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More on Zagreb coindices of graphs

Hongbo Hua[a], Ali Reza Ashrafi[b,c], Libing Zhang[a]

[a]*Faculty of Mathematics and Physics, Huaiyin Institute of Technology, Huai'an, Jiangsu 223003, P.R. China*
[b]*Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I.R. Iran*
[c]*School of Mathematics, Institute for Research in Fundamental Sciences (IPM), P.O. Box: 19395-5746, Tehran, I.R. Iran*

Abstract. For a nontrivial graph G, its first and second Zagreb coindices are defined, respectively, as $\overline{M}_1(G) = \sum_{uv\notin E(G)} (d_G(u) + d_G(v))$ and $\overline{M}_2(G) = \sum_{uv\notin E(G)} d_G(u)d_G(v)$, where $d_G(x)$ is the degree of vertex x in G. In this paper, we explore further properties of Zagreb coindices. First, we investigate Zagreb coindices of two classes of composite graphs, namely, Mycielski graph and edge corona, and we present explicit formulas for Zagreb coindices of these two composite graphs. Then we we give two estimations on Zagreb coindices of graphs in terms of the number of pendent vertices and Merrifield-Simmons index, respectively. Finally, we give several Nordhaus-Gaddum type bounds for the first Zagreb coindex.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, let $d_G(v)$ be the degree of a vertex v in G.

A graph invariant is a function defined on a graph which is independent of the labeling of its vertices. Till now, hundreds of different graph invariants have been employed in QSAR/QSPR studies, some of which have been proved to be successful (see [23]). Among those successful invariants, there are two invariants called the *first Zagreb index* and the *second Zagreb index* (see [7, 9, 15, 17, 19, 21, 22, 24, 27–29]), defined as

$$M_1(G) = \sum_{u\in V(G)} (d_G(u))^2 \ \text{ and } \ M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v),$$

respectively.

In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v)).$$

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Email addresses: hongbo.hua@gmail.com (Hongbo Hua), ashrafi@kashanu.ac.ir (Ali Reza Ashrafi), libing.zhang@163.com (Libing Zhang)

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs, Došlić [8] proposed the *first Zagreb coindex* and *second Zagreb coindex* as

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

respectively.

It is well known that many graphs arise from simpler graphs via various graph operations. Hence, it is important and of interest to understand how certain invariants of such composite graphs are related to the corresponding invariants of the original graphs.

Ashrafi et al. [2] explored basic mathematical properties of Zagreb coindices and, in particular, presented explicit formulas for these new graph invariants under several graph operations, such as, union, join, Cartesian product, disjunction product, vertex corona and so on. Ashrafi et al. [3] determined the extremal values of Zagreb coindices over some special classes of graphs. Hossein-Zadeh et al. [10] obtained some new extremal values of Zagreb coindices over some special classes of graphs. Hua and Zhang [14] revealed some relations between Zagreb coindices and some other distance-based topological indices.

In this paper, we explore further properties of Zagreb coindices. In Section 2, we investigate Zagreb coindices of two classes of composite graphs, namely, Mycielski graph and edge corona, and we present explicit formulas for Zagreb coindices of these two composite graphs. In Section 3, we we present two estimations on Zagreb coindices in terms of the number of pendent vertices and Merrifield-Simmons index, respectively. In Section 4, we give several Nordhaus-Gaddum type bounds for the first Zagreb coindex.

2. Mycielski graph and edge corona of two graphs

We begin with some notations and terminology used in the proof of our results.

Let the n vertices of the given graph G be $v_1, v_2, \ldots, v_n$. Mycielski [20] introduced the following composite graph, which is well-studied by authors in [4–6].

Definition 2.1. *The* **Mycielski graph** $\mu(G)$ *of G contains G itself as an isomorphic subgraph, together with $n+1$ additional vertices: a vertex u_i corresponding to each vertex v_i of G, and another vertex w. Each vertex u_i is connected by an edge to w, so that these vertices form a subgraph in the form of a star $K_{1,n}$. In addition, for each edge v_iv_j of G, the Mycielski graph includes two edges, u_iv_j and v_iu_j.*

By Definition 2.1, if G has n vertices and m edges, then $\mu(G)$ has $2n+1$ vertices and $3m+n$ edges. Moreover, we have the following lemma by Definition 2.1.

