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The first and second Zagreb indices of some graph operations

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ABSTRACT

In this paper some exact expressions for the first and second Zagreb indices of graph operations containing the Cartesian product, composition, join, disjunction and symmetric difference of graphs will be presented. We apply some of our results to compute the Zagreb indices of arbitrary C_4 tube, C_4 torus and q-multi-walled polyhex nanotorus.

1. Introduction

Throughout this paper we consider only simple connected graphs, i.e. connected graphs without loops and multiple edges. For a graph G, $V(G)$ and $E(G)$ denote the set of all vertices and edges, respectively. For a graph G, the degree of a vertex v is the number of edges incident to v and denoted by $\deg_G(v)$.

A topological index $Top(G)$ of a graph G, is a number with this property that for every graph H isomorphic to G, $Top(H) = Top(G)$. The Wiener index is the first and most studied topological indices, both from theoretical point of view and applications. It is equal to the sum of distances between all pairs of vertices of the respective graph, see for details [3,4,19].

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic, [6]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2,$$

$$M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v).$$

We encourage the reader to consult [1,7,16,22–24] for historical background, computational techniques and mathematical properties of Zagreb indices.

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If $G_1, G_2, \ldots, G_n$ are graphs then we denote $G_1 \times \cdots \times G_n$ by $\bigotimes_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\bigotimes_{i=1}^{n} G_i$ by G^n. The Wiener index of the Cartesian product graphs

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was studied in [5,17]. In [15], Klavzar, Rajapakse and Gutman computed the Szeged index of the Cartesian product graphs. The present authors, [10–14,20], computed some exact formulae for the hyper-Wiener, vertex PI, edge Wiener, edge PI and edge Szeged indices of some graph operations.

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. If $G = \underbrace{H + \cdots + H}_{n \text{ times}}$ then we denote G by nH.

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V_1 \times V_2$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or ($u_1 = u_2$ and v_1 is adjacent with v_2), see [8, p. 185].

The disjunction $G \vee H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ and (u_1, v_1) is adjacent with (u_2, v_2) whenever $u_1u_2 \in E(G)$ or $v_1v_2 \in E(H)$.

The symmetric difference $G \oplus H$ of two graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $E(G \oplus H) = \{(u_1, u_2)(v_1, v_2) \mid u_1v_1 \in E(G) \text{ or } u_2v_2 \in E(H) \text{ but not both}\}$. In [17], Sagan et al. computed some exact formulae for the Wiener polynomial of various graph operations containing Cartesian product, composition, join, disjunction and symmetric difference of graphs. In [10], the present authors computed vertex and edge PI indices of the join and composition of graphs. Here the Padmakar–Ivan (PI) index of a graph G is defined as $\mathrm{PI}(G) = \sum_{e \in E(G)} [n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ denotes the number of edges lying closer to the vertex u than the vertex v, and $n_{ev}(e|G)$ is the number of edges lying closer to the vertex v than the vertex u. In this definition, edges equidistant from both ends of the edge $e = uv$ are not counted, see for detail [20,9]. The aim of this paper is to continue this program for computing the Zagreb indices of these operations on graphs.

Throughout this paper our notation is standard and taken mainly from [2,18]. K_n denotes a complete graph on n vertices. IF H and G are graphs in which $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ then we call H to be a subgraph of G. H is called a spanning subgraph of G, if $V(H) = V(G)$. If H is a spanning subgraph of G then we write $H \leq_{ss} G$. A graph G is called to be quasi multi-walled nanotorus (q-multi-walled nanotorus as short), if G is isomorphic to the Cartesian product of a path P_n and an arbitrary nanotorus T, see [21].

2. The first Zagreb index of graph operations

In this section, some exact formulae for the first Zagreb index of the Cartesian product, composition, join, disjunction and symmetric difference of graphs are presented. We begin with the following crucial lemma related to distance properties of some graph operations.

