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GENERALIZED ZAGREB INDEX OF PRODUCT GRAPHS

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Abstract. The generalized Zagreb index is an extension of both ordinary and variable Zagreb indices. In this paper, we present exact formulae for the values of the generalized Zagreb index for product graphs. Results are applied to some graphs of general and chemical interest such as nanotubes and nanotori.

1. Introduction

The concept of the variable topological indices was proposed as an alternative way of characterizing hetero-atoms in molecules, but also to assess the structural differences, such as, for example, the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes. The idea behind the variable topological indices is that the variables are determined during the regression so that the standard error of estimate for a studied property is as small as possible. Several topological indices have already been generalized in their variable forms but here we consider Zagreb indices.

Let G be a finite simple graph with vertex set $V(G)$ and edge set $E(G)$. The *first and second Zagreb indices* are among the oldest topological indices, and were introduced by Gutman and Trinajstić [15] and Gutman *et. al.*. [14], respectively. These indices have since been used to study molecular complexity, chirality, ZE–isomerism, and hetero–systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models. For details on their theory and applications see the recent

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surveys [1, 13] and the references quoted there in. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively and defined as

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 = \sum_{uv\in E(G)} [d_G(u) + d_G(v)],$$

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

where $d_G(u)$ denotes the degree of the vertex u in G which is the number of vertices incident to u. For more information on Zagreb indices, see the recent survey [6] and the references quoted therein.

At the very beginning of development of chemical graph theory, Gutman and Trinajstić [15] considered also an invariant defined as the sum of cubes of vertex degrees. The invariant was then completely forgotten and received no attention until very recently, when Furtula and Gutman [10] revived it under the name of *forgotten topological index* or *F-index*. The F-index of a graph G is defined as

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2].$$

We refer the reader to [7, 8, 12, 27, 31] for more information on F-index.

The *first and second variable Zagreb indices* were introduced in 2004 by Li *et al.* [21, 22] as

$$M_1^{(r)}(G) = \sum_{u\in V(G)} d_G(u)^r = \sum_{uv\in E(G)} [d_G(u)^{r-1} + d_G(v)^{r-1}],$$

$$M_2^{(r)}(G) = \sum_{uv\in E(G)} [d_G(u)d_G(v)]^r,$$

where r is a variable parameter. It is easy to see that, $M_1^{(2)}(G) = M_1(G)$, $M_2^{(1)}(G) = M_2(G)$, and $M_1^{(3)}(G) = F(G)$. We refer the reader to [26, 29, 32] for more results on variable Zagreb indices.

The *generalized Zagreb index* [3] which is a generalization of both ordinary and variable Zagreb indices was introduced in 2011. The generalized Zagreb index $M_{\{r,s\}}(G)$ of a graph G is defined as

$$M_{\{r,s\}}(G) = \sum_{uv\in E(G)} [d_G(u)^r d_G(v)^s + d_G(u)^s d_G(v)^r],$$

where r and s are variable parameters. It is easy to see that, $M_{\{r,s\}}(G) = M_{\{s,r\}}(G)$, $M_{\{0,0\}}(G) = 2\,|E(G)|$ and $M_{\{0,-1\}}(G) = |V(G)|$. Also,

$$M_{\{r-1,0\}}(G) = M_1^{(r)}(G),\ M_{\{r,r\}}(G) = 2M_2^{(r)}(G).$$

In particular,

$$M_{\{1,0\}}(G) = M_1(G),\ M_{\{2,0\}}(G) = F(G),\ M_{\{1,1\}}(G) = 2M_2(G).$$

The *redefined third Zagreb index* was proposed in 2013 by Ranjini *et al.* [28] as

$$ReZG_3(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)[d_G(u) + d_G(v)].$$

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A few years later the same index was proposed in [20] under the name *second Gourava index*. It is easy to see that, $ReZG_3(G) = M_{\{1,2\}}(G)$, so the redefined third Zagreb index can be considered as a special case of the generalized Zagreb index. For more information on the generalized Zagreb index, see the recent papers [11, 17, 18, 23].

Graph products play an important rule in many areas like Human Genetics, a dynamic location problem, networks, etc. [16]. In this paper, we consider the standard graph products namely union, sum, corona product, lexicographic product, direct product, Cartesian product, strong product, disjunction, and symmetric difference and present exact formulae for the values of the generalized Zagreb index for the resulting product graphs. Results are applied to some interesting classes of chemical graphs and nanostructures by specializing components in graph products. Using these results, one can deduce the formulae for the first and second variable Zagreb indices (for nonnegative integer parameters) and the formulae for redefined third Zagreb index of the standard graph products. Moreover, by these results, most parts of the papers [19] and [30] on the first and second Zagreb indices of graph operations and the paper [8] on the F-index of graph operations are generalized. The readers interested in more information on computing topological indices of graph products can be referred to [2, 4, 5, 9, 24, 25].

2. **Results and discussion**

In this section, we compute the generalized Zagreb index $M_{\{r,s\}}$ for standard product graphs where the parameters r and s are considered to be nonnegative integers. We denote the components of each graph product by G_1 and G_2 which are considered to be finite simple graphs without isolated vertices. For a given graph G_i, its vertex and edge sets are denoted by $V(G_i)$ and $E(G_i)$, respectively, and the cardinality of $V(G_i)$ is denoted by n_i, where $i = 1, 2$.