Lemma 2.2. *Let G be a nontrivial graph of order n and size m, and let $\mu(G)$ be its Mycielski graph. Then, for each $i = 1, \ldots, n$, we have $d_{\mu(G)}(v_i) = 2d_G(v_i)$, $d_{\mu(G)}(u_i) = d_G(v_i) + 1$ and $d_{\mu(G)}(w) = n$.*

Let $\|n-1\|_G$ denote the number of vertices of degree $n-1$ in G. Now, we are in a position to state and prove the result of the Mycielski graph.

Theorem 2.3. *Let G be a nontrivial graph of order n and size m. Then*

(i) $\overline{M}_1(\mu(G)) = \frac{n^2-n-2m+6}{2}\overline{M}_1(G) + mM_1(G) + 4m^2 - 2mn^2 + 2mn + 11m + \frac{n^4-2n^3+4n^2+3n}{2} - (n-1)\|n-1\|_G$;

(ii) $\overline{M}_2(\mu(G)) = \frac{n^2-n-2m}{2}\overline{M}_1(G) + \frac{n^2-n-2m+12}{2}\overline{M}_2(G) + (m+2)M_1(G) + mM_2(G) + 3m^2 - mn^2 + 5mn + 12m + \frac{n^2(n-1)^2}{4} - 2(n-1)\|n-1\|_G$.

Proof. As stated in Definition 2.1, we label all vertices in $\mu(G)$ as $v_1, \ldots, v_n; u_1, \ldots, u_n; w$, where $v_1, \ldots, v_n$ are also vertices in the underlying graph G.

By Lemma 2.1, for each v_i in G, we have $d_{\mu(G)}(v_i) = 2d_G(v_i)$, $d_{\mu(G)}(u_i) = d_G(v_i) + 1$ and $d_{\mu(G)}(w) = n$.

Suppose that $v_iv_j \notin E(G)$. Then $v_iu_j \notin E(G)$ and $u_iv_j \notin E(G)$ by the structure of Mycielski graph. So, there are five types of nonadjacent vertex pairs in $\mu(G)$ subjecting to the above assumption, namely,

- Type 1: The nonadjacent vertex pairs $\{v_i, v_j\}$ in $\mu(G)$;
- Type 2: The nonadjacent vertex pairs $\{u_i, u_j\}$ in $\mu(G)$;
- Type 3: The nonadjacent vertex pairs $\{u_i, v_i\}$ in $\mu(G)$ for each $i = 1, \ldots, n$;
- Type 4: The nonadjacent vertex pairs $\{u_i, v_j\}$ in $\mu(G)$;
- Type 5: The nonadjacent vertex pairs $\{w, v_i\}$ in $\mu(G)$ for each $i = 1, \ldots, n$.

To complete the proof, it is sufficient to consider the respective contribution of the above five types of nonadjacent vertex pairs both to $\overline{M}_1(G^*)$ and to $\overline{M}_2(G^*)$.

The total contribution of nonadjacent vertex pairs of type 1 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$ are, respectively, given by

$$\begin{aligned}\sum_{v_iv_j\notin E(\mu(G))}(d_{\mu(G)}(v_i)+d_{\mu(G)}(v_j)) &= \sum_{v_iv_j\notin E(G)}(2d_G(v_i)+2d_G(v_j))\\ &= 2\sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_j))\\ &= 2\overline{M}_1(G)\end{aligned}$$

and

$$\begin{aligned}\sum_{v_iv_j\notin E(\mu(G))}d_{\mu(G)}(v_i)d_{\mu(G)}(v_j) &= \sum_{v_iv_j\notin E(G)}(2d_G(v_i))\cdot(2d_G(v_j))\\ &= 4\sum_{v_iv_j\notin E(G)}d_G(v_i)d_G(v_j)\\ &= 4\overline{M}_2(G).\end{aligned}$$

Now, we consider the total contribution of nonadjacent vertex pairs of type 2 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$, respectively. There are the following two distinct cases.

