n+1}{3}$.
- $W_e(P_n) = \binom{n}{3}$
- $W^{\mathcal{E}}(P_n) = \frac{1}{6}n(n-1)(4n-5)$.

5. For any complete bipartite graph $K_{a,b}$ with $a, b \geq 2$,

- $W(K_{a,b}) = (a+b)(a+b-1) - ab$.
- $W_e(K_{a,b}) = \frac{1}{2}ab(2ab-a-b)$
- $W^{\mathcal{E}}(K_{a,b}) = (a+b)\big(a+b+\frac{1}{2}ab-1\big) + ab(ab-3)$.

3. Entire Wiener index for trees

In this section, we obtain the exact formula of the entire Wiener index $W^{\mathcal{E}}(T_n)$ of a tree T_n with n vertices in terms of the Wiener index $W(T_n)$ and we find its relation with some other versions of $W(T_n)$ and with Gutman index $Gut(T_n)$.

Theorem 1. *Let T_n be a tree on $n \geq 3$ vertices. Then*

$$W^{\mathcal{E}}(T_n) = 4W(T_n) - 3\binom{n}{2}.$$

Proof. Let T_n be a tree on $n \geq 3$ vertices. Then

$$\begin{aligned} W^{\mathcal{E}}(T_n) &= W(T_n) + W_e(T_n) + \sum_{\substack{\{v,e\} \in B(T_n) \\ v \in V(T_n),\, e \in E(T_n)}} d(v,e) \\ &= W(T_n) + W_e(T_n) + \sum_{v \in V(T_n)} \sum_{e \in E(T_n)} d(v,e). \end{aligned}$$

For a fixed vertex $v \in V(T_n)$, we have

$$\sum_{e \in E(T_n)} d(v,e) = \sum_{u \in V(T_n)} d(v,u) - (n-1) = d_{T_n}(v) - (n-1),$$

where $d_{T_n}(v) = \sum_{u \in V(T_n)} d(v,u)$. Since $W_e(T_n) = W(T_n) - \binom{n}{2}$, [4], then

$$\begin{aligned} W^{\mathcal{E}}(T_n) &= 2W(T_n) - \binom{n}{2} + \sum_{v \in V(T_n)} d_{T_n}(v) - n(n-1) \\ &= 4W(T_n) - 3\binom{n}{2}. \end{aligned}$$

□

In [21], it has been proven that, for any tree T_n, $W(T_n) = \sum_{e \in E(T_n)} N_2(T_n - e)$, where $N_2(T_n - e)$ denotes to the product of the numbers of vertices of the two components of T_n obtained by deleting the edge $e \in E(T_n)$. Therefore, for $W^{\mathcal{E}}(T_n)$ we have the following result.

Theorem 2. *For any tree T_n on $n \geq 3$ vertices,*

$$W^{\mathcal{E}}(T_n) = 4\sum_{e \in E(T_n)} N_2(T_n - e) - 3\binom{n}{2}.$$

Also, Skrekovski and Gutman in [18] have been introduced a vertex version of the Wiener index theorem for trees and they extended the result for any connected graph as in the following two theorems.

Theorem 3 ([18]). *Let T_n be a tree on n vertices. Then*

$$W(T_n) = \sum_{v \in V(T_n)} N_2(T_n - v) + \binom{n}{2}.$$

Theorem 4 ([18]). *Let G be a connected graph on n vertices. Then*

$$W(G) = \sum_{v \in V(G)} B(v) + \binom{n}{2}.$$

Note that $B(x) = \sum_{\substack{u,v \in V(G)\setminus\{x\} \\ u \neq v}} \dfrac{\sigma_{u,v}(x)}{\sigma_{u,v}}$ is the betweenness centrality of a vertex $x \in V(G)$, where $\sigma_{u,v}$ denotes the total number of shortest (u,v)-paths in G and $\sigma_{u,v}(x)$ represents the number of shortest (u,v)-paths passing through the vertex x. Thus one can see easily for any tree T_n, $W(L(T_n)) = \sum_{v \in V(T_n)} N_2(T_n - v)$. According to Theorem 1 and Theorem 3, we get our vertex version of the entire Wiener index of trees.

Theorem 5. *Let T_n be a tree on $n \geq 3$ vertices. Then*

$$W^{\mathcal{E}}(T_n) = 4 \sum_{v \in V(T_n)} N_2(T_n - v) + \binom{n}{2}.$$

A formula discovered in [7] deserves to be mentioned:

Theorem 6 ([7]). *Let T_n be a tree on n vertices. Then*

$$W(T_n) = \binom{n+1}{3} - \sum_{v \in V(T_n)} N_3(T_n - v),$$

where $N_3(T_n - v)$ denotes the product of the number of vertices of the triplets components of T_n obtained by deleting the vertex $v \in V(T_n)$.