2.1. **Union.** The *union* $\bigcup_{i=1}^{n} G_i$ of graphs $G_1, G_2, \ldots, G_n$ with disjoint vertex sets $V(G_1), V(G_2), \ldots, V(G_n)$ is a graph with the vertex set $\bigcup_{i=1}^{n} V(G_i)$ and the edge set $\bigcup_{i=1}^{n} E(G_i)$. In the case that $G_1 = G_2 = \ldots = G_k = G$, we denote $\bigcup_{i=1}^{n} G_i$ by nG. Let $G = \bigcup_{i=1}^{n} G_i$. It is easy to see that, the degree $d_G(u)$ of a vertex u is equal to the degree of u in the component G_i, $1 \le i \le n$, that contains it.

In the following theorem, an exact formula is obtained for the generalized Zagreb index of the union of $G_1, G_2, \ldots, G_n$. The result follows easily from the definition, so the proof is omitted.

Theorem 2.1.

$$M_{\{r,s\}}(\bigcup_{i=1}^{n} G_i) = \sum_{i=1}^{n} M_{\{r,s\}}(G_i). \tag{2.1}$$

In particular, $M_{\{r,s\}}(nG) = nM_{\{r,s\}}(G)$.

It is clear from Theorem 2.1 that, we can restrict our attention to connected graphs, since for a graph with several connected components its generalized Zagreb index is equal to the product of the indices of its components.

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2.2. **Sum.** The *sum* G_1+G_2 of graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ is a graph union $G_1 \cup G_2$ together with all the edges joining $V(G_1)$ and $V(G_2)$. The sum of two graphs is also known as their *join*. The degree of a vertex u of G_1+G_2 is given by

$$d_{G_1+G_2}(u) = \begin{cases} d_{G_1}(u)+n_2 & u \in V(G_1), \\ d_{G_2}(u)+n_1 & u \in V(G_2). \end{cases}$$

We first consider the case when one of the components in sum is single vertex. For a given graph G, the graph K_1+G is called the *suspension* of G, where K_1 denotes a single vertex. In the following theorem, we compute the generalized Zagreb index of the suspension of graphs.

Theorem 2.2. *Let G be a finite simple graph of order n without isolated vertices. Then*

$$M_{\{r,s\}}(K_1+G) = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}M_{\{i,j\}}(G) + n^s\sum_{i=0}^{r}\binom{r}{i}M_1^{(i)}(G) + n^r\sum_{i=0}^{s}\binom{s}{i}M_1^{(i)}(G). \tag{2.2}$$

Proof. By definition of the generalized Zagreb index,

$$\begin{aligned} M_{\{r,s\}}(K_1+G) &= \sum_{uv\in E(K_1+G)} \left[d_{K_1+G}(u)^r d_{K_1+G}(v)^s + d_{K_1+G}(u)^s d_{K_1+G}(v)^r\right] \\ &= \sum_{uv\in E(G)} \left[\left(d_G(u)+1\right)^r\left(d_G(v)+1\right)^s + \left(d_G(u)+1\right)^s\left(d_G(v)+1\right)^r\right] \\ &\quad + \sum_{u\in V(G)} \left[n^s\left(d_G(u)+1\right)^r + n^r\left(d_G(u)+1\right)^s\right] \\ &= \sum_{uv\in E(G)} \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\left[d_G(u)^i d_G(v)^j + d_{G_1}(u)^j d_G(v)^i\right] \\ &\quad + \sum_{u\in V(G)} \left[n^s\sum_{i=0}^{r}\binom{r}{i}d_G(u)^i + n^r\sum_{i=0}^{s}\binom{s}{i}d_G(u)^i\right], \end{aligned}$$

which is easily transformed into Eq. (2.2). □

Now, we tackle the case when the components in sum are not singleton.

Theorem 2.3.

$$\begin{aligned} M_{\{r,s\}}(G_1+G_2) = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\Big[& n_2^{i+j}M_{\{r-i,s-j\}}(G_1) + n_1^{i+j}M_{\{r-i,s-j\}}(G_2) \\ &+ n_1^j n_2^i M_1^{(r-i)}(G_1)M_1^{(s-j)}(G_2) + n_1^i n_2^j M_1^{(s-j)}(G_1)M_1^{(r-i)}(G_2)\Big]. \end{aligned} \tag{2.3}$$

Proof. By definition of the generalized Zagreb index,

$$M_{\{r,s\}}(G_1+G_2) = \sum_{uv\in E(G_1+G_2)} \left[d_{G_1+G_2}(u)^r d_{G_1+G_2}(v)^s + d_{G_1+G_2}(u)^s d_{G_1+G_2}(v)^r\right].$$

We partition the above sum into three sums as follows.

