

THIRD ZAGREB INDICES AND ITS COINDICES OF TWO CLASSES OF GRAPHS

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ABSTRACT. In this paper, we compute the formulae for the third Zagreb indices and its coindices for two classes of graphs such as edge corona product graph, double graph and k^{th} iterated double graph.

1. Introduction

Throughout this paper we consider simple and connected graphs. Let $d_G(v)$ be the degree of a vertex v in G . A *chemical graph* is a graph whose vertices denote atoms and edges denote bonds between those atoms of any underlying chemical structure. A *topological index* for a (chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. Topological indices and graph invariants based on the distances between vertices of a graph or vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications. These indices may be used to derive quantitative structure-property or structure-activity relationships (QSPR/QSAR). The Wiener index is the first and most studied topological indices, both from theoretical point of view and applications.

For a (molecular) graph G , The *first Zagreb index* $M_1(G)$ is the equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* $M_2(G)$ is the equal to the sum of the products of the degrees of pairs of adjacent

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vertices, that is,

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

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

The *first* and *second Zagreb coindices* were first introduced by Ashrafi et al. [2]. They are defined as follows:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v)), \quad \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v).$$

The *third Zagreb index* of a graph G is defined as

$$M_3(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

This graph invariant is also known as *irregularity* of G , see [1, 9, 6]. The *third Zagreb coindex* was introduced by Veylaki et al. [8]. This index of G is defined as

$$\overline{M}_3(G) = \sum_{uv \notin E(G)} |d_G(u) - d_G(v)|.$$

Khalifeh et al. [4] obtained the first and second Zagreb indices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs. Ashrafi et al. [2] obtained the first and second Zagreb coindices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs. In [7, 5], the hyper and third Zagreb indices of some graph operations are obtained. In [8], the mathematical properties for the third and hyper-Zagreb coindices of graph operations containing the Cartesian product and composition are explained. In this paper, we compute the formulae for the third Zagreb indices and its coindices of edge corona product graph, double graph and k^{th} iterated double graph.

2. Edge corona product

Hou and Shiu [3] introduced a kind of new graph operation, namely, edge corona product. The *edge corona product* $G \bullet H$ of G and H is defined as the graph obtained by taking one copy of G and p copies of H , and then joining two end vertices of the i^{th} edge of G to every vertex in the i^{th} copy of H . In [3], the adjacency spectrum and Laplacian spectrum of edge corona product of G and H were presented in terms of the spectrum and Laplacian spectrum of G and H , respectively. Now we compute the third Zagreb index and its coindex of edge corona product of two graphs.

THEOREM 2.1. *Let G and H be two connected graphs with n_1 and n_2 vertices, m_1 and m_2 edges, respectively. Then*

$$M_3(G \bullet H) \leq (n_2 + 1)M_3(G) + m_1M_3(H) + n_2(n_2 + 1)M_1(G) + 2m_1(m_2 + n_2).$$

PROOF. By the definition of edge corona product, for each vertex $x \in V(G)$, we have

$$G \bullet H(x) = d_G(x)(|V(H)| + 1)$$

and for each vertex $y \in V(H_i)$, $d_{G \bullet H}(y) = d_H(y) + 2$. Clearly,

$$|V(G \bullet H)| = |V(G)| + |E(G)||V(H)|.$$

By the definition of third Zagreb index

$$\begin{aligned} M_3(G \bullet H) &= \sum_{xy \in E(G \bullet H)} |d_{G \bullet H}(x) - d_{G \bullet H}(y)| \\ &= \sum_{xy \in E(G)} |(n_2 + 1)d_G(x) - (n_2 + 1)d_G(y)| \\ &+ \sum_{i=1}^{m_1} \sum_{xy \in E(H)} |d_H(x) + 2 - (d_H(y) + 2)| \\ &+ \sum_{xy \in E(G)} \sum_{u \in V(H)} |((n_2 + 1)d_G(x) + (n_2 + 1)d_G(y)) - (d_H(u) + 2)| \\ &\leq (n_2 + 1)^2 \sum_{xy \in E(G)} |d_G(x) - d_G(y)| + m_1 \sum_{xy \in E(H)} |d_H(x) - d_H(y)| \\ &+ \sum_{xy \in E(G)} \sum_{u \in V(H)} (n_2 + 1)(d_G(x) + d_G(y) + \sum_{xy \in E(G)} \sum_{u \in V(H)} (d_H(u) + 2)) \\ &= (n_2 + 1)M_3(G) + m_1M_3(H) + n_2(n_2 + 1)M_1(G) + 2m_1(m_2 + n_2). \end{aligned}$$