Lemma 1. *Let G and H be graphs. Then we have:*

(a)

$$\begin{aligned} |V(G \times H)| &= |V(G \vee H)| = |V(G[H])| \\ &= |V(G \oplus H)| = |V(G)||V(H)|, \\ |E(G \times H)| &= |E(G)||V(H)| + |V(G)||E(H)|, \\ |E(G + H)| &= |E(G)| + |E(H)| + |V(G)||V(H)|, \\ |E(G[H])| &= |E(G)||V(H)|^2 + |E(H)||V(G)|, \\ |E(G \vee H)| &= |E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 2|E(G)||E(H)|, \\ |E(G \oplus H)| &= |E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 4|E(G)||E(H)|. \end{aligned}$$

(b) *$G \times H$ is connected if and only if G and H are connected,*
(c) *If (a, c) and (b, d) are vertices of $G \times H$ then $d_{G \times H}((a, c), (b, d)) = d_G(a, b) + d_H(c, d)$,*
(d) *The Cartesian product, join, composition, disjunction and symmetric difference of graphs are associative and all of them are commutative except from composition.*
(e)

$$d_{G+H}(u, v) = \begin{cases} 0 & u = v \\ 1 & uv \in E(G) \text{ or } uv \in E(H) \text{ or} \\ & (u \in V(G)\ \&\ v \in V(H)) \\ 2 & \text{otherwise}, \end{cases}$$

(f)

$$d_{G[H]}((a, b), (c, d)) = \begin{cases} d_G(a, c) & a \neq c \\ 0 & a = c\ \&\ b = d \\ 1 & a = c\ \&\ bd \in E(H) \\ 2 & a = c\ \&\ bd \notin E(H), \end{cases}$$

(g)

$$d_{G\vee H}((a,b),(c,d)) = \begin{cases} 0 & a=c\ \&\ b=d \\ 1 & ac\in E(G) \text{ or } bd\in E(H) \\ 2 & \text{otherwise}, \end{cases}$$

(h)

$$d_{G\oplus H}((a,b),(c,d)) = \begin{cases} 0 & a=c\ \&\ b=d \\ 1 & ac\in E(G) \text{ or } bd\in E(H) \text{ but not both} \\ 2 & \text{otherwise}, \end{cases}$$

(i) $\deg_{G\times H}((a,b)) = \deg_G(a) + \deg_H(b)$,
(j) $\deg_{G[H]}((a,b)) = |V(H)|\deg_G(a) + \deg_H(b)$,
(k)

$$\deg_{G+H}(a) = \begin{cases} \deg_G(a) + |V(H)| & a\in V(G) \\ \deg_H(a) + |V(G)| & a\in V(H), \end{cases}$$

(l) $\deg_{G\vee H}((a,b)) = |V(H)|\deg_G(a) + |V(G)|\deg_H(b) - \deg_G(a)\deg_H(b)$,
(m) $\deg_{G\oplus H}((a,b)) = |V(H)|\deg_G(a) + |V(G)|\deg_H(b) - 2\deg_G(a)\deg_H(b)$.

Proof. The parts (a–e) are consequence of definitions and some well-known results of the book of Imrich and Klavzar, [8]. For the proof of (f–m) we refer to [13]. □

From now on, we write $\deg(u)$ as $\deg_G(u)$, if there is no confusion.

Theorem 1. *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$ and $E_i = E(G_i)$, $1 \le i \le n$, and $V = V(\bigotimes_{i=1}^n G_i)$. Then $M_1\left(\bigotimes_{i=1}^n G_i\right) = |V|\sum_{i=1}^n \frac{M_1(G_i)}{|V_i|} + 4|V|\sum_{i\neq j, i,j=1}^n \frac{|E_i||E_j|}{|V_i||V_j|}$. In particular, $M_1(G^n) = n|V(G)|^{n-2}(M_1(G)|V(G)| + 4(n-1)|E(G)|^2)$.*

Proof. We first prove the case $n = 2$. By Lemma 1(i), $\deg_{G_1\times G_2}(a,b) = \deg_{G_1}(a) + \deg_{G_2}(b)$. So, $M_1(G_1\times G_2) = \sum_{a\in V_1}\sum_{b\in V_2}[\deg_{G_1}(a)^2 + \deg_{G_2}(b)^2 + 2\deg_{G_1}(a)\deg_{G_2}(b)] = |V_1|M_1(G_2) + |V_2|M_1(G_2) + 8|E_1||E_2|$. On the other hand, by Lemma 1(a) and an inductive argument, one can see that $|E(\bigotimes_{i=1}^n G_i)| = |V|\sum_{i=1}^n \frac{|E_i|}{|V_i|}$ and $|V| = \prod_{i=1}^n |V_i|$. We now apply Lemma 1(d) to deduce that

$$\begin{aligned} M_1\left(\bigotimes_{i=1}^{n} G_i\right) &= M_1\left(\bigotimes_{i=1}^{n-1} G_i \times G_n\right) \\ &= |V|\sum_{i=1}^{n-1}\frac{M_1(G_i)}{|V_i|} + 4|V|\sum_{i\neq j, i,j=1}^{n-1}\frac{|E_i||E_j|}{|V_i||V_j|} + \frac{|V|}{|V_n|}M_1(G_n) + 8\left|E\left(\bigotimes_{i=1}^{n-1} G_i\right)\right||E_n| \\ &= |V|\sum_{i=1}^{n}\frac{M_1(G_i)}{|V_i|} + 4|V|\sum_{i\neq j, i,j=1}^{n}\frac{|E_i||E_j|}{|V_i||V_j|}. \end{aligned}$$