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The first sum S_1 is taken over all edges $uv \in E(G_1)$,

$$\begin{aligned} S_1 = &\sum_{uv\in E(G_1)} \big[\big(d_{G_1}(u)+n_2\big)^r\big(d_{G_1}(v)+n_2\big)^s+\big(d_{G_1}(u)+n_2\big)^s\big(d_{G_1}(v)+n_2\big)^r\big] \\ = &\sum_{uv\in E(G_1)} [\sum_{i=0}^{r}\binom{r}{i} d_{G_1}(u)^{r-i}n_2^i \sum_{j=0}^{s}\binom{s}{j} d_{G_1}(v)^{s-j}n_2^j \\ &+\sum_{j=0}^{s}\binom{s}{j} d_{G_1}(u)^{s-j}n_2^j \sum_{i=0}^{r}\binom{r}{i} d_{G_1}(v)^{r-i}n_2^i] \\ = &\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j} n_2^{i+j} M_{\{r-i,s-j\}}(G_1). \end{aligned}$$

The second sum S_2 is taken over all edges $uv \in E(G_2)$. By symmetry,

$$S_2 = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j} n_1^{i+j} M_{\{r-i,s-j\}}(G_2).$$

The third sum S_3 is taken over all vertices $u \in V(G_1)$ and $v \in V(G_2)$,

$$S_3 = \sum_{u\in V(G_1)}\sum_{v\in V(G_2)} \big[\big(d_{G_1}(u)+n_2\big)^r\big(d_{G_2}(v)+n_1\big)^s+\big(d_{G_1}(u)+n_2\big)^s\big(d_{G_2}(v)+n_1\big)^r\big].$$

Using the same argument as in the calculation of S_1, we obtain

$$S_3 = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\big[n_1^j n_2^i M_1^{(r-i)}(G_1)M_1^{(s-j)}(G_2)+n_1^i n_2^j M_1^{(s-j)}(G_1)M_1^{(r-i)}(G_2)\big].$$

Eq. (2.3) is obtained by adding the quantities S_1, S_2 and S_3. □

2.3. **Corona product.** The *corona product* $G_1 \circ G_2$ of graphs G_1 and G_2 is a graph obtained by taking one copy of G_1 and n_1 copies of G_2 and joining the ith vertex of G_1 to every vertex in ith copy of G_2, for $i = 1, 2, \ldots, n_1$. We denote the ith copy of G_2 by G_2^i, $1 \le i \le n_1$. The degree of a vertex $u \in V(G_1 \circ G_2)$ is given by

$$d_{G_1\circ G_2}(u) = \begin{cases} d_{G_1}(u)+n_2 & u \in V(G_1), \\ d_{G_2}(u)+1 & u \in V(G_2^i),\ 1 \le i \le n_1. \end{cases}$$

In the following theorem, we compute the generalized Zagreb index of the corona product of G_1 and G_2. The proof follows much in the same way as in the previous case, and we omit it.

Theorem 2.4.

$$\begin{aligned} M_{\{r,s\}}(G_1\circ G_2) = &\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\big[n_2^{r-i+s-j}M_{\{i,j\}}(G_1)+n_1 M_{\{i,j\}}(G_2) \\ &+n_2^{r-i}M_1^{(i)}(G_1)M_1^{(j)}(G_2)+n_2^{s-j}M_1^{(i)}(G_2)M_1^{(j)}(G_1)\big]. \end{aligned} \tag{2.4}$$

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2.4. **Lexicographic product.** The *lexicographic product* $G_1[G_2]$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1)\times V(G_2)$ and vertex (u_1,u_2) is adjacent with vertex (v_1,v_2) whenever u_1 is adjacent with v_1 in G_1 or $u_1=v_1$ and u_2 is adjacent with v_2 in G_2. The lexicographic product of two graphs is also known as their *composition*. The degree of a vertex (u_1,u_2) of $G_1[G_2]$ is given by

$$d_{G_1[G_2]}\big((u_1,u_2)\big)=n_2d_{G_1}(u_1)+d_{G_2}(u_2).$$

Theorem 2.5.

$$M_{\{r,s\}}(G_1[G_2])=\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}n_2^{i+j}\big[M_1^{(i+j)}(G_1)M_{\{r-i,s-j\}}(G_2)+M_{\{i,j\}}(G_1)M_1^{(r-i)}(G_2)M_1^{(s-j)}(G_2)\big]. \tag{2.5}$$

Proof. By definition of the generalized Zagreb index,

$$M_{\{r,s\}}(G_1[G_2])=\sum_{(u_1,u_2)(v_1,v_2)\in E(G_1[G_2])}\big[d_{G_1[G_2]}\big((u_1,u_2)\big)^r d_{G_1[G_2]}\big((v_1,v_2)\big)^s + d_{G_1[G_2]}\big((u_1,u_2)\big)^s d_{G_1[G_2]}\big((v_1,v_2)\big)^r\big].$$

We partition the above sum into two sums S_1 and S_2.

