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SOME RESULTS ON WIENER INDEX, HYPER-WIENER INDEX AND ZAGREB INDEX

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Abstract

A topological index is a real number derived from the structure of a graph, which is invariant under graph isomorphism. Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds. In this paper, some topological indices such as Wiener index, hyper-Wiener index and Zagreb index of a generalized join of some certain graphs are obtained.

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1 Introduction

Let $G = (V, E)$ be a simple connected graph and $V(G)$ and $E(G)$ denote the vertex set and edge set of G, respectively. For a vertex v of G, $\mathrm{N}_G(v)$ denotes the set of vertices of G that are adjacent to v in G, and we denote $|\mathrm{N}_G(v)|$ by $\mathrm{d}_G(v)$. For distinct vertices u and v of G, we write $u \sim v$ if u and v are adjacent in G and the edge e between u and v will be denoted by $e = uv$. Also the *distance* between two distinct vertices u and v in G, denoted by $\mathrm{d}_G(u, v)$, is the length of the shortest path connecting u and v, if such a path exists; otherwise, we set $\mathrm{d}_G(u, v) := \infty$. A *topological index* is a real number derived from the structure of a graph, which is invariant under graph isomorphism. Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds. The first and second *Zagreb indices* of a graph denoted by $M_1(G)$ and $M_2(G)$, respectively, are degree based topological indices introduced more than thirty years ago by I. Gutman and N. Trinajstic [8]. They are defined as

$$M_1(G) = \sum_{e=uv\in E(G)} (\mathrm{d}_G(u) + \mathrm{d}_G(v)) = \sum_{v\in V(G)} \mathrm{d}_G^2(v),$$
$$M_2(G) = \sum_{e=uv\in E(G)} \mathrm{d}_G(u)\mathrm{d}_G(v).$$

These indices were introduced to study the structure-dependency of the total π-electron energy (ε). It was found that ε depends on $M_1(G)$ and thus provides a measure of carbon skeleton of the underlying molecules.

The *Hyper Zagreb index* of a graph denoted by $HM(G)$, was introduced in [12], as a new version of Zagreb index. For a graph G, the Hyper Zagreb index is defined as follows:

$$HM(G) = \sum_{e=uv\in E(G)} (\mathrm{d}_G(u) + \mathrm{d}_G(v))^2.$$

In [13], the authors considered the multiplicative variants of molecular structure. When this idea is applied to Zagreb indices, one arrives at their multiplicative versions $\Pi_1(G)$ and $\Pi_2(G)$, defined as

$$\Pi_1(G) = \prod_{v\in V(G)} d^2(v) \text{ and } \Pi_2(G) = \prod_{uv\in E(G)} d(u)d(v).$$

Finally, Eliasi et al. [4] defined a multiplicative version of M_1 as

$$\Pi_1^*(G) = \prod_{uv\in E(G)} (d(u) + d(v)),$$

and is called as the *multiplicative sum Zagreb index* by Xu and Das [15].

The *Wiener index*, $W(G)$, is equal to the count of all shortest distances in a graph (cf. [14]). In other words, $W(G) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$. Wiener number was defined in 1947 by an American chemist H. Wiener. He used this index to estimate the boiling point of Alkans. There are many situations in communication, facility location, cryptology, architecture etc. where the Wiener index of the corresponding graph or the average distance is of great interest. One of these problems, for example, is to find a spanning tree with minimum average distance. The Wiener index is one of the most studied topological indices, both from a theoretical point of view and applications, see for details [3], [5], [7] and [16].

The *hyper-Wiener index* of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al. [10], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. It is $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d^2(u,v)$, where $d^2(u,v) = d(u,v)^2$. We encourage the reader to consult [1], [2], [6] and [9] for the mathematical properties of hyper-Wiener index and its applications in chemistry.

In Section 2 of the paper, we study Wiener index and hyper-Wiener index of a generalized join of some certain graphs. In Section 3, the first and second Zagreb indices and their multiplicative versions of a generalized join of some certain graphs are investigated, and also the Hayper Zagreb index is obtained.

All graphs considered in this paper are connected and simple. We say that G is an *empty graph* if $E(G) = \emptyset$. Also, K_n and $\overline{K_n}$ denote the complete graph with n vertices and its complement, respectively, and P_n denotes the path with n vertices.