The second part is a simple substitution of above equation. □

It is easy to see that $M_1(C_n) = 4n$, $n \ge 3$, $M_1(P_1) = 0$ and $M_1(P_n) = 4n-6$, $n > 1$. Furthermore, if G is a connected graph with n vertices, then $M_1(G) \le (n-1)^2 n$, with equality if and only if G is isomorphic to a complete graph with n vertices. Suppose T_n denotes the set of all trees with exactly n vertices. Then it is easy to see that the path P_n and the star S_n have the minimum and maximum of M_1 in T_n, respectively. On the other hand, if H is a subgraph of G then $M_1(H) \le M_1(G)$. Therefore, the minimum of M_1 on the set of all connected graphs with n vertices is the same as the minimum of M_1 on $T(n)$. This implies that P_n and K_n take the minimum and maximum Zagreb index M_1 on the set of all connected graphs with n vertices.

Example 1. Consider the graph G whose vertices are the N-tuples $b_1b_2\cdots b_N$ with $b_i \in \{0, 1, \ldots, n_i - 1\}$, $n_i \ge 2$, and let two vertices be adjacent if the corresponding tuples differ in precisely one place. Such a graph is called a Hamming graph. It is well-known fact that a graph G is a Hamming graph if and only if it can be written in the form $G = \bigotimes_{i=1}^N K_{n_i}$ and so the Hamming graph G is usually denoted as $H_{n_1,\ldots,n_N}$. Apply the previous theorem to compute the first Zagreb index of a Hamming graph. Then $M_1(G) = M_1(\bigotimes_{i=1}^N K_{n_i}) = (\prod_{i=1}^N n_i)(\sum_{i=1}^N (n_i - 1))^2$. The case that $n_1 = n_2 = \cdots = n_N = 2$, the graph G is well-knows as a hypercube of dimension N and denoted by Q_N. By our calculation, $M_1(Q_N) = N^2 2^N$.

Example 2. In [20], the authors computed PI index of C_4 tubes and tori. In this example, we compute the first Zagreb index of these molecular graphs. Suppose R and S denote a C_4 tube and torus, respectively. Then $R = P_n \times C_m$ and $S = C_k \times C_m$, $k, m \ge 3$ and $n \ge 2$. By above calculations and Theorem 1, we have $M_1(R) = 16mn - 14m$ and $M_1(S) = 16mk$.

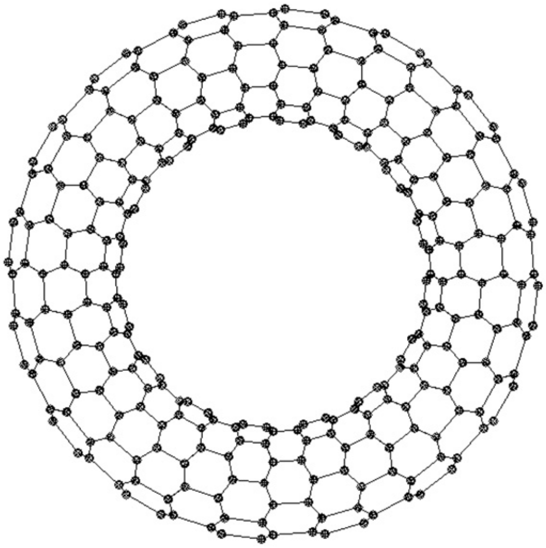

Fig. 1. The graph of a nanotorus.

Example 3. Let $T = T[p, q]$ be the molecular graph of a nanotorus, Fig. 1. Then T has exactly pq vertices, $3/2(pq)$ edges, $M_1(T) = 9|V(T)|$ and for a q-multi-walled nanotorus $G = P_n \times T$, $M_1(G) = (13n-6)|V(T)|+8(n-1)|E(T)| = pq(25n-18)$.

Theorem 2. *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$, $E_i = E(G_i)$, $1 \le i \le n$, $G = G_1 + G_2 + \cdots + G_n$ and $V = V(G)$. Then*

$$M_1(G) = \sum_{i=1}^{n}(M_1(G_i) + |V_i|(|V| - |V_i|)^2 + 4|E_i|(|V| - |V_i|)).$$

In particular, $M_1(nH) = nM_1(H) + n(n-1)^2|V(H)|^3 + 4n(n-1)|E(H)||V(H)|$.