□

THEOREM 2.2. *Let G and H be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$\begin{aligned} \overline{M}_3(G \bullet H) &= \\ &= m_1 \overline{M}_3(H) + (n_2 + 1) \overline{M}_3(H) + n_2(n_2 + 1)M_1(G) + \\ &+ 2(m_2 + n_2)(n_1^2 - 2m_1) - 2n_1n_2m_1(n_2 + 1). \end{aligned}$$

PROOF. Let x_{ij} be the j th vertex in the i th copy of H , $i = 1, 2, \dots, m_1, j = 1, 2, \dots, n_2$, and let y_k be the k th in $G, k = 1, 2, \dots, n_1$. Also let x_j be the j th vertex in H .

By the definition of edge corona, for each vertex x_{ij} , we have

$$d_{G \bullet H}(x_{ij}) = d_H(x_j) + 2$$

and for every vertex y_k in G we have

$$d_{G \bullet H}(y_k) = d_G(y_k)n_2 + d_G(y_k) = (n_2 + 1)d_G(y_k).$$

Now, we consider the following four cases of nonadjacent vertex pairs in $G \bullet H$.

Case 1: The nonadjacent vertex pairs $\{x_{ij}; x_{ih}\}$, $1 \leq i \leq m_1, 1 \leq j < h \leq n_2$, and it is assumed that $x_jx_h \notin E(H)$.

$$\begin{aligned} \sum_{i=1}^{m_1} \sum_{x_{ij}x_{ih} \notin E(G \bullet H)} |d_{G \bullet H}(x_{ij}) - d_{G \bullet H}(x_{ih})| &= \sum_{i=1}^{m_1} \sum_{x_jx_h \notin E(H)} |d_H(x_j) + 2 - d_H(x_h) - 2| \\ &= m_1 \overline{M}_3(H). \end{aligned}$$

Case 2: The nonadjacent vertex pairs $\{y_k, y_s\}, 1 \leq k < s \leq n_1$ and it is assumed that $y_k y_s \notin E(G)$.

$$\begin{aligned} \sum_{y_k y_s \notin E(G \bullet H)} |d_{G \bullet H}(y_k) - d_{G \bullet H}(y_s)| &= \sum_{y_k y_s \notin E(G)} |(n_2 + 1)d_G(y_k) - (n_2 + 1)d_G(y_s)| \\ &= (n_2 + 1)\overline{M}_3(G). \end{aligned}$$

Case 3: The nonadjacent vertex pairs $\{x_{ij}, y_k\}, 1 \leq i \leq m_1, 1 \leq j \leq n_2, 1 \leq k \leq n_1$, and it is assumed that the i th edge $e_i, 1 \leq i \leq m_1$ in G does not pass through y_k .

Note that each vertex y_k is adjacent to all vertices of $d_G(y_k)$ copies of H , that is, each y_k is not adjacent to any vertex of $m_1 - d_G(y_k)$ copies of H . Hence

$$\begin{aligned} \sum_{j=1}^{n_2} |d_H(x_j) + 2 - (n_2 + 1)d_G(y_k)| &\leq \sum_{j=1}^{n_2} (d_H(x_j) + 2 - (n_2 + 1)d_G(y_k)) \\ (2.1) \qquad \qquad \qquad &= 2m_2 + 2n_2 - (n_2 + 1)n_2 d_G(y_k). \end{aligned}$$