2 Wiener index and hyper-Wiener index

In this section, first we recall the definition of a generalized join of graphs. For two graphs H_1 and H_2 with disjoint vertex sets, the *join* $H_1 \vee H_2$ of the graphs H_1 and H_2 is the graph obtained from the union of H_1 and H_2 by adding new edges from each vertex of H_1 to every vertex of H_2. The concept of join graph is generalized (in [11], it is called as a generalized composition graph). Let G be a graph on k vertices with $V(G) = \{v_1, v_2, \ldots, v_k\}$, and let $H_1, H_2, \ldots, H_k$ be k pairwise disjoint graphs. The *G-generalized join graph* $G[H_1, H_2, \ldots, H_k]$ of $H_1, H_2, \ldots, H_k$ is the graph formed by replacing each vertex v_i of G by the graph H_i and then joining each vertex of H_i to each vertex of H_j whenever $v_i \sim v_j$ in the graph G. Now, if the graph G consists of two adjacent vertices, then the G-generalized join graph $G[H_1, H_2]$ coincides with the join $H_1 \vee H_2$ of the graphs H_1 and H_2.

In the rest of the paper, in the G-generalized join graph $G[H_1, H_2, \ldots, H_k]$, we assume that each H_i is either a complete graph or it is an empty graph, and without loss of generality, we assume that $H_1, \ldots, H_t$ are complete graphs and $H_{t+1}, \ldots, H_k$ are empty graphs, where $0 \leqslant t \leqslant k$. Also, we always assume that there exists $1 \leqslant i \leqslant k$ such that $|H_i| > 1$.

In the following theorem, we study the Wiener index and hyper-Wiener index of $G' = G[H_1, H_2, \ldots, H_k]$, where G is isomorphic to the path P_k.

Theorem 2.1. *Assume that $G' = P_k[H_1, H_2, \ldots, H_k]$, where $k > 1$. Then*

$$W(G') = \frac{1}{2}\sum_{i=1}^{k} |H_i|\Delta_{H_i}$$

and

$$WW(G') = \frac{1}{4}\sum_{i=1}^{k} |H_i|\Delta_{H_i} + \frac{1}{4}\sum_{i=1}^{k} |H_i|\Delta'_{H_i},$$

where for $1 \leqslant i \leqslant t$, we have

$$\Delta_{H_i} = |H_i| - 1 + \sum_{j=1}^{k} |i-j||H_j| \quad \text{and} \quad \Delta'_{H_i} = |H_i| - 1 + \sum_{j=1}^{k} (i-j)^2|H_j|,$$

and for $t+1 \leqslant i \leqslant k$, we have

$$\Delta_{H_i} = 2(|H_i|-1)+\sum_{j=1}^{k}|i-j||H_j| \text{ and } \Delta'_{H_i} = 4(|H_i|-1)+\sum_{j=1}^{k}(i-j)^2|H_j|.$$

Proof. Assume that $h \in H_i$, for some $1 \leqslant i \leqslant k$. Then we have

$$\sum_{x\in V(G')} \mathrm{d}(h,x) = \sum_{x\in H_i} \mathrm{d}(h,x) + \sum_{x\in V(G')\setminus H_i} \mathrm{d}(h,x)$$

$$= \sum_{x\in H_i} \mathrm{d}(h,x) + \sum_{j=1}^{k} |i-j||H_j|$$

$$= \begin{cases} n-1+\sum_{j=1}^{k} |i-j||H_j| & H_i \cong K_n \\ 2(n-1)+\sum_{j=1}^{k} |i-j||H_j| & H_i \cong \overline{K}_n. \end{cases}$$

It is easy to see that for each $h, h' \in H_i$, $\sum_{x\in V(G')} \mathrm{d}(h,x) = \sum_{x\in V(G')} \mathrm{d}(h',x)$. Let $\Delta_{H_i} = \sum_{x\in V(G')} \mathrm{d}(h,x)$, for some $h \in H_i$. Thus we have

$$\sum_{h\in H_i} \sum_{x\in V(G')} \mathrm{d}(h,x) = |H_i|\Delta_{H_i}.$$

Therefore

$$W(G') = \frac{1}{2}\sum_{i=1}^{k} |H_i|\Delta_{H_i}.$$

Now let $h \in H_i$, for some $1 \leqslant i \leqslant k$. Then we have

$$\sum_{x\in V(G')} \mathrm{d}^2(h,x) = \sum_{x\in H_i} \mathrm{d}^2(h,x) + \sum_{x\in V(G')\setminus H_i} \mathrm{d}^2(h,x)$$

$$= \sum_{x\in H_i} \mathrm{d}^2(h,x) + \sum_{j=1}^{k} (i-j)^2|H_j|$$

$$= \begin{cases} n-1+\sum_{j=1}^{k} (i-j)^2|H_j| & H_i \cong K_n \\ 4(n-1)+\sum_{j=1}^{k} (i-j)^2|H_j| & H_i \cong \overline{K}_n. \end{cases}$$