According to Theorem 6 and Theorem 1, we have

Theorem 7. *Let T_n be a tree on $n \geq 3$ vertices. Then*

$$W^{\mathcal{E}}(T_n) = \frac{n(n-1)(4n-5)}{6} - 4 \sum_{v \in V(T_n)} N_3(T_n - v).$$

In the following theorem, we obtain the relation between the entire Wiener index and Gutman index for trees:

Theorem 8. *For a tree T_n on $n \geq 3$ vertices,*

$$W^{\mathcal{E}}(T_n) = Gut(T_n) + \binom{n-1}{2}.$$

Proof. Gutman, in [9], has stated the relation between $W(T_n)$ and $Gut(T_n)$ for a tree T_n on n vertices as

$$Gut(T_n) = 4W(T_n) - (2n-1)(n-1).$$

Hence, by Theorem 1, our result is established. □

4. Entire Wiener index of Kragujevac trees

In this section, we study the entire Wiener index of a special class of trees called the Kragujevac trees. The formal definition of a Kragujevac tree was introduced in [1]. Let B_1, B_2, $B_3, \cdots$ be branches whose structure is depicted in Figure 1.

Definition 2 ([10]). Let $d \geq 2$ be an integer. Let $\beta_1, \beta_2, \ldots, \beta_d$ be rooted trees specified in Figure 1, i.e., $\beta_1, \beta_2, \ldots, \beta_d \in \{B_2, B_3, \ldots, B_k\}$. A proper Kragujevac tree Kg is a tree possessing a vertex w of degree d, adjacent to the roots of $\beta_1, \beta_2, \ldots, \beta_d$. The vertex w is said to be the central vertex of Kg, whereas d is the degree of Kg. The subgraphs $\beta_1, \beta_2, \ldots, \beta_d$ are the branches of Kg. Recall that some (or all) branches of Kg may be mutually isomorphic.

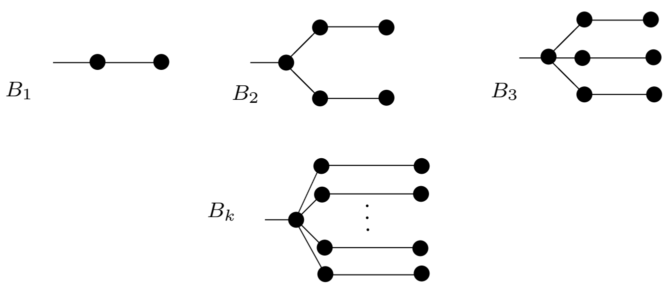

Figure 1. **The branches of proper Kragujevac trees**

The branch B_k has $2k+1$ vertices for $k>1$ and 2 vertices for $k=1$. Therefore, if in the Kragujevac tree Kg specified in Definition 2, $\beta_i \cong B_{k_i}$, $i=1,2,\cdots,d$, then its order is

$$n(Kg) = d+1+2\sum_{i=1}^{d} k_i = 1+\sum_{i=1}^{d}(2k_i+1).$$

Theorem 9. *Let Kg be a proper Kragujevac tree on n vertices. Then*

$$\begin{aligned} W^{\mathcal{E}}(Kg) =& 24\sum_{i=1}^{d} k_i^2 + (14d-5)\sum_{i=1}^{d} k_i + 14\sum_{j=1}^{d}\sum_{\substack{i=1\\ i\neq j}}^{d} k_i + 40\sum_{j=1}^{d} k_j \sum_{\substack{i=1\\ i\neq j}}^{d} k_i \\ & -\frac{3}{2}\Big(\sum_{i=1}^{d}(2k_i+1)\Big)^2 + \frac{d(8d-3)}{2}. \end{aligned}$$

Proof. By using Theorem 1, we need only to find $W(Kg)$. We compute $W(Kg)$ as follows:

1. Compute the sum of distances between the central vertex w and all the other vertices (denoted by $d(w)$).
2. Compute the Weiner index of each branch separately ($W(\beta_i)$, $i=1,2,\ldots,d$).
3. Compute the sum of distances between the vertices of each branch with all the vertices of other branches, alternately, except the central vertex w.

By simple computations one can find that, $d(w) = \sum_{i=1}^{d}(5k_i+1)$ and $W(\beta_i) = 6k_i^2 - 2k_i$, where $i=1,2,\ldots,d$.
Now, in the branch number j denote to the center vertex by u_j, the pendent vertices by v_{jl} and the support vertices by s_{jl} ($j=1,2,\ldots,d$) and ($l=1,2,\ldots,k_i$). Also, denote by α_j to the sum that mentioned in (3) for each branch. Therefore,

$$\alpha_j = d(u_j)+d(s_j)+d(v_j) = \sum_{\substack{i=1\\ i\neq j}}^{d}(7k_i+2) + k_j\sum_{\substack{i=1\\ i\neq j}}^{d}(9k_i+3) + k_j\sum_{\substack{i=1\\ i\neq j}}^{d}(11k_i+4).$$

where $d(u_j)$, $d(s_j)$ and $d(v_j)$ denote to the sum of distances between the center vertex, the support vertices and the pendent vertices, respectively, in the branch j with all the vertices of other branches, alternately, except the central vertex w (note that $d(s_j) = \sum_{l=1}^{k_j} d(s_{jl})$, $d(v_j) = \sum_{l=1}^{k_j} d(v_{jl})$). Hence,

$$\begin{aligned} W(Kg) =& d(w) + \sum_{i=1}^{d} W(\beta_i) + \frac{1}{2}\sum_{j=1}^{d}\alpha_j \\ =& \sum_{i=1}^{d}(5k_i+1) + \sum_{i=1}^{d}(6k_i^2-2k_i) + \frac{1}{2}\sum_{j=1}^{d}\sum_{\substack{i=1\\ i\neq j}}^{d}(7k_i+2) + \frac{1}{2}\sum_{j=1}^{d}k_j\sum_{\substack{i=1\\ i\neq j}}^{d}(20k_i+7) \\ =& 6\sum_{i=1}^{d}k_i^2 + \frac{1}{2}(7d-1)\sum_{i=1}^{d}k_i + \frac{7}{2}\sum_{j=1}^{d}\sum_{\substack{i=1\\ i\neq j}}^{d}k_i + 10\sum_{j=1}^{d}k_j\sum_{\substack{i=1\\ i\neq j}}^{d}k_i + d^2. \end{aligned}$$