Proof. By Lemma 1(d), $G \cong G_i + (G_1 + \cdots G_{i-1} + G_{i+1} + \cdots + G_n)$ and $|V| = \sum_{i=1}^{n} |V_i|$. So $\deg_G(v) = \deg_{G_i}(v) + |V| - |V_i|$, for each $v \in V_i$. Thus $M_1(G) = \sum_{i=1}^{n} \sum_{j=1}^{|V_i|}(\deg_{G_i}(v_j) + \sum_{k\neq i,k=1}^{n} |V_k|)^2 = \sum_{i=1}^{n}(M_1(G_i) + |V_i|(|V| - |V_i|)^2 + 4|E_i|(|V| - |V_i|))$. The second part is a direct consequence of above equation. □

Example 4. Consider a complete n-partite graph $G = K_{m_1,m_2,\ldots,m_n}$ containing $v = |V(G)|$ vertices, Fig. 2. By definition of this graph, $V = V(G)$ can be partitioned into subsets $V_1, V_2, \ldots, V_n$ of V such that for every i, $1 \le i \le n$, there is no edge between the vertices of V_i. It is easy to see that $K_{m_1,m_2,\ldots,m_n}$ is the join of n empty graphs $G_1, \ldots, G_n$ with exactly $m_1, \ldots, m_n$ vertices, respectively. So by previous theorem $M_1(K_{m_1,m_2,\ldots,m_n}) = (\sum m_i)^3 + \sum m_i^3 - 2(\sum m_i)(\sum m_i^2)$.

Theorem 3. *Let G and H be graphs. Then*

(a)

$$M_1(G[H]) = |V(H)|^3 M_1(G) + |V(G)|M_1(H) + 8|V(H)||E(H)||E(G)|,$$

(b)

$$M_1(G \vee H) = (|V(G)||V(H)|^2 - 4|E(H)||V(H)|)M_1(G) + M_1(H)M_1(G) + (|V(H)||V(G)|^2 - 4|E(G)||V(G)|)M_1(H) + 8|E(G)||E(H)||V(G)||V(H)|,$$

(c)

$$M_1(G \oplus H) = (|V(G)||V(H)|^2 - 8|E(H)||V(H)|)M_1(G) + 4M_1(G)M_1(H) + (|V(H)||V(G)|^2 - 8|E(G)||V(G)|)M_1(H) + 8|E(G)||E(H)||V(G)||V(H)|.$$

Proof. Apply Lemma 1(j), we have $M_1(G[H]) = \sum_{a\in V(G)} \sum_{b\in V(H)}[|V(H)|^2 \deg_G(a)^2 + 2|V(H)| \deg_G(a) \deg_H(b) + \deg_H(b)^2] = |V(H)|^3 M_1(G) + |V(G)| M_1(H) + 8|V(H)||E(H)||E(G)|$. To prove (b) and (c) it is enough to apply Lemma 1(l & m) and similar arguments as above. □

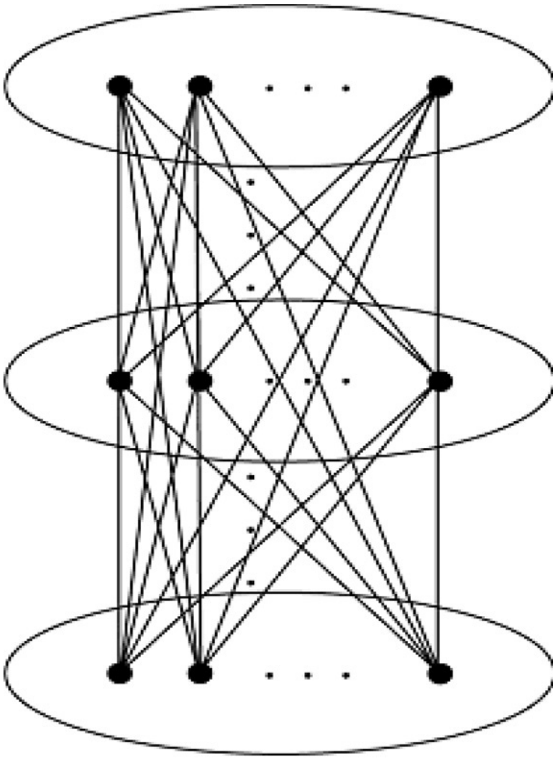

Fig. 2. The complete n-partite graph.