Clearly for each $h, h' \in H_i$, $\sum_{x\in V(G')} \mathrm{d}^2(h,x) = \sum_{x\in V(G')} \mathrm{d}^2(h',x)$. Let $\Delta'_{H_i} = \sum_{x\in V(G')} \mathrm{d}^2(h,x)$, for some $h \in H_i$. Thus we have

$$\sum_{h\in H_i} \sum_{x\in V(G')} \mathrm{d}^2(h,x) = |H_i|\Delta'_{H_i}.$$

Therefore

$$WW(G') = \frac{1}{4}\sum_{i=1}^{k} |H_i|\Delta_{H_i} + \frac{1}{4}\sum_{i=1}^{k} |H_i|\Delta'_{H_i}.$$

□

We end this section with the following theorem which determines the Wiener index and hyper-Wiener index of $G' = G[H_1, H_2, \ldots, H_n]$, where G is isomorphic to the complete graph K_n.

Theorem 2.2. *Let $G' = K_n[H_1, H_2, \ldots, H_n]$, where $n > 1$. Then*

$$W(G') = \frac{1}{2}\sum_{i=1}^{n} |H_i|\Delta_{H_i}$$

and

$$WW(G') = \frac{1}{4}\sum_{i=1}^{n} |H_i|\Delta_{H_i} + \frac{1}{4}\sum_{i=1}^{n} |H_i|\Delta'_{H_i},$$

where for $1 \leqslant i \leqslant n$,

$$\Delta_{H_i} = \begin{cases} t-1+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong K_t \\ 2(t-1)+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong \overline{K_t} \end{cases}$$

and

$$\Delta'_{H_i} = \begin{cases} t-1+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong K_t \\ 4(t-1)+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong \overline{K_t}. \end{cases}$$

Proof. Let $h, h' \in H_i$, for some $1 \leqslant i \leqslant n$. Then we have

$$\sum_{x\in V(G')} \mathrm{d}(h,x) = \sum_{x\in H_i} \mathrm{d}(h,x) + \sum_{x\in V(G')\setminus H_i} 1$$

$$= \sum_{x\in H_i} \mathrm{d}(h,x) + \sum_{j=1,j\neq i}^{n} |H_j|$$

$$= \begin{cases} t-1+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong K_t \\ 2(t-1)+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong \overline{K_t} \end{cases}$$

$$= \sum_{x\in V(G')} \mathrm{d}(h',x)$$

Let $\Delta_{H_i} = \sum_{x\in V(G')} \mathrm{d}(h,x)$, for some $h \in H_i$. Thus we have

$$\sum_{h\in H_i} \sum_{x\in V(G')} \mathrm{d}(h,x) = |H_i|\Delta_{H_i}.$$

Therefore

$$W(G') = \frac{1}{2}\sum_{i=1}^{n} |H_i|\Delta_{H_i}.$$

Now, for $h, h' \in H_i$, where $1 \leqslant i \leqslant n$, we have

$$\sum_{x\in V(G')} \mathrm{d}^2(h,x) = \sum_{x\in H_i} \mathrm{d}^2(h,x) + \sum_{x\in V(G')\setminus H_i} 1$$

$$= \sum_{x\in H_i} \mathrm{d}^2(h,x) + \sum_{j=1,j\neq i}^{n} |H_j|$$

$$= \begin{cases} t-1+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong K_t \\ 4(t-1)+\sum_{j=1,j\neq i}^{n} |H_j| & H_i \cong \overline{K_t} \end{cases}$$

$$= \sum_{x\in V(G')} \mathrm{d}^2(h',x)$$

Let $\Delta'_{H_i} = \sum_{x\in V(G')} \mathrm{d}^2(h,x)$, for some $h \in H_i$. Thus we have

$$\sum_{h\in H_i} \sum_{x\in V(G')} \mathrm{d}^2(h,x) = |H_i|D'_{H_i}.$$

Therefore

$$WW(G') = \frac{1}{4}\sum_{i=1}^{n} |H_i|\Delta_{H_i} + \frac{1}{4}\sum_{i=1}^{n} |H_i|\Delta'_{H_i}.$$