This completes the proof. □

5. Entire Wiener index of subdivision and k-subdivision graphs

Let G be a graph. It is useful to define some new graph relatedly to G in many areas of graph theory. Some examples are the line graph, total graph and subdivision graphs. In some sources, these kinds of graphs are named as derived graphs. Now we deal with the subdivision graphs and their entire Wiener indices. The subdivision graph of G is obtained by simply adding a new vertex to every edge of G. It is used in some chemical calculations.

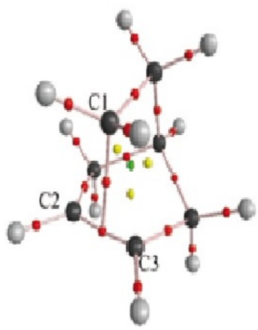

Figure 2: A subdivision graph

Theorem 10. *Let G be a connected graph on n vertices and m edges and let $S(G)$ be the subdivision graph of G. Then*

$$W^{\mathcal{E}}(G) = \frac{1}{2}\big(W(S(G)) - nm\big).$$

Proof. Let $S(G)$ be the subdivision graph of a connected graph G. Suppose u and v be any two vertices in G. Clearly $d_{S(G)}(u,v) = 2d_G(u,v)$. Also, denote the vertex in $V(S(G)) - V(G)$ that subdivides the edge $e \in E(G)$ by w_e. Therefore for any two edges e and f in $E(G)$, we have $d_{S(G)}(w_e,w_f) = 2d_G(e,f)$. Finally, for any $v \in V(G)$ and $w_e \in V(S(G)) - V(G)$ we have $d_{S(G)}(v,w_e) = 2d_G(v,e) + 1$. Hence

$$\begin{aligned}
W(S(G)) &= \sum_{\{x,y\}\subseteq V(S(G))} d_{S(G)}(x,y) \\
&= \sum_{\{u,v\}\subseteq V(G)} d_{S(G)}(u,v) + \sum_{\{w_e,w_f\}\subseteq V(S(G))-V(G)} d_{S(G)}(w_e,w_f) \\
&+ \sum_{\substack{\{v,w_e\}\subseteq V(S(G)) \\ v\in V(G),\, w_e\in V(S(G))-V(G)}} d_{S(G)}(v,w_e) \\
&= 2W(G) + 2W(L(G)) + 2\sum_{\{v,e\}\subseteq B(G)} d(v,e) + nm \\
&= 2W^{\mathcal{E}}(G) + nm.
\end{aligned}$$

□

In [2, 19, 20], a generalization of the subdivision graph named as k-subdivision graph was introduced and several properties of this new derived graph class was studied. The k-subdivision graph of G is obtained by adding k new vertices onto every edge of G. Here we calculate the entire Wiener indices of the k-subdivision graphs:

Theorem 11. *Let $S^k(G)$ be the k-subdivision graph of a connected graph G. Then*

$$\begin{aligned} W(S^k(G)) =& k(k+1)W^{\mathcal{E}}(G) + (1-k^2)W(G) + k(k^2-1)W(L(G)) \\ &+ \frac{k(k+1)}{2}|V(G)||E(G)| + |E(G)|W(P_k). \end{aligned}$$

Proof. Suppose u and v be any two vertices in G. Clearly that $d_{S^k(G)}(u,v) = (k+1)d_G(u,v)$. Denote the vertices in $V(S^k(G)) - V(G)$ that subdivides the edge $e \in E(G)$ by w_e^i, where $i = 1, 2, \ldots, k$. Then the sum of distances between any vertex u in G and the k-subdivision vertices of an edge e in G is

$$d_{S^k(G)}(u, w_e) = \sum_{i=1}^{k} d_{S^k(G)}(u, w_e^i) = k(k+1)d_G(u,e) + \frac{k(k+1)}{2}.$$

Also, for any two different edges e and f, the sum of distances between their k-subdivision vertices is given by

$$d_{S^k(G)}(w_e, w_f) = \sum_{i=1}^{k}\sum_{j=1}^{k} d_{S^k(G)}(w_e^i, w_f^j) = k^2(k+1)d_G(e,f).$$