The line graph $L(G)$ of a graph G is a graph such that each vertex of $L(G)$ represents an edge of G and any two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G. Suppose $L^0(G) = G, L^1(G) = L(G)$ and $L^n(G) = L(L^{n-1}(G))$. Then we have $2|E(L^n(G))| = M_1(L^{n-1}(G)) - 2|E(L^{n-1}(G))|$. To see this, we notice that every edge of $L^{n-1}(G)$ is a vertex of $L^n(G)$ and so $\sum_{v\in V(L^n(G))} \deg_{L^n(G)}(v) = \sum_{uv\in E(L^{n-1}(G))}[\deg_{L^{n-1}(G)}(u) + \deg_{L^{n-1}(G)}(v) - 2] = M_1(L^{n-1}(G)) - 2|E(L^{n-1}(G))|$. Thus using the values of $M_1(G), M_1(L(G)), \ldots, M_1(L^{n-1}(G))$, one can compute the size of $E(L(G)), E(L^2(G)), \ldots, E(L^n(G))$.

In the end of this section we prove a simple inequality between $PI(G)$, $M_1(G)$ and $|E(L(G))|$. To do this, we assume that $V(G) = \{v_1, v_2, \ldots, v_n\}$. Then

$$\begin{aligned} PI(G) &= \sum_{e\in E(G)} [n_{eu}(e|G) + n_{ev}(e|G)] \\ &\geq \sum_{uv\in E(G)} (\deg(v) + \deg(u) - 2) \\ &= \sum_{i=1}^{n} \deg(v_i)^2 - 2|E(G)| \\ &= M_1(G) - 2|E(G)| = 2|E(L(G))|. \end{aligned}$$

3. The second Zagreb index of graph operations

In this section, the second Zagreb index of the Cartesian product, composition, join and disjunction of graphs are investigated. We begin again with the Cartesian product of graphs.

Theorem 4. *Let G and H be graphs. Then* $M_2(G \times H) = |V(G)|M_2(H) + |V(H)|M_2(G) + 3|E(H)|M_1(G) + 3|E(G)|M_1(H)$.

Proof. By Lemma 1(i),

$$\begin{aligned} M_2(G \times H) &= \sum_{(a,b)(c,d)\in E(G\times H)} \deg_{G\times H}(a, b) \deg_{G\times H}(c, d) \\ &= \sum_{u\in V(G)} \sum_{bd\in E(H)} (\deg_G(u) + \deg_H(b))(\deg_G(u) + \deg_H(d)) \end{aligned}$$

$$+\sum_{v\in V(H)}\sum_{ac\in E(G)}(\deg_G(a)+\deg_H(v))(\deg_G(c)+\deg_H(v))$$
$$=|V(G)|M_2(H)+|V(H)|M_2(G)+3|E(H)|M_1(G)+3|E(G)|M_1(H).\quad\square$$

A graph G is called r-regular, if for every $u,v\in V(G)$, $\deg(u)=\deg(v)=r$. It is clear that if G is r-regular then $M_2(G)=\frac{r}{2}M_1(G)=\frac{nr^3}{2}$, where $n=|V(G)|$. In the special case that $r=n-1$ or 2, we have $M_2(K_n)=\frac{n(n-1)^3}{2}$ and $M_2(C_n)=M_1(C_n)=4n$. On the other hand, $M_2(P_n)=4(n-2)$, $n>2$. Moreover, $M_2(P_1)=0$ and $M_2(P_2)=1$.

Corollary. Let $G_1,G_2,\ldots,G_n$ be graphs with $V_i=V(G_i)$ and $E_i=E(G_i)$, $1\le i\le n$, and $V=V(\bigotimes_{i=1}^n G_i)$ and $E=E(\bigotimes_{i=1}^n G_i)$. Then $M_2\left(\bigotimes_{i=1}^n G_i\right)=|V|\sum_{i=1}^n(\frac{M_2(G_i)}{|V_i|}+3M_1(G_i)(\frac{|E|}{|V_i|}-\frac{|V||E_i|}{|V_i|^2}))+4|V|\sum_{\substack{i,j,k=1\\ i\ne j,i\ne k,j\ne k}}^n\frac{|E_i||E_j||E_k|}{|V_i||V_j||V_k|}$. In particular, $M_2(H^n)=n|V(H)|^{n-3}(|V(H)|^2M_2(G)+3(n-1)|E(H)||V(H)|M_1(H)+4(n-1)(n-2)|E(H)|^3)$.