□

3 Zagreb index

In this section, we investigate the first and second Zagreb indices and their multiplicative versions, and also the Hayper Zagreb index of $G[H_1, H_2, \dots, H_k]$. Since each H_i is either a complete graph or it is an empty graph, without loss of generality, we assume that $H_1, \dots, H_t$ are complete graphs and $H_{t+1}, \dots, H_k$ are empty graphs, where $0 \leqslant t \leqslant k$.

In the following theorem, we study the first and second Zagreb indices of $G[H_1, H_2, \dots, H_k]$.

Theorem 3.1. *Let* $G' = G[H_1, H_2, \dots, H_k]$, *where* $k > 1$. *Then*

$$M_1(G') = \sum_{i=1}^{k} |H_i| \mathrm{d}^2_{G'}(v_i)$$

and

$$M_2(G') = \sum_{e=v_iv_j \in E(G)} |H_i||H_j| \mathrm{d}_{G'}(v_i) \mathrm{d}_{G'}(v_j) + \sum_{i=1}^{t} \frac{|H_i|(|H_i|-1)}{2} \mathrm{d}^2_{G'}(v_i).$$

Proof. For each two distinct vertices x and y in H_i, where $1 \leqslant i \leqslant k$, we have $\mathrm{d}_{G'}(x) = \mathrm{d}_{G'}(y)$. So we have $\sum_{x \in H_i} \mathrm{d}^2_{G'}(x) = |H_i| \mathrm{d}^2_{G'}(v_i)$. Therefore we have

$$M_1(G') = \sum_{v \in V(G')} \mathrm{d}^2_{G'}(v) = \sum_{i=1}^{k} |H_i| \mathrm{d}^2_{G'}(v_i).$$

Note that for each edge $e = v_iv_j \in E(G)$, we have $|H_i||H_j|$ edges in G'. Also $H_1, \dots, H_t$ are complete graphs, where $0 \leqslant t \leqslant k$. Hence the second Zagreb index of G' reads as follows:

$$M_2(G') = \sum_{e=v_iv_j \in E(G)} |H_i||H_j| \mathrm{d}_{G'}(v_i) \mathrm{d}_{G'}(v_j) + \sum_{i=1}^{t} \frac{|H_i|(|H_i|-1)}{2} \mathrm{d}^2_{G'}(v_i).$$

□

The following proposition, which determines the Hyper Zagreb index of $G' = G[H_1, H_2, \dots, H_k]$, is obtained simillar to the second Zagreb index.

Proposition 3.2. *The Hyper Zagreb index of* $G' = G[H_1, H_2, \ldots, H_k]$ *is*

$$HM(G') = \sum_{e=v_iv_j\in E(G)} |H_i||H_j|(\mathrm{d}_{G'}(v_i)+\mathrm{d}_{G'}(v_j))^2+\sum_{i=1}^{t} 2|H_i|(|H_i|-1)\mathrm{d}^2_{G'}(v_i).$$

We end this section with the following corollary which is about the multiplicative versions of Zagreb indices.

Corollary 3.3. *Assume that* $G' = G[H_1, H_2, \ldots, H_k]$*, where* $k > 1$*. Then the following holds:*

(i) $\Pi_1(G') = \prod_{i=1}^{k}(\mathrm{d}_{G'}(v_i))^{2|H_i|}$.

(ii) $\Pi_2(G') = \prod_{e=v_iv_j\in E(G)}(\mathrm{d}_{G'}(v_i))^{|H_i|}(\mathrm{d}_{G'}(v_j))^{|H_j|}\prod_{i=1}^{t}\mathrm{d}_{G'}(v_i)^{|H_i|(|H_i|-1)}$.

(iii) $\Pi_1^*(G') = \prod_{e=v_iv_j\in E(G)}(\mathrm{d}_{G'}(v_i)+\mathrm{d}_{G'}(v_j))^{|H_i||H_j|}\prod_{i=1}^{t}(2\mathrm{d}_{G'}(v_i))^{\frac{|H_i|(|H_i|-1)}{2}}$.

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