Now, it remains to determine the distances between the k-subdivision vertices on each edge which are equal to each other and is denoted by $W(P_k)$ for each edge in G. Hence

$$\begin{aligned} W(S^k(G)) =& \sum_{\{x,y\}\subseteq V(S^k(G))} d_{S^k(G)}(x,y) \\ =& \sum_{\{u,v\}\subseteq V(G)} d_{S^k(G)}(u,v) + \sum_{\{w_e,w_f\}\subseteq V(S^k(G))-V(G)} d_{S^k(G)}(w_e,w_f) \\ &+ \sum_{\substack{\{v,w_e\}\subseteq V(S^k(G)) \\ v\in V(G),\, w_e\in V(S^k(G))-V(G)}} d_{S^k(G)}(v,w_e) + \sum_{e\in E(G)} W(P_k) \\ =& (k+1)W(G) + k^2(k+1)W(L(G)) + k(k+1)\sum_{\{v,e\}\subseteq B(G)} d(v,e) \\ &+ \frac{k(k+1)}{2}|V(G)||E(G)| + |E(G)|W(P_k) \\ =& k(k+1)W^{\mathcal{E}}(G) + (1-k^2)W(G) + k(k^2-1)W(L(G)) \\ &+ \frac{k(k+1)}{2}|V(G)||E(G)| + |E(G)|W(P_k). \end{aligned}$$

□

6. Bounds for the entire Wiener index

Our first result gives the maximum and minimum values of the entire Wiener index of any tree:

Theorem 12. *For any tree T_n on n vertices, we have*

$$W^{\mathcal{E}}(S_n) \leq W^{\mathcal{E}}(T_n) \leq W^{\mathcal{E}}(P_n).$$

Our next result shows that the minimum value of the entire Wiener index for any graph G is attained for star graph, but the maximum value is attained for the complete graph:

Theorem 13. *For any graph G on n vertices,*

$$W^{\mathcal{E}}(S_n) \leq W^{\mathcal{E}}(G) \leq W^{\mathcal{E}}(K_n).$$

Theorem 14. *Let G be a connected graph on n vertices and m edges. Then*

$$\frac{Gut(G)-m}{4}+\frac{D^{'}(G)}{2}-\frac{nm}{2} \leq W^{\mathcal{E}}(G)-W(G) \leq \frac{Gut(G)-m}{4}+\frac{D^{'}(G)}{2}+\frac{m(m-1)}{2}.$$

Moreover, the equality of the lower bound is attained if and only if G is a tree.

Proof. Let u be a vertex and $e = xy$ be an edge in G. By Definition 1, we have

$$\frac{1}{2}\big(d(u,x)+d(u,y)-1\big) \leq d(u,e) \leq \frac{1}{2}\big(d(u,x)+d(u,y)\big).$$

Therefore,

$$\begin{aligned}\sum_{v\in V(G)}\sum_{e\in E(G)} d(v,e) \leq& \frac{1}{2}\sum_{v\in V(G)}\sum_{xy\in E(G)}\big(d(u,x)+d(u,y)\big)\\ =&\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}\big(d(u)+d(v)\big)d(u,v)=\frac{1}{2}D^{'}(G).\end{aligned}$$

Then

$$\frac{1}{2}D^{'}(G)-\frac{nm}{2} \leq \sum_{v\in V(G)}\sum_{e\in E(G)} d(v,e) \leq \frac{1}{2}D^{'}(G).$$

From [22], we have

$$\frac{1}{4}\big(Gut(G)-m\big) \leq W\big(L(G)\big) \leq \frac{1}{4}\big(Gut(G)-m\big)+\frac{m(m-1)}{2}$$

which completes the proof. □

7. Entire Wiener index of the join and corona product of two graphs

In this section, we get $W^{\mathcal{E}}$ for the Join $G_1 \vee G_2$ and the Corona product $G_1 \circ G_2$ of two connected graphs G_1 and G_2.

The join $G_1 \vee G_2$ of two graphs G_1 and G_2 with disjoint vertex sets $|V(G_1)| = n_1$, $|V(G_2)| = n_2$ and edge sets $|E(G_1)| = m_1$, $|E(G_2)| = m_2$ is the graph on the vertex set $V(G_1) \cup V(G_2)$ and the edge set $E(G_1) \cup E(G_2) \cup \{u_1u_2 : u_1 \in V(G_1), u_2 \in V(G_2)\}$. Hence, the join of two graphs is obtained by connecting each vertex of one graph to each vertex of the other graph, while keeping all edges of both graphs.

Theorem 15. *Let G_1 and G_2 be two connected graphs. Then*

$$\begin{aligned} W^{\mathcal{E}}(G_1 \vee G_2) \leq & \frac{3\big(m_1^2 + m_2^2\big)}{2} - 2\big(M_1(G_1) + M_1(G_2)\big) + (n_1 - 1)(2n_2m_1 + n_1) \\ & + (n_2 - 1)(2n_1m_2 + n_2) - \frac{13(m_1 + m_2)}{2} + \frac{n_1n_2(2n_1n_2 + n_1 + n_2 - 2)}{2} \\ & + 2(n_1m_1 + n_2m_2) + 2m_1m_2 + n_1m_2 + n_2m_1, \end{aligned}$$

and

$$\begin{aligned} W^{\mathcal{E}}(G_1 \vee G_2) \geq & \big(m_1^2 + m_2^2\big) - \frac{3\big[M_1(G_1) + M_1(G_2)\big]}{2} + (n_1 - 1)(2n_2m_1 + n_1) \\ & + (n_2 - 1)(2n_1m_2 + n_2) - 7(m_1 + m_2) + \frac{n_1n_2(2n_1n_2 + n_1 + n_2 - 2)}{2} \\ & + 2(n_1m_1 + n_2m_2) + 2m_1m_2 + n_1m_2 + n_2m_1, \end{aligned}$$

with the equality holding in the lower inequality if and only if G_1 and G_2 of diameter less than or equal three.