Note that each vertex y_k is adjacent to all vertices of $d_G(y_k)$ copies of H , that is, each y_k is not adjacent to any vertex of $m_1 - d_G(y_k)$ copies of H . Hence

$$\begin{aligned} \sum_{j=1}^{n_2} |d_H(x_j) + 2 - (n_2 + 1)d_G(y_k)| &\leq \sum_{j=1}^{n_2} (d_H(x_j) + 2 - (n_2 + 1)d_G(y_k)) \\ (2.2) \qquad \qquad \qquad &= 2m_2 + 2n_2 - (n_2 + 1)n_2 d_G(y_k). \end{aligned}$$

Case 4: The nonadjacent vertex pairs $\{x_{ij}, x_{\ell h}\}, 1 \leq i < \ell \leq m_1, 1 \leq j, h \leq n_2$.

$$\begin{aligned} \sum_{x_{ij} x_{\ell h} \notin E(G \bullet H)} |d_{G \bullet H}(x_{ij}) - d_{G \bullet H}(x_{\ell h})| &= \frac{m_1(m_1 - 1)}{2} \sum_{j=1}^{n_2} \sum_{h=1}^{n_2} |d_H(x_j) - d_H(x_h)| \\ &\leq \frac{m_1(m_1 - 1)}{2} \sum_{j=1}^{n_2} (n_2 d_H(x_j) - 2m_2) = 0. \end{aligned}$$

From the above four cases of nonadjacent vertex pairs, we can obtain the desired result. This completes the proof. \square

2.1. Double and its k^{th} iteration graphs. Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$. The vertices of the double graph G^* are given by the two sets $X = \{x_1, x_2, \dots, x_n\}$ and $Y = \{y_1, y_2, \dots, y_n\}$. Thus for each vertex $v_i \in V(G)$, there are two vertices x_i and y_i in $V(G^*)$. The *double graph* G^* includes the initial edge set of each copies of G , and for any edge $v_i v_j \in E(G)$, two more edges $x_i y_j$ and $x_j y_i$ are added. For a given vertex v in G , let

$$D_G(v) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v)).$$

In this section, we compute the third Zagreb index and its coindex of double graph and its iterated graph.

THEOREM 2.3. *Let G be a connected graph with n vertices and m edges. Then $\overline{M}_3(G^*) = 8\overline{M}_3(G)$.*

PROOF. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Suppose that x_i and y_i are the corresponding clone vertices, in G^* , of v_i for each $i = 1, 2, \dots, n$. For any given vertex v_i in G and its clone vertices x_i and y_i , there exists $d_{G^*}(x_i) = d_{G^*}(y_i) = 2d_G(v_i)$ by the definition of double graph.

For $v_i, v_j \in V(G)$, if $v_i v_j \notin E(G)$, then

$$x_i x_j \notin E(G), y_i y_j \notin E(G), x_i y_j \notin E(G) \text{ and } y_i x_j \notin E(G).$$

So we need only to consider total contribution of the following three types of nonadjacent vertex pairs to calculate $\overline{M}_3(G)$.

Case 1: The nonadjacent vertex pairs $\{x_i, x_j\}$ and $\{y_i, y_j\}$, where $v_i v_j \notin E(G)$.

$$\begin{aligned} \sum_{y_i y_j \notin E(G^*)} |d_{G^*}(y_i) - d_{G^*}(y_j)| &= \sum_{x_i x_j \notin E(G^*)} |d_{G^*}(x_i) - d_{G^*}(x_j)| \\ &= \sum_{v_i v_j \notin E(G)} |2d_G(v_i) - 2d_G(v_j)| \\ &= 2\overline{M}_3(G). \end{aligned}$$

Case 2: The nonadjacent vertex pairs $\{x_i, y_i\}$ for each $i = 1, 2, \dots, n$.

$$\sum_{i=1}^n |d_{G^*}(x_i) - d_{G^*}(y_i)| = \sum_{i=1}^n |2d_G(v_i) - 2d_G(v_i)| = 0.$$

Case 3: The nonadjacent vertex pairs $\{x_i, y_j\}$ and $\{y_i, x_j\}$, where $v_i v_j \notin E(G)$.