The first sum S_1 is taken over all edges $(u_1,u_2)(v_1,v_2)\in E(G_1[G_2])$ such that $u_1\in V(G_1)$ and $u_2v_2\in E(G_2)$,

$$\begin{aligned}S_1&=\sum_{u_1\in V(G_1)}\sum_{u_2v_2\in E(G_2)}\big[\big(n_2d_{G_1}(u_1)+d_{G_2}(u_2)\big)^r\big(n_2d_{G_1}(u_1)+d_{G_2}(v_2)\big)^s\\&\quad+\big(n_2d_{G_1}(u_1)+d_{G_2}(u_2)\big)^s\big(n_2d_{G_1}(u_1)+d_{G_2}(v_2)\big)^r\big]\\&=\sum_{u_1\in V(G_1)}\sum_{u_2v_2\in E(G_2)}\Big[\sum_{i=0}^{r}\binom{r}{i}n_2^id_{G_1}(u_1)^id_{G_2}(u_2)^{r-i}\sum_{j=0}^{s}\binom{s}{j}n_2^jd_{G_1}(u_1)^jd_{G_2}(v_2)^{s-j}\\&\quad+\sum_{j=0}^{s}\binom{s}{j}n_2^jd_{G_1}(u_1)^jd_{G_2}(u_2)^{s-j}\sum_{i=0}^{r}\binom{r}{i}n_2^id_{G_1}(u_1)^id_{G_2}(v_2)^{r-i}\Big]\\&=\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}n_2^{i+j}M_1^{(i+j)}(G_1)M_{\{r-i,s-j\}}(G_2).\end{aligned}$$

The second sum S_2 is taken over all edges $(u_1,u_2)(v_1,v_2)\in E(G_1[G_2])$ such that $u_1v_1\in E(G_1)$ and $u_2,v_2\in V(G_2)$,

$$\begin{aligned}S_2=\sum_{u_1v_1\in E(G_1)}\sum_{u_2\in V(G_2)}\sum_{v_2\in V(G_2)}&\big[\big(n_2d_{G_1}(u_1)+d_{G_2}(u_2)\big)^r\big(n_2d_{G_1}(v_1)+d_{G_2}(v_2)\big)^s\\&+\big(n_2d_{G_1}(u_1)+d_{G_2}(u_2)\big)^s\big(n_2d_{G_1}(v_1)+d_{G_2}(v_2)\big)^r\big].\end{aligned}$$

Using the same argument as in the calculation of S_1, we obtain

$$S_2=\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}n_2^{i+j}M_{\{i,j\}}(G_1)M_1^{(r-i)}(G_2)M_1^{(s-j)}(G_2).$$

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Eq. (2.5) is obtained by adding the quantities S_1 and S_2. □

2.5. **Direct product.** The *direct product* $G_1 \times G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1)\times V(G_2)$ and two vertices (u_1,u_2) and (v_1,v_2) are adjacent if and only if $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$. The direct product of two graphs is also known as their *tensor product*, *Kronecker product*, *categorical product*, *cardinal product*, *relational product*, or *conjunction*. The degree of a vertex (u_1,u_2) of $G_1 \times G_2$ is given by

$$d_{G_1\times G_2}\big((u_1,u_2)\big) = d_{G_1}(u_1)d_{G_2}(u_2).$$

Theorem 2.6.

$$M_{\{r,s\}}(G_1 \times G_2) = M_{\{r,s\}}(G_1)M_{\{r,s\}}(G_2). \tag{2.6}$$

Proof. By definition of the generalized Zagreb index,

$$\begin{aligned}
M_{\{r,s\}}(G_1 \times G_2) = &\sum_{(u_1,u_2)(v_1,v_2)\in E(G_1\times G_2)} \Big[d_{G_1\times G_2}\big((u_1,u_2)\big)^r d_{G_1\times G_2}\big((v_1,v_2)\big)^s \\
&+ d_{G_1\times G_2}\big((u_1,u_2)\big)^s d_{G_1\times G_2}\big((v_1,v_2)\big)^r\Big] \\
= &\sum_{u_1v_1\in E(G_1)} \sum_{u_2v_2\in E(G_2)} \Big[\big(d_{G_1}(u_1)d_{G_2}(u_2)\big)^r\big(d_{G_1}(v_1)d_{G_2}(v_2)\big)^s \\
&+ \big(d_{G_1}(u_1)d_{G_2}(u_2)\big)^s\big(d_{G_1}(v_1)d_{G_2}(v_2)\big)^r \\
&+ \big(d_{G_1}(u_1)d_{G_2}(v_2)\big)^r\big(d_{G_1}(v_1)d_{G_2}(u_2)\big)^s \\
&+ \big(d_{G_1}(u_1)d_{G_2}(v_2)\big)^s\big(d_{G_1}(v_1)d_{G_2}(u_2)\big)^r\Big] \\
= &\sum_{u_1v_1\in E(G_1)} \Big[d_{G_1}(u_1)^r d_{G_1}(v_1)^s + d_{G_1}(u_1)^s d_{G_1}(v_1)^r\Big] \\
&\sum_{u_2v_2\in E(G_2)} \Big[d_{G_2}(u_2)^r d_{G_2}(v_2)^s + d_{G_2}(u_2)^s d_{G_2}(v_2)^r\Big] \\
= &M_{\{r,s\}}(G_1)M_{\{r,s\}}(G_2),
\end{aligned}$$

and Eq. (2.6) holds. □

Note that Eq. (2.6) remains valid if r and s are arbitrary real numbers.