Proof. By the definition of the entire Wiener index, we have

$$\begin{aligned} W^{\mathcal{E}}(G_1 \vee G_2) = & \sum_{\{x,y\} \in B(G_1 \vee G_2)} d_{G_1 \vee G_2}(x, y) \\ = & W(G_1 \vee G_2) + W_e(G_1 \vee G_2) + \sum_{u \in V(G_1 \vee G_2)} \sum_{e \in E(G_1 \vee G_2)} d_{G_1 \vee G_2}(u, e). \end{aligned}$$

From [23], we have

$$W(G_1 \vee G_2) = \sum_{\{u,v\} \subseteq V(G_1 \vee G_2)} d_{G_1 \vee G_2}(u, v) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - (m_1 + m_2).$$

Also, we have

$$\begin{aligned}
W_e(G_1 \vee G_2) &= \sum_{\{e,f\}\subseteq E(G_1\vee G_2)} d_{G_1\vee G_2(e,f)} \\
&= \sum_{\{e,f\}\subseteq E(G_1)} d_{G_1\vee G_2}(e,f) + \sum_{\{e,f\}\subseteq E(G_2)} d_{G_1\vee G_2}(e,f) \\
&+ \sum_{\substack{\{e,f\}\subseteq E(G_1\vee G_2) \\ e\in E(G_1),\, f\in E(G_2)}} d_{G_1\vee G_2}(e,f) \\
&+ \sum_{\substack{\{e,f\}\subseteq E(G_1\vee G_2) \\ e\in E(G_1),\, f\notin E(G_1\cup G_2)}} d_{G_1\vee G_2}(e,f) + \sum_{\substack{\{e,f\}\subseteq E(G_1\vee G_2) \\ e\in E(G_2),\, f\notin E(G_1\cup G_2)}} d_{G_1\vee G_2}(e,f) \\
&+ \sum_{\substack{\{e,f\}\subseteq E(G_1\vee G_2) \\ e,f\notin E(G_1\cup G_2)}} d_{G_1\vee G_2}(e,f).
\end{aligned}$$

Since for any two edges e and f in $G_1 \vee G_2$, we have:

$$d_{G_1\vee G_2}(e,f) = \begin{cases} 1, & \text{if } e \text{ and } f \text{ are adjacent;} \\ 3, & \text{if } e,f\in E(G_1) \textit{ or } e,f\in E(G_2) \textit{ and} \\ & \quad d_{G_1}(e,f) > 2 \textit{ or } d_{G_2}(e,f) > 2; \\ 2, & \text{Otherwise,} \end{cases} \tag{1}$$

then

$$\begin{aligned}
W_e(G_1 \vee G_2) \leq &\frac{1}{2}\sum_{e\in E(G_1)} \left[\deg_{G_1}(e) + 3(m_1 - \deg_{G_1}(e) - 1)\right] \\
&+ \frac{1}{2}\sum_{e\in E(G_2)} \left[\deg_{G_2}(e) + 3(m_2 - \deg_{G_2}(e) - 1)\right] \\
&+ 2m_1m_2 + m_1\left[2n_2 + 2(n_1n_2 - 2n_2)\right] \\
&+ m_2\left[2n_1 + 2(n_1n_2 - 2n_1)\right] + \frac{n_1n_2}{2}(n_1+n_2-2) + n_1n_2(n_1n_2 - n_1 - n_2 + 1) \\
= &\frac{3(m_1^2+m_2^2)}{2} - \left(M_1(G_1) + M_1(G_2)\right) + \frac{m_1+m_2}{2} + 2m_1m_2 + 2n_2m_1(n_1-1) \\
&+ 2n_1m_2(n_2-1) + \frac{n_1n_2}{2}(2n_1n_2 - n_1 - n_2),
\end{aligned}$$

where $M_1(G_1)$, $M_2(G_2)$ are the first Zagreb index of G_1 and G_2, respectively. Finally, we have