Proof. By Theorems 1 and 4 and an inductive argument, we have

$$M_2\left(\bigotimes_{i=1}^{n+1}G_i\right)=M_2\left(\bigotimes_{i=1}^{n}G_i\times G_{n+1}\right)$$
$$=|V_{n+1}|\left(|V|\sum_{i=1}^n\frac{M_2(G_i)}{|V_i|}+\sum_{i=1}^n 3M_1(G_i)\left(\frac{|E|}{|V_i|}-\frac{|V||E_i|}{|V_i|^2}\right)+4|V|\sum_{\substack{i,j,k=1\\ i\ne j,i\ne k,j\ne k}}^n\frac{|E_i||E_j||E_k|}{|V_i||V_j||V_k|}\right)$$
$$+|V|M_2(G_{n+1})+3|E|M_1(G_{n+1})+3|E_{n+1}|\left(|V|\sum_{i=1}^n\frac{M_1(G_i)}{|V_i|}+4|V|\sum_{i\ne j,i,j=1}^n\frac{|E_i||E_j|}{|V_i||V_j|}\right)$$
$$=|V||V_{n+1}|\sum_{i=1}^{n+1}\left[\frac{M_2(G_i)}{|V_i|}+3M_1(G_i)\left(\frac{|V_{n+1}||E|+|E_{n+1}||V|}{|V_i|}-\frac{|V||V_{n+1}||E_i|}{|V_i|^2}\right)\right]$$
$$+4|V||V_{n+1}|\sum_{\substack{i,j,k=1\\ i\ne j,i\ne k,j\ne k}}^{n+1}\frac{|E_i||E_j||E_k|}{|V_i||V_j||V_k|}.$$

For the second part, it is enough to substitute $G_1,\ldots,G_n$ by H. $\square$

Example 5. In Example 2, we compute the first Zagreb index of C_4 tubes and tori. In this example, the second Zagreb index of these molecular graphs are computed. With notation as Example 1, we have $M_2(R)=32mn-38n$ and $M_2(S)=32mk$, $m,n,k\ge 3$.

Example 6. In Example 1, the first Zagreb index of Hamming graphs are computed. By previous corollary, one can see that

$$M_2(H_{m_1,m_2,\ldots,m_n})=\frac{\prod_{i=1}^n m_i}{2}\left(\sum_{i=1}^n(m_i-1)^3+3\sum_{i\ne j,i,j=1}^n m_i(m_i-1)(m_j-1)\right)$$
$$+\frac{\prod_{i=1}^n m_i}{2}\left(\sum_{\substack{i,j,k=1\\ i\ne j,i\ne k,j\ne k}}^n(m_i-1)(m_j-1)(m_k-1)\right).$$

Example 7. Let $T=T[p,q]$ be the molecular graph of a nanotorus, Fig. 1. Then $M_2(T)=9|E(T)|=\frac{27}{2}pq$ and for a q-multi-walled nanotorus $G(n)=P_n\times T$, $M_2(G(n))=(31n-35)|V(T)|+(21n-18)|E(T)|=\frac{pq}{2}(125n-124)$, when $n>2$. On the other hand, $M_2(G(1))=\frac{27}{2}pq$ and $M_2(G(2))=24|E(T)|+28|V(T)|=64pq$.

Theorem 5. *Let $G_1,G_2,\ldots,G_n$ be graphs with $V_i=V(G_i)$, $E_i=E(G_i)$, $1\le i\le n$, $G=G_1+G_2+\cdots+G_n$ and $V=V(G)$. Then*

$$M_2(G)=\sum_{i=1}^n[M_2(G_i)+(|V|-|V_i|)(M_1(G_i)+(|V|-|V_i|)|E_i|)]-\frac{1}{2}\sum_{i=1}^n[2|E_i|+|V_i|(|V|-|V_i|)]^2$$
$$+\frac{1}{2}\left[\sum_{i=1}^n(2|E_i|+|V_i|(|V|-|V_i|))\right]^2.$$

In particular, if $G_1 = \cdots = G_n = H$ *then* $M_2(nH) = nM_2(H)+n(n-1)|V(H)|(M_1(H)+(n-1)|V(H)||E(H)|)+\binom{n}{2}(2|E(H)|+(n-1)|V(H)|^2)^2$.