2.6. **Cartesian product.** The *Cartesian product* $G_1 \Box G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1)\times V(G_2)$ and two vertices (u_1,u_2) and (v_1,v_2) are adjacent if and only if $[u_1 = v_1$ and $u_2v_2 \in E(G_2)]$ or $[u_2 = v_2$ and $u_1v_1 \in E(G_1)]$. The degree of a vertex (u_1,u_2) of $G_1 \Box G_2$ is given by

$$d_{G_1\Box G_2}\big((u_1,u_2)\big) = d_{G_1}(u_1) + d_{G_2}(u_2).$$

Theorem 2.7.

$$M_{\{r,s\}}(G_1 \Box G_2) = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\big[M_{\{r-i,s-j\}}(G_1)M_1^{(i+j)}(G_2) + M_{\{r-i,s-j\}}(G_2)M_1^{(i+j)}(G_1)\big]. \tag{2.7}$$

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Proof. By definition of the generalized Zagreb index,

$$M_{\{r,s\}}(G_1\Box G_2) = \sum_{(u_1,u_2)(v_1,v_2)\in E(G_1\Box G_2)} \Big[d_{G_1\Box G_2}\big((u_1,u_2)\big)^r d_{G_1\Box G_2}\big((v_1,v_2)\big)^s + d_{G_1\Box G_2}\big((u_1,u_2)\big)^s d_{G_1\Box G_2}\big((v_1,v_2)\big)^r\Big].$$

We partition the above sum into two sums S_1 and S_2.

The first sum S_1 is taken over all edges $(u_1,u_2)(v_1,v_2) \in E(G_1\Box G_2)$ such that $u_1v_1 \in E(G_1)$ and $u_2 = v_2$,

$$\begin{aligned} S_1 &= \sum_{u_1v_1\in E(G_1)}\sum_{u_2\in V(G_2)} \Big[\big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)^r\big(d_{G_1}(v_1)+d_{G_2}(u_2)\big)^s \\ &\quad + \big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)^s\big(d_{G_1}(v_1)+d_{G_2}(u_2)\big)^r\Big] \\ &= \sum_{u_1v_1\in E(G_1)}\sum_{u_2\in V(G_2)}\sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j}\Big[d_{G_1}(u_1)^{r-i}d_{G_1}(v_1)^{s-j}d_{G_2}(u_2)^{i+j} \\ &\quad + d_{G_1}(u_1)^{s-j}d_{G_1}(v_1)^{r-i}d_{G_2}(u_2)^{i+j}\Big] \\ &= \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j} M_{\{r-i,s-j\}}(G_1)M_1^{(i+j)}(G_2). \end{aligned}$$

The second sum S_2 is taken over all edges $(u_1,u_2)(v_1,v_2) \in E(G_1\Box G_2)$ such that $u_1 = v_1$ and $u_2v_2 \in E(G_2)$. By symmetry,

$$S_2 = \sum_{i=0}^{r}\sum_{j=0}^{s}\binom{r}{i}\binom{s}{j} M_{\{r-i,s-j\}}(G_2)M_1^{(i+j)}(G_1).$$

Eq. (2.7) is obtained by adding the quantities S_1 and S_2. □

2.7. **Strong product.** The *strong product* $G_1 \boxtimes G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1,u_2) and (v_1,v_2) are adjacent if and only if $[u_1 = v_1 \textit{ and } u_2v_2 \in E(G_2)]$ or $[u_2 = v_2 \textit{ and } u_1v_1 \in E(G_1)]$ or $[u_1v_1 \in E(G_1) \textit{ and } u_2v_2 \in E(G_2)]$. The strong product of two graphs is also known as their *normal product* or *AND product*. The degree of a vertex (u_1,u_2) of $G_1 \boxtimes G_2$ is given by

$$d_{G_1\boxtimes G_2}\big((u_1,u_2)\big) = d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2).$$

Theorem 2.8.

$$\begin{aligned} M_{\{r,s\}}(G_1\boxtimes G_2) &= \sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k}\binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l}\Big[M_{\{r-j,s-l\}}(G_1)M_1^{(i+k)}(G_2) \\ &\quad + M_{\{r-j,s-l\}}(G_2)M_1^{(i+k)}(G_1) + M_{\{r-j,s-l\}}(G_1)M_{\{i,k\}}(G_2)\Big]. \end{aligned} \tag{2.8}$$

Proof. By definition of the generalized Zagreb index,

$$M_{\{r,s\}}(G_1 \boxtimes G_2) = \sum_{(u_1,u_2)(v_1,v_2)\in E(G_1\boxtimes G_2)} \left[d_{G_1\boxtimes G_2}\big((u_1,u_2)\big)^r d_{G_1\boxtimes G_2}\big((v_1,v_2)\big)^s + d_{G_1\boxtimes G_2}\big((u_1,u_2)\big)^s d_{G_1\boxtimes G_2}\big((v_1,v_2)\big)^r\right].$$

We partition the above sum into three sums S_1, S_2 and S_3.