$$\begin{aligned}
\sum_{u\in V(G_1\vee G_2)}\sum_{e\in E(G_1\vee G_2)} d_{G_1\vee G_2}(u,e) =& \sum_{u\in V(G_1)}\sum_{e\in E(G_1)} d_{G_1\vee G_2}(u,e)\\
&+\sum_{u\in V(G_2)}\sum_{e\in E(G_2)} d_{G_1\vee G_2}(u,e)\\
&+\sum_{u\in V(G_1)}\sum_{e\in E(G_2)} d_{G_1\vee G_2}(u,e)\\
&+\sum_{u\in V(G_2)}\sum_{e\in E(G_1)} d_{G_1\vee G_2}(u,e)\\
&+\sum_{u\in V(G_1\cup G_2)}\sum_{e\notin E(G_1\cup G_2)} d_{G_1\vee G_2}(u,e)\\
=&\sum_{u\in V(G_1)}\sum_{v\in N_{G_1}(u)}\big(\deg_{G_1}(v)-1\big)\\
&+\sum_{u\in V(G_2)}\sum_{v\in N_{G_2}(u)}\big(\deg_{G_2}(v)-1\big)\\
&+2\sum_{u\in V(G_1)}\Bigg[m_1-\deg_{G_1}(u)-\sum_{v\in N_{G_1}(u)}\deg_{G_1}(v)\Bigg]\\
&+2\sum_{u\in V(G_2)}\Bigg[m_2-\deg_{G_2}(u)-\sum_{v\in N_{G_2}(u)}\deg_{G_2}(v)\Bigg]\\
&+n_1m_2+n_2m_1+n_1(n_1n_2-n_2)+n_2(n_1n_2-n_1)\\
=&M_1(G_1)-2m_1+M_1(G_2)-2m_2\\
&+2\big[n_1m_1-2m_1-M_1(G_1)\big]\\
&+2\big[n_2m_2-2m_2-M_1(G_2)\big]+n_1m_2+n_2m_1\\
&+n_1(n_1n_2-n_2)+n_2(n_1n_2-n_1)\\
=&2(n_1m_1+n_2m_2)-\big(M_1(G_1)+M_1(G_2)\big)-6(m_1+m_2)\\
&+n_1m_2+n_2m_1+n_1n_2(n_1+n_2-2).
\end{aligned}$$

For the equality of the lower inequality, note that, if the diameter of G_1 and G_2 less than or equal three, then Eqn. (1) will be as follows:

$$d_{G_1\vee G_2}(e,f)=\begin{cases}1, & \text{if } e \text{ and } f \text{ are adjacent;}\\ 2, & \text{Otherwise.}\end{cases}$$

Hence, the equality holds if and only if the diameter of G_1 and G_2 less than or equal three. This completes the proof. □

Example 2.

$$
\begin{aligned}
W^{\mathcal{E}}(C_{n_1} \vee C_{n_2}) \leq & \frac{3\big(n_1^2+n_2^2\big)}{2} - 2\big(4n_1+4n_2\big) + (n_1-1)(2n_2n_1+n_1) \\
& + (n_2-1)(2n_1n_2+n_2) - \frac{13(n_1+n_2)}{2} + \frac{n_1n_2(2n_1n_2+n_1+n_2-2)}{2} \\
& + 2(n_1^2+n_2^2) + 4n_1n_2, \\
= & \frac{7\big(n_1^2+n_2^2\big)}{2} + n_1(n_1-1)(2n_2+1) + n_2(n_2-1)(2n_1+1) - \frac{29(n_1+n_2)}{2} \\
& + \frac{n_1n_2(2n_1n_2+n_1+n_2+6)}{2},
\end{aligned}
$$

and

$$
\begin{aligned}
W^{\mathcal{E}}(C_{n_1} \vee C_{n_2}) \geq & \big(n_1^2+n_2^2\big) - \frac{3\big[4n_1+4n_2\big]}{2} + (n_1-1)(2n_2n_1+n_1) \\
& + (n_2-1)(2n_1n_2+n_2) - 7(n_1+n_2) + \frac{n_1n_2(2n_1n_2+n_1+n_2-2)}{2} \\
& + 2(n_1^2+n_2^2) + 4n_1n_2 \\
= & 3\big(n_1^2+n_2^2\big) + n_1(n_1-1)(2n_2+1) + n_2(n_2-1)(2n_1+1) - 13(n_1+n_2) \\
& + \frac{n_1n_2(2n_1n_2+n_1+n_2+6)}{2}.
\end{aligned}
$$

The corona product $G_1 \circ G_2$ of two graphs G_1 and G_2, where $|V(G_1)| = n_1$, $|V(G_2)| = n_2$ and $|E(G_1)| = m_1$, $|E(G_2)| = m_2$ is the graph obtained by taking $|V(G_1)|$ copies of G_2 and joining the ith vertex of G_1 to each vertex of the i-th copy of G_2. Obviously, $|V(G_1 \circ G_2)| = n_1(n_2+1)$ and $|E(G_1 \circ G_2)| = m_1 + n_1(m_2+n_2)$.

Theorem 16. *Let G_1 and G_2 be two connected graphs. Then*

$$
\begin{aligned}
W^{\mathcal{E}}(G_1 \circ G_2) \leq & (2n_2+m_2+1)W^{\mathcal{E}}(G_1) + [m_2^2+4n_2^2+4n_2m_2+2n_2+m_2]W(G_1) \\
& + (2n_2+m_2)\big[n_1m_1 - W_e(G_1)\big] + n_1^2(n_2+m_2) + 4n_1m_2(n_2-2) \\
& + \frac{n_1n_2(n_1n_2+4n_2-5)}{2} - n_1\big(M_1(G_1)+M_1(G_2)\big) + \frac{n_1m_2(3m_2+1)}{2} \\
& + \frac{n_1(n_1-1)}{2}\big[3m_2^2+4n_2^2+8n_2m_2\big],
\end{aligned}
$$

and

$$
\begin{aligned}
W^{\mathcal{E}}(G_1 \circ G_2) \geq & (2n_2+m_2+1)W^{\mathcal{E}}(G_1) + [m_2^2+4n_2^2+4n_2m_2+2n_2+m_2]W(G_1) \\
& + (2n_2+m_2)\big[n_1m_1 - W_e(G_1)\big] + n_1^2(n_2+m_2) + 4n_1m_2(n_2-2) \\
& + \frac{n_1n_2(n_1n_2+4n_2-5)}{2} - \frac{n_1}{2}\big(M_1(G_1)+2M_1(G_2)\big) + n_1m_2^2 \\
& + \frac{n_1(n_1-1)}{2}\big[3m_2^2+4n_2^2+8n_2m_2\big],
\end{aligned}
$$

with the equality holding in the lower inequality if and only if G_2 of diameter less than or equal three.