For each x_i , there exist $n - 1 - d_G(v_i)$ vertices in the set $\{y_1, y_2, \dots, y_n\}$, among which every vertex together with x_i compose a nonadjacent vertex pairs of G^* . The total contribution of these $n - 1 - d_G(v_i)$ nonadjacent vertex pairs to calculate $M_3(G^*)$ is

$$\begin{aligned} \sum_{x_i y_j \notin E(G^*)} |d_{G^*}(x_i) - d_{G^*}(y_j)| &= \sum_{v_i v_j \notin E(G^*)} |2d_G(v_i) - 2d_G(v_j)| \\ &= 2D_G(v_i). \end{aligned}$$

Hence

$$\begin{aligned} \sum_{i \neq j, x_i y_j \notin E(G^*)} |d_{G^*}(x_i) - d_{G^*}(y_j)| &= \sum_{i=1}^n 2D_G(v_i) \\ &= 4\overline{M}_3(G). \end{aligned}$$

Hence

$$\begin{aligned} \overline{M}_3(G^*) &= \sum_{x_i x_j \notin E(G^*)} |d_{G^*}(x_i) - d_{G^*}(x_j)| + \sum_{y_i y_j \notin E(G^*)} |d_{G^*}(y_i) - d_{G^*}(y_j)| \\ &+ \sum_{i=1}^n |d_{G^*}(x_i) - d_{G^*}(y_i)| + \sum_{i \neq j, x_i y_j \notin E(G^*)} |d_{G^*}(x_i) - d_{G^*}(y_j)| \\ &= 8\overline{M}_3(G). \end{aligned}$$

□

THEOREM 2.4. *Let G be a simple connected graph and let G^{k*} be its k^{th} iterated double graph. Then $\overline{M}_3(G^{k*}) = 8^k \overline{M}_3(G)$.*

PROOF. Let G be a simple connected graph with n vertices m edges. Then the number of vertices and edges of G^* are $2n$ and $4m$. From the structure of G^{k*} , $|V(G^{k*})| = 2^k n$ and $|E(G^{k*})| = 4^k m$.

By Theorem 2.3, and the definition of k^{th} iterated double graph, for $k \geq 1$, we have $\overline{M}_3(G^{k*}) = 8\overline{M}_3(G^{(k-1)*})$.

By the recursive relations, we obtain

$$\begin{aligned} \overline{M}_3(G^{k*}) &= 8\overline{M}_3(G^{(k-1)*}) = 8\left(8\overline{M}_3(G^{(k-2)*})\right) = 8^2\overline{M}_3(G^{(k-2)*}) = 8^3\overline{M}_3(G^{(k-2)*}) \\ &\dots \\ &\overline{M}_3(G^{k*}) = 8^k \overline{M}_3(G). \end{aligned}$$

□

Next we obtain the third Zagreb indices of G^* and G^{k*} .

THEOREM 2.5. *The third Zagreb index of the double graph G^* of a graph G is given by $M_3(G^*) = 8M_3(G)$.*

PROOF. From the definition of double graph it is clear that

$$d_{G^*}(x_i) = d_{G^*}(y_i) = 2d_G(v_i),$$

where $v_i \in V(G)$ and $x_i, y_i \in V(G^*)$ are corresponding clone vertices of v_i . Therefore

$$\begin{aligned} M_3(G^*) &= \sum_{uv \in E(G^*)} |d_{G^*}(u) - d_{G^*}(v)| \\ &= \sum_{x_i x_j \in E(G^*)} |d_{G^*}(x_i) - d_{G^*}(x_j)| + \sum_{y_i y_j \in E(G^*)} |d_{G^*}(y_i) - d_{G^*}(y_j)| \\ &+ \sum_{x_i y_j \in E(G^*)} |d_{G^*}(x_i) - d_{G^*}(y_j)| + \sum_{x_j y_i \in E(G^*)} |d_{G^*}(x_j) - d_{G^*}(y_i)| \\ &= 4 \sum_{v_i v_j \in E(G)} |2d_G(v_i) - 2d_G(v_j)| \\ &= 8M_3(G). \end{aligned}$$

□

A similar argument of Theorem 2.4, we have the following.

THEOREM 2.6. *The third Zagreb index of the k^{th} iterated double graph G^{k*} is $M_3(G^{k*}) = 8^k M_3(G)$.*

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