The first sum S_1 is taken over all edges $(u_1,u_2)(v_1,v_2) \in E(G_1 \boxtimes G_2)$ such that $u_1v_1 \in E(G_1)$ and $u_2 = v_2$,

$$\begin{aligned}
S_1 = &\sum_{u_1v_1\in E(G_1)} \sum_{u_2\in V(G_2)} \Big[\big(d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(u_1)d_{G_2}(u_2)\big)^r \big(d_{G_1}(v_1)+d_{G_2}(u_2)+d_{G_1}(v_1)d_{G_2}(u_2)\big)^s \\
&+ \big(d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(u_1)d_{G_2}(u_2)\big)^s \big(d_{G_1}(v_1)+d_{G_2}(u_2)+d_{G_1}(v_1)d_{G_2}(u_2)\big)^r\Big] \\
= &\sum_{u_1v_1\in E(G_1)} \sum_{u_2\in V(G_2)} [\sum_{i=0}^{r}\binom{r}{i} d_{G_1}(u_1)^{r-i} \sum_{j=0}^{i}\binom{i}{j} d_{G_2}(u_2)^j d_{G_1}(u_1)^{i-j} d_{G_2}(u_2)^{i-j} \\
&\sum_{k=0}^{s}\binom{s}{k} d_{G_1}(v_1)^{s-k} \sum_{l=0}^{k}\binom{k}{l} d_{G_2}(u_2)^l d_{G_1}(v_1)^{k-l} d_{G_2}(u_2)^{k-l} \\
&+ \sum_{k=0}^{s}\binom{s}{k} d_{G_1}(u_1)^{s-k} \sum_{l=0}^{k}\binom{k}{l} d_{G_2}(u_2)^l d_{G_1}(u_1)^{k-l} d_{G_2}(u_2)^{k-l} \\
&\sum_{i=0}^{r}\binom{r}{i} d_{G_1}(v_1)^{r-i} \sum_{j=0}^{i}\binom{i}{j} d_{G_2}(u_2)^j d_{G_1}(v_1)^{i-j} d_{G_2}(u_2)^{i-j}] \\
= &\sum_{u_1v_1\in E(G_1)} \sum_{u_2\in V(G_2)} \sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k} \binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l} \big[d_{G_1}(u_1)^{r-j} d_{G_1}(v_1)^{s-l} d_{G_2}(u_2)^{i+k} \\
&+ d_{G_1}(u_1)^{s-l} d_{G_1}(v_1)^{r-j} d_{G_2}(u_2)^{i+k}\big] \\
= &\sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k} \binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l} M_{\{r-j,s-l\}}(G_1) M_1^{(i+k)}(G_2).
\end{aligned}$$

The second sum S_2 is taken over all edges $(u_1,u_2)(v_1,v_2) \in E(G_1 \boxtimes G_2)$ such that $u_1 = v_1$ and $u_2v_2 \in E(G_2)$. By symmetry,

$$S_2 = \sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k} \binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l} M_{\{r-j,s-l\}}(G_2) M_1^{(i+k)}(G_1).$$

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The third sum S_3 is taken over all edges $(u_1,u_2)(v_1,v_2)\in E(G_1\boxtimes G_2)$ such that $u_1v_1\in E(G_1)$ and $u_2v_2\in E(G_2)$,

$$S_3=\sum_{u_1v_1\in E(G_1)}\sum_{u_2v_2\in E(G_2)}\Big[\big(d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(u_1)d_{G_2}(u_2)\big)^r\big(d_{G_1}(v_1)+d_{G_2}(v_2)+d_{G_1}(v_1)d_{G_2}(v_2)\big)^s$$
$$+\big(d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(u_1)d_{G_2}(u_2)\big)^s\big(d_{G_1}(v_1)+d_{G_2}(v_2)+d_{G_1}(v_1)d_{G_2}(v_2)\big)^r$$
$$+\big(d_{G_1}(v_1)+d_{G_2}(u_2)+d_{G_1}(v_1)d_{G_2}(u_2)\big)^r\big(d_{G_1}(u_1)+d_{G_2}(v_2)+d_{G_1}(u_1)d_{G_2}(v_2)\big)^s$$
$$+\big(d_{G_1}(v_1)+d_{G_2}(u_2)+d_{G_1}(v_1)d_{G_2}(u_2)\big)^s\big(d_{G_1}(u_1)+d_{G_2}(v_2)+d_{G_1}(u_1)d_{G_2}(v_2)\big)^r\Big].$$

Using the same argument as in the calculation of S_1, we obtain

$$S_3=\sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k}\binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l}M_{\{r-j,s-l\}}(G_1)M_{\{i,k\}}(G_2).$$

Eq. (2.8) is obtained by adding the quantities S_1, S_2 and S_3. □

2.8. **Disjunction.** The *disjunction* $G_1\vee G_2$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1)\times V(G_2)$ and vertex (u_1,u_2) is adjacent with vertex (v_1,v_2) whenever $u_1v_1\in E(G_1)$ or $u_2v_2\in E(G_2)$ or both. The disjunction of two graphs is also known as their *co-normal product* or *OR product*. The degree of a vertex (u_1,u_2) of $G_1\vee G_2$ is given by

$$d_{G_1\vee G_2}\big((u_1,u_2)\big)=n_2d_{G_1}(u_1)+n_1d_{G_2}(u_2)-d_{G_1}(u_1)d_{G_2}(u_2).$$

Using the same argument as in the proof of Theorem 2.8, we can get the following result.