Proof. By the definition of the entire Wiener index, we have

$$\begin{aligned}
W^{\mathcal{E}}(G_1\circ G_2) =& \sum_{\{x,y\}\in B(G_1\circ G_2)} d_{G_1\circ G_2}(x,y)\\
=& W^{\mathcal{E}}(G_1) + \sum_{\substack{\{u,y\}\in B(G_1\circ G_2)\\ u\in V(G_1),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(u,y)\\
&+ \sum_{\substack{\{e,y\}\in B(G_1\circ G_2)\\ e\in E(G_1),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(e,y) + \sum_{\substack{\{u,y\}\in B(G_1\circ G_2)\\ u\in V(G_2),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(u,y)\\
&+ \sum_{\substack{\{e,y\}\in B(G_1\circ G_2)\\ e\in E(G_2),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(e,y) + \sum_{\substack{\{e,f\}\subseteq E(G_1\circ G_2)\\ e\notin E(G_1),\, f\notin E(G_2)}} d_{G_1\circ G_2}(e,f).
\end{aligned} \tag{2}$$

Now, we compute the summations in Eqn. (2) as follows:

$$\begin{aligned}
\sum_{\substack{\{u,y\}\in B(G_1\circ G_2)\\ u\in V(G_1),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(u,y) =& n_1n_2 + n_1m_2 + 2n_2 \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u,v)+1)\\
&+ 2m_2 \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u,v)+1)\\
&+ 2n_2 \sum_{\{u,v\}\subseteq V(G_1)} d_{G_1}(u,v)\\
=& n_1^2(n_2+m_2) + 2(2n_2+m_2)W(G_1).
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{\{e,y\}\in B(G_1\circ G_2)\\ e\in E(G_1),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(e,y) =& \sum_{v\in V(G_2)} \sum_{\substack{\{u,e\}\in B(G_1)\\ u\in V(G_1),\, e\in E(G_1)}} \big(d_{G_1}(u,e)+1\big)\\
&+ \sum_{f\in E(G_2)} \sum_{\substack{\{u,e\}\in B(G_1)\\ u\in V(G_1),\, e\in E(G_1)}} \big(d_{G_1}(u,e)+1\big)\\
=& (2n_2+m_2)\Bigg[n_1m_1 + \sum_{u\in V(G_1)} \sum_{e\in E(G_1)} d_{G_1}(u,e)\Bigg]\\
=& (2n_2+m_2)\big[n_1m_1 + W^{\mathcal{E}}(G_1) - W(G_1) - W_e(G_1)\big].
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{\{u,y\}\in B(G_1\circ G_2)\\ u\in V(G_2),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(u,y) =& \frac{n_1}{2}\Bigg[\sum_{u\in V(G_2)} \deg_{G_2}(u) + 2\sum_{u\in V(G_2)} \big[n_2 - \deg_{G_2}(u) - 1\big]\Bigg]\\
&+ n_1 \sum_{u\in V(G_2)} \sum_{w\in N_{G_2}(u)} \big(\deg_{G_2}(w) - 1\big) + n_1n_2(n_2-1)\\
&+ 2n_1 \sum_{u\in V(G_2)} \big[m_2 - \deg_{G_2}(u) - \sum_{w\in N_{G_2}(u)} \deg_{G_2}(w)\big]\\
&+ n_2^2 \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u,v)+2)\\
&+ 2n_2^2 \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u,v)+1)\\
&+ 2n_2m_2 \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u,v)+2)\\
=& 2n_1n_2(n_2-1) + (3n_2^2 + 2n_2m_2)W(G_1) - n_1M_1(G_1)\\
&+ 2n_1m_2(n_2-3) + 2n_1n_2(n_1-1)(n_2+m_2).
\end{aligned}$$

Since for any two edges e and f both in one copy of G_2, we have:

$$d_{G_1\circ G_2}(e,f)=\begin{cases}1, & \text{if } e \text{ and } f \text{ are adjacent;}\\ 2, & \text{if } d_{G_2}(e,f)=2;\\ 3, & \text{Otherwise,}\end{cases} \tag{3}$$

then

$$\begin{aligned}\sum_{\substack{\{e,y\}\in B(G_1\circ G_2)\\ e\in E(G_2),\, y\notin V(G_1)\cup E(G_1)}} d_{G_1\circ G_2}(e,y) \leq & \frac{n_1}{2}\Big[\sum_{e\in E(G_2)}\deg_{G_2}(e)+3\sum_{e\in E(G_2)}\big[m_2-\deg_{G_2}(e)-1\big]\Big]\\ &+2n_1m_2(n_2-2)+2n_1m_2\\ &+m_2^2\sum_{\{u,v\}\subseteq V(G_1)}\big(d_{G_1}(u,v)+3\big)\\ &+2n_2m_2\sum_{\{u,v\}\subseteq V(G_1)}\big(d_{G_1}(u,v)+2\big)\\ =&\frac{n_1}{2}\Big[3m_2^2+m_2-2M_1(G_2)\Big]+(m_2^2+2n_2m_2)W(G_1)\\ &+\frac{n_1(n_1-1)}{2}\big[3m_2^2+4n_2m_2\big]+2n_1m_2(n_2-1).\end{aligned}$$