Proof. There are two type of edges in $G_1 + \cdots + G_n$. Both of the ends of a first type edge belong to G_i, for some i. An edge of second type connects a vertex of G_i to a vertex of G_j, $i \neq j$. So by Lemma 1(k) and this fact that $G \cong G_i + (G_1 + \cdots G_{i-1} + G_{i+1} + \cdots + G_n)$, $\deg_G(v) = \deg_{G_i}(v) + |V| - |V_i|$, for each $v \in V_i$. Thus

$$\begin{aligned} M_2(G) &= \sum_{ab\in E} \deg_G(a)\deg_G(b) \\ &= \sum_{i=1}^{n}\sum_{uv\in E_i}(\deg_{G_i}(u) + |V| - |V_i|)(\deg_{G_i}(v) + |V| - |V_i|) \\ &\quad + \frac{1}{2}\sum_{i\neq j,i,j=1}^{n}\sum_{u\in V_i}\sum_{v\in V_j}(\deg_{G_i}(u) + |V| - |V_i|)(\deg_{G_j}(v) + |V| - |V_j|) \\ &= \sum_{i=1}^{n}(M_2(G_i) + (|V| - |V_i|)M_1(G_i) + |E_i|(|V| - |V_i|)^2) \\ &\quad + \frac{1}{2}\sum_{i\neq j,i,j=1}^{n}[2|E_i| + |V_i|(|V| - |V_i|)][2|E_j| + |V_j|(|V| - |V_j|)], \end{aligned}$$

as desired. The second part is a direct consequence of above equation. □

Example 8. Consider a complete n-partite graph $G = K_{m_1,m_2,\ldots,m_n}$ containing $v = |V(G)|$ vertices. By definition, $K_{m_1,m_2,\ldots,m_n}$ is the join of n empty graphs $G_1, \ldots, G_n$ with exactly $m_1, \ldots, m_n$ vertices, respectively. So by Theorem 5, $M_2(K_{m_1,m_2,\ldots,m_n}) = \binom{\frac{(\sum_{i=1}^{n} m_i)^2-\sum_{i=1}^{n} m_i^2}{2}}{2}$.

Theorem 6. *Let G and H be graphs. Then*

(a)

$$M_2(G[H]) = |V(H)|^4M_2(G) + |V(G)|M_2(H) + 3|V(H)|^2|E(H)||M_1(G)| + 2|V(H)||E(G)|M_1(H) + 4|E(G)||E(H)|^2,$$

(b)

$$\begin{aligned} M_2(G \vee H) &= ((|V(G)|^2 - 2|E(G)|)^2 - 2|V(G)|^2|E(G)|)M_2(H) \\ &\quad + ((|V(H)|^2 - 2|E(H)|)^2 - 2|V(H)|^2|E(H)|)M_2(G) \\ &\quad + (2|V(G)|^2|V(H)||E(G)| - 4|E(G)|^2|V(H)|)M_1(H) \\ &\quad + (2|V(H)|^2|V(G)||E(H)| - 4|E(H)|^2|V(G)|)M_1(G) \\ &\quad - |V(G)||V(H)|M_1(H)M_1(G) + 2|V(H)|M_2(G)M_1(H) \\ &\quad + 2|V(G)|M_2(H)M_1(G) - 2M_2(H)M_2(G) + 4|E(H)||E(G)|(|V(H)|^2|E(G)| + |V(G)|^2|E(H)|). \end{aligned}$$

Proof. (a) By Lemma 1(j),

$$\begin{aligned} M_2(G[H]) &= \sum_{w\in V(G)}\sum_{uv\in E(H)}(|V(H)|\deg_G(w) + \deg_H(u))(|V(H)|\deg_G(w) + \deg_H(v)) \\ &\quad + \sum_{ab\in E(G)}\sum_{v\in V(H)}\sum_{u\in V(H)}(|V(H)|\deg_G(a) + \deg_H(u))(|V(H)|\deg_G(b) + \deg_H(v)) \\ &= |V(H)|^4M_2(G) + |V(G)|M_2(H) + 3|V(H)|^2|E(H)||M_1(G)| + 2|V(H)||E(G)|M_1(H) + 4|E(G)||E(H)|^2. \end{aligned}$$