Theorem 2.9.

$$M_{\{r,s\}}(G_1\vee G_2)=\sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k}\binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l}(-1)^{l+j}n_1^{i-j+k-l}n_2^{r-i+s-k}\big[M_{\{r-i+j,s-k+l\}}(G_1)$$
$$M_1^{(i)}(G_2)M_1^{(k)}(G_2)+M_{\{i,k\}}(G_2)M_1^{(r-i+j)}(G_1)M_1^{(s-k+l)}(G_1)$$
$$-M_{\{r-i+j,s-k+l\}}(G_1)M_{\{i,k\}}(G_2)\big].$$

2.9. **Symmetric difference.** The *symmetric difference* $G_1\oplus G_2$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1)\times V(G_2)$ and vertex (u_1,u_2) is adjacent with vertex (v_1,v_2) whenever $u_1v_1\in E(G_1)$ or $u_2v_2\in E(G_2)$ but not both. The degree of a vertex $(u_1,u_2)\in V(G_1\oplus G_2)$ is given by

$$d_{G_1\oplus G_2}\big((u_1,u_2)\big)=n_2d_{G_1}(u_1)+n_1d_{G_2}(u_2)-2d_{G_1}(u_1)d_{G_2}(u_2).$$

In the following theorem, the generalized Zagreb index of $G_1\oplus G_2$ is computed. The proof follows much in the same way as in the previous cases, and we omit it.

Theorem 2.10.

$$M_{\{r,s\}}(G_1 \oplus G_2) = \sum_{i=0}^{r}\sum_{j=0}^{i}\sum_{k=0}^{s}\sum_{l=0}^{k}\binom{r}{i}\binom{i}{j}\binom{s}{k}\binom{k}{l}(-2)^{l+j}n_1^{i-j+k-l}n_2^{r-i+s-k}\big[M_{\{r-i+j,s-k+l\}}(G_1) M_1^{(i)}(G_2)M_1^{(k)}(G_2) + M_{\{i,k\}}(G_2)M_1^{(r-i+j)}(G_1)M_1^{(s-k+l)}(G_1) - 2M_{\{r-i+j,s-k+l\}}(G_1)M_{\{i,k\}}(G_2)\big].$$

3. Examples and applications

In this section, we find exact formulae for the generalized Zagreb index of some classes of chemical graphs, especially for some nanotubes and nanotori, by specializing components in graph products.

Let P_n, C_n and K_n denote the $n-$vertex path, cycle, and complete graph, respectively. It is easy to see that,

$$M_{\{r,s\}}(P_n) = \begin{cases} 2 & n = 2, \\ 2^{r+1} + 2^{s+1} + (n-3)2^{r+s+1} & n \geq 3, \end{cases}$$
$$M_{\{r,s\}}(C_n) = n2^{r+s+1}, \quad M_{\{r,s\}}(K_n) = n(n-1)^{r+s+1}.$$

Example 3.1 The *fan graph* F_{n+1} on $n+1$ vertices is the suspension of P_n. Using Eq. (2.2), we obtain

$$M_{\{r,s\}}(F_{n+1}) = M_{\{r,s\}}(K_1 + P_n) = 2^{r+1}(3^s + n^s) + 2^{s+1}(3^r + n^r) + (n-2)(3^r n^s + 3^s n^r) + 2(n-3)3^{r+s}, \quad n \geq 3.$$

Example 3.2 The *wheel graph* W_{n+1} on $n+1$ vertices is the suspension of C_n. Using Eq. (2.2), we obtain

$$M_{\{r,s\}}(W_{n+1}) = M_{\{r,s\}}(K_1 + C_n) = n\big[2 \times 3^{r+s} + 3^r n^s + 3^s n^r\big].$$

Example 3.3 The *windmill graph* $D_n^{(m)}$ is the graph obtained by taking m copies of K_{n-1} with a vertex in common. The case $n = 3$ therefore corresponds to the *Dutch windmill graph*. One can easily see that, the windmill graph $D_n^{(m)}$ is the suspension of mK_{n-1}. Using Eq. (2.1), we obtain

$$M_{\{r,s\}}(mK_{n-1}) = mM_{\{r,s\}}(K_{n-1}) = m(n-1)(n-2)^{r+s+1}.$$

Now by Eq. (2.2), the generalized Zagreb index of the windmill graph $D_n^{(m)}$ is equal to

$$M_{\{r,s\}}(D_n^{(m)}) = (n-1)^{r+s+1}[m^{r+1} + m^{s+1} + m(n-2)].$$

In particular, for the Dutch windmill graph, we obtain

$$M_{\{r,s\}}(D_3^{(m)}) = 2^{r+s+1}m(m^r + m^s + 1).$$

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Example 3.4 For a given graph G, the graph $K_2 \circ G$ is called the *bottleneck graph* of G. Let $|V(G)| = n$. Using Eq. (2.4), the generalized Zagreb index of $K_2 \circ G$ is given by

$$M_{\{r,s\}}(K_2 \circ G) = 2(n+1)^{r+s} + 2(n+1)^r \sum_{i=0}^{r} \binom{r}{i} M_1^{(i)}(G) + 2(n+1)^s \sum_{i=0}^{s} \binom{s}{i} M_1^{(i)}(G) + 2 \sum_{i=0}^{r} \sum_{j=0}^{s} \binom{r}{i}\binom{s}{j} M_{\{i,j\}}(G).$$