Finally,

$$\begin{aligned}\sum_{\substack{\{e,f\}\subseteq E(G_1\circ G_2)\\ e,f\notin E(G_1),\, e,f\notin E(G_2)}} d_{G_1\circ G_2}(e,f) =& \frac{n_1n_2(n_2-1)}{2}+n_2^2\sum_{\{u,v\}\subseteq V(G_1)}\big(d_{G_1}(u,v)+1\big)\\ =&\frac{n_1n_2(n_1n_2-1)}{2}+n_2^2W(G_1).\end{aligned}$$

For the equality of the lower inequality, note that, if the diameter of G_1 and G_2 less than or equal three, then Eqn. (3) will be as follows:

$$d_{G_1\circ G_2}(e,f)=\begin{cases}1, & \text{if } e \text{ and } f \text{ are adjacent;}\\ 2, & \text{Otherwise.}\end{cases}$$

Hence, the equality holds if and only if the diameter of G_2 less than or equal three. This completes the proof. □

Example 3.

$$\begin{aligned}W^{\mathcal{E}}(G_1\circ K_2)=&6W^{\mathcal{E}}(G_1)+30W(G_1)+5\big[n_1m_1-W_e(G_1)\big]+n_1(3n_1+1)\\ &+\frac{2n_1(2n_1+3)}{2}-\frac{n_1}{2}\big(M_1(G_1)+4\big)+\frac{35n_1(n_1-1)}{2}.\end{aligned}$$

References

[1] M.B. Ahmadi, S.A. Hosseini, and P.S. Nowbandegani, *On trees with minimal atom bond connectivity index*, MATCH Commun. Math. Comput. Chem. **69** (2013), 559–563.

[2] M. Ascioglu and I.N. Cangul, *Sigma index and forgotten index of the subdivision and r-subdivision graphs*, Proceedings of the Jangjeon Mathematical Society **21** (2018), no. 3, 375–383.

[3] M. Azari, *Multiplicative sum Zagreb index of chain and chain-cycle graphs*, J. Inform. Optim. Sci. **40** (2019), no. 7, 1529–1541.

[4] F. Buckley, *Mean distance in line graphs*, Congr. Numer. **32** (1981), 153–162.

[5] A.A. Dobrynin, R. Entringer, and I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001), no. 3, 211–249.

[6] A.A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert, *Wiener index of hexagonal systems*, Acta Appl. Math. **72** (2002), no. 3, 247–294.

[7] J.K. Doyle and J.E. Graver, *Mean distance in a graph*, Discrete Math. **17** (1977), no. 2, 147–154.

[8] R.C. Entringer, *Distance in graphs: Trees*, J. Comb. Math. Comb. Comput. **24** (1997), 65–84.

[9] I. Gutman, *Selected properties of the Schultz molecular topological index*, J. Chem. Inf. Coumput. Sci. **34** (1994), no. 5, 1087–1089.

[10] ______, *Kragujevac trees and their energy*, Ser. A: Appl. Math. Inform. Mech. **6** (2014), no. 2, 71–79.

[11] I. Gutman, A.M. Naji, and N.D. Soner, *On leap Zagreb indices of graphs*, Commun. Comb. Optim. **2** (2017), no. 2, 99–117.

[12] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer Science & Business Media, 2012.

[13] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.

[14] 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.

[15] F. Harary, *Graph Theory*, Addison-Wesley, Reading Mass, 1969.

[16] A. Iranmanesh, I. Gutman, O. Khormali, and A. Mahmiani, *The edge versions of the Wiener index*, MATCH Commun. Math. Comput. Chem. **61** (2009), no. 3, 663–672.

[17] S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003), no. 2, 113–124.

[18] R. Škrekovski and I. Gutman, *Vertex version of the Wiener Theorem*, MATCH Commun. Math. Comput. Chem. **72** (2014), no. 1, 295–300.

[19] M. Togan, A. Yurttas, and I.N. Cangul, *Some formulae and inequalities on several Zagreb indices of r-subdivision graphs*, Enlightments of Pure and Applied

Mathematics (EPAM) **1** (2015), no. 1, 29–45.

[20] ______, *Zagreb and multiplicative Zagreb indices of r-subdivision graphs of double graphs*, Scientia Magna **12** (2017), no. 1, 115–119.

[21] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947), no. 1, 17–20.

[22] B. Wu, *Wiener index of line graphs*, MATCH Commun. Math. Comput. Chem. **64** (2010), no. 3, 699–706.

[23] Y.-N. Yeh and I. Gutman, *On the sum of all distances in composite graphs*, Discrete Math. **135** (1994), no. 1-3, 359–365.

[24] B. Zhou, *Zagreb indices*, MATCH Commun. Math. Comput. Chem. **52** (2004), no. 1, 13–118.