(b) By Lemma 1(l), we have

$$\begin{aligned} M_2(G \vee H) &= \sum_{a\in V(G)}\sum_{c\in V(G)}\sum_{bd\in E(H)}\deg_{G\vee H}(a,b)\deg_{G\vee H}(c,d) + \sum_{b\in V(H)}\sum_{d\in V(H)}\sum_{ac\in E(G)}\deg_{G\vee H}(a,b)\deg_{G\vee H}(c,d) \\ &\quad - 2\sum_{ac\in E(G)}\sum_{bd\in E(H)}\deg_{G\vee H}(a,b)\deg_{G\vee H}(c,d) \\ &= \sum_{a\in V(G)}\sum_{c\in V(G)}\sum_{bd\in E(H)}[|V(G)||V(H)|(\deg_G(a)\deg_H(d) + \deg_H(b)\deg_G(c)) + \deg_G(a)\deg_G(c)\deg_H(b)\deg_H(d) \\ &\quad + |V(H)|^2\deg_G(a)\deg_G(c) + |V(G)|^2\deg_H(b)\deg_H(d) - |V(H)|\deg_G(a)\deg_G(c)(\deg_H(d) + \deg_H(b)) \end{aligned}$$

$$- |V(G)| \deg_H(b) \deg_H(d)(\deg_G(a) + \deg_G(c))] + \sum_{b\in V(H)} \sum_{d\in V(H)} \sum_{ac\in E(G)} [|V(G)||V(H)|(\deg_G(a) \deg_H(d)$$
$$+ \deg_H(b) \deg_G(c)) + \deg_G(a) \deg_G(c) \deg_H(b) \deg_H(d) + |V(H)|^2 \deg_G(a) \deg_G(c) + |V(G)|^2 \deg_H(b) \deg_H(d)$$
$$- |V(H)| \deg_G(a) \deg_G(c)(\deg_H(d) + \deg_H(b)) - |V(G)| \deg_H(b) \deg_H(d)(\deg_G(a) + \deg_G(c))]$$
$$- \sum_{ac\in E(G)} \sum_{bd\in E(H)} [|V(G)||V(H)|(\deg_G(a) + \deg_H(d))(\deg_H(b) + \deg_G(c)) + 2 \deg_G(a) \deg_G(c) \deg_H(b) \deg_H(d)$$
$$+ 2|V(H)|^2 \deg_G(a) \deg_G(c) + 2|V(G)|^2 \deg_H(b) \deg_H(d) - 2|V(H)| \deg_G(a) \deg_G(c)(\deg_H(d) + \deg_H(b))$$
$$- 2|V(G)| \deg_H(b) \deg_H(d)(\deg_G(a) + \deg_G(c))],$$

which completes the proof. □

Finally, using a similar method, one can prove the following exact formula for the second Zagreb index of symmetric difference of graphs:

Theorem 7. *Let G and H be graphs. Then*

$$\begin{aligned} M_2(G \oplus H) = {} & ((|V(G)|^2 - 2|E(G)|)^2 - 4|V(G)|^2|E(G)|)M_2(H) + ((|V(H)|^2 - 2|E(H)|)^2 - 4|V(H)|^2|E(H)|)M_2(G) \\ & + (2|V(G)|^2|V(H)||E(G)| - 8|E(G)|^2|V(H)|)M_1(H) + (2|V(H)|^2|V(G)||E(H)| - 8|E(H)|^2|V(G)|)M_1(G) \\ & - 2|V(G)||V(H)|M_1(H)M_1(G) + 8|V(H)|M_2(G)M_1(H) \\ & + 8|V(G)|M_2(H)M_1(G) - 16M_2(H)M_2(G) + 4|E(H)||E(G)|(|V(H)|^2|E(G)| + |V(G)|^2|E(H)|) \end{aligned}$$

We end the paper with the following simple but elegant lemma:

Lemma 2. *Let H be a subgraph of G then $M_1(H) \le M_1(G)$ and $M_2(H) \le M_2(G)$.*

Using Lemma 2, one can see that for arbitrary connected graphs G and H, since $G \times H \le_{ss} G[H] \le_{ss} G \vee H$, $M_1(G \times H) \le M_1(G[H]) \le M_1(G \vee H)$, $M_2(G \times H) \le M_2(G[H]) \le M_2(G \vee H)$, $M_1(G \times H) \le M_1(H[G]) \le M_1(G \vee H)$ and $M_2(G\times H) \le M_2(H[G]) \le M_2(G\vee H)$. On the other hand, $G\times H \le_{ss} G\oplus H \le_{ss} G\vee H$ and so $M_1(G\times H) \le M_1(G\oplus H) \le M_1(G\vee H)$ and $M_2(G \times H) \le M_2(G \oplus H) \le M_2(G \vee H)$. By previous lemma, clearly K_n has the maximum Zagreb index M_2 on the set of all connected graphs with n vertices. It is also easy to prove the path P_n and the star S_n have the minimum and maximum of M_2 between n-vertex trees, respectively. Therefore, by Lemma 2, the minimum of M_2 on the set of all connected graphs with n vertices is the same as the minimum of M_2 on n-vertex trees.

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