In particular, for the bottleneck graph of P_n, we obtain

$$M_{\{r,s\}}(K_2 \circ P_n) = 2(n+1)^{r+s} + 2(n+1)^r \left[2^{r+1} + (n-2)3^r\right] + 2(n+1)^s \left[2^{s+1} + (n-2)3^s\right] + 2^{s+2}3^r + 2^{r+2}3^s + 4(n-3)3^{r+s}, \qquad n \geq 3.$$

Example 3.5 Using Eq. (2.5), we can obtain the generalized Zagreb index of the *fence graph* $P_n[P_2]$ and *closed fence graph* $C_n[P_2]$. For $n \geq 3$,

$$M_{\{r,s\}}(P_n[P_2]) = (10n - 28)5^{r+s} + 4 \times 3^{r+s} + 8(5^r 3^s + 5^s 3^r)$$

and

$$M_{\{r,s\}}(C_n[P_2]) = 2n5^{r+s+1}.$$

Example 3.6 Let $G = P_n \square P_m$ be the *rectangular grid*. Using Eq. (2.7), we obtain

$$M_{\{r,s\}}(G) = (n+m-4)(2^{2s+1}3^r + 2^{2r+1}3^s) + 2^{s+3}3^r + 2^{r+3}3^s + 4(n+m-6)3^{r+s} + (2nm - 5n - 5m - 12)2^{2r+2s+1}, \quad n, m \geq 3.$$

The graph $P_2 \square P_{n+1}$ made by n squares is called the *ladder graph* on $2n + 2$ vertices and denoted by L_n. This graph is also the molecular graph related to polyomino structures and called the *linear polyomino chain*. By the above formula, the generalized Zagreb index of the linear polyomino chain is given by

$$M_{\{r,s\}}(L_n) = (n-1)(2^{2s+1}3^r + 2^{2r+1}3^s) + 2^{s+3}3^r + 2^{r+3}3^s + 4(n-3)3^{r+s} - (n+23)2^{2r+2s+1}, \quad n \geq 3.$$

Example 3.7 Let $R = P_n \square C_m$. Then $R = TUC_4(m, n)$ is a C_4-*nanotube*. By Eq. (2.7),

$$M_{\{r,s\}}(R) = m[4 \times 3^{r+s} + 2^{2r+1}3^s + 2^{2s+1}3^r + (2n-5)2^{2r+2s+1}], \quad n \geq 3.$$

Example 3.8 Let $S = C_n \square C_m$. Then $S = TC_4(m, n)$ is a C_4-*nanotorus*. By Eq. (2.7),

$$M_{\{r,s\}}(S) = nm4^{r+s+1}.$$

Example 3.9 A graph Q_T is said to be a *quasi multi-walled nanotorus*, if it is isomorphic to the Cartesian product of a path and an arbitrary nanotorus T. Let T be a nanotorus such that the degree of all of its vertices is 3. Then

$$M_{\{r,s\}}(T) = 2 \times 3^{r+s} e,$$

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where $e = |E(T)|$. Let $Q^k_T = P_k \square T$ be the quasi multi-walled nanotorus related to T. By Eq. (2.7),

$$M_{\{r,s\}}(Q^k_T) = \frac{e}{3}\big[3 \times 4^{r+s+1} + 4^{s+1}5^r + 4^{r+1}5^s + (10k-24)5^{r+s}\big],\ k \geq 3.$$

In particular, let $G = TUZC_6(p,q)$ be an arbitrary *zigzag polyhex nanotube*, where p is the number of horizontal hexagons in each row and q is the number of horizontal zigzag lines in the molecular graph of G. Let $T = TZC_6(p,q)$ be the nanotorus related to G. It is easy to see that, the degree of all vertices of this nanotorus is equal to 3 and $|E(T)| = 3pq$. So, by our calculation,

$$M_{\{r,s\}}(Q^k_T) = pq[3 \times 4^{r+s+1} + 4^{s+1}5^r + 4^{r+1}5^s + (10k-24)5^{r+s}], \quad k \geq 3.$$

4. Concluding remarks

The generalized Zagreb index is a degree-based graph invariant that generalizes much used ordinary and variable Zagreb indices. In this paper, we study this invariant under several graph products and apply our results to compute it for some classes of graphs by specializing components in graph products. However, much work still needs to be done. For example, one could try to establish some extremal graphs with respect to the generalized Zagreb index in a given class of graphs in which some graph parameters are fixed. It would also be interesting to find some relations between the generalized Zagreb index and other topological indices.

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