Case 2.4. *$u_iu_j \notin E(\mu(G))$ and $v_iv_j \notin E(G)$.*

In this case, we have

$$\begin{aligned}\sum_{u_iu_j\notin E(\mu(G))}(d_{\mu(G)}(u_i)+d_{\mu(G)}(u_j)) &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_j)+2)\\ &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_j))+2\left[\binom{n}{2}-m\right]\\ &= \overline{M}_1(G)+n(n-1)-2m\end{aligned}$$

and

$$\begin{aligned}\sum_{v_iv_j\notin E(\mu(G))}d_{\mu(G)}(v_i)d_{\mu(G)}(v_j) &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+1)\cdot(d_G(v_j)+1)\\ &= \sum_{v_iv_j\notin E(G)}d_G(v_i)d_G(v_j)+\sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_j))+\\ &\quad\left[\binom{n}{2}-m\right]\\ &= \overline{M}_1(G)+\overline{M}_2(G)+\frac{n(n-1)}{2}-m.\end{aligned}$$

Case 2.5. *$u_iu_j \notin E(\mu(G))$, but $v_iv_j \in E(G)$.*

In this case, we have

$$\begin{aligned}\sum_{u_iu_j\notin E(\mu(G))}(d_{\mu(G)}(u_i)+d_{\mu(G)}(u_j)) &= \sum_{v_iv_j\in E(G)}(d_G(v_i)+d_G(v_j)+2)\\ &= \sum_{v_iv_j\in E(G)}(d_G(v_i)+d_G(v_j))+2m\\ &= M_1(G)+2m\end{aligned}$$

and

$$\begin{aligned}\sum_{v_iv_j\notin E(\mu(G))}d_{\mu(G)}(v_i)d_{\mu(G)}(v_j) &= \sum_{v_iv_j\in E(G)}(d_G(v_i)+1)\cdot(d_G(v_j)+1)\\ &= \sum_{v_iv_j\in E(G)}d_G(v_i)d_G(v_j)+\sum_{v_iv_j\in E(G)}(d_G(v_i)+d_G(v_j))+m\\ &= M_1(G)+M_2(G)+m.\end{aligned}$$

Note that for any $1 \le i, j \le n$, $i \ne j$, we always have $u_iu_j \notin E(\mu(G))$. There are m edges $v_iv_j \in E(G)$ and $\binom{n}{2} - m$ nonadjacent vertex pairs $\{v_i, v_j\}$ in G as well as $\mu(G)$. By above analysis, the total contributions of nonadjacent vertex pairs of type 2 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$ are, respectively, given by

$$\left[\binom{n}{2}-m\right](\overline{M}_1(G)+n(n-1)-2m)+m(M_1(G)+2m)$$

and

$$\left[\binom{n}{2}-m\right](\overline{M}_1(G)+\overline{M}_2(G)+\frac{n(n-1)}{2}-m)+m(M_1(G)+M_2(G)+m).$$

The total contribution of nonadjacent vertex pairs of type 3 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$ are, respectively, given by

$$\begin{aligned}\sum_{i=1}^{n}(d_{\mu(G)}(u_i)+d_{\mu(G)}(v_i)) &= \sum_{i=1}^{n}(2d_G(v_i)+d_G(v_i)+1)\\ &= 3\sum_{i=1}^{n}d_G(v_i)+n\\ &= 6m+n\end{aligned}$$

and

$$\begin{aligned}\sum_{i=1}^{n}d_{\mu(G)}(u_i)d_{\mu(G)}(v_i) &= \sum_{i=1}^{n}2d_G(v_i)(d_G(v_i)+1)\\ &= 2\sum_{i=1}^{n}(d_G(v_i))^2+2\sum_{i=1}^{n}d_G(v_i)\\ &= 2M_1(G)+4m.\end{aligned}$$

The total contribution of nonadjacent vertex pairs of type 4 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$ are, respectively, given by

$$\begin{aligned}\sum_{u_iv_j\notin E(\mu(G))}(d_{\mu(G)}(u_i)+d_{\mu(G)}(v_j)) &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+1+2d_G(v_j))\\ &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_j))+\left[\binom{n}{2}-m\right]+\\ &\quad \sum_{v_iv_j\notin E(G)} d_G(v_j)\\ &= \overline{M}_1(G)+\frac{n(n-1)}{2}-m+\sum_{v_k\in V(G)} d_G(v_k)-\\ &\quad (n-1)\|n-1\|_G\\ &= \overline{M}_1(G)+\frac{n(n-1)}{2}+m-(n-1)\|n-1\|_G,\end{aligned}$$

and

$$\begin{aligned}\sum_{v_iv_j\notin E(\mu(G))} d_{\mu(G)}(v_i)d_{\mu(G)}(v_j) &= \sum_{v_iv_j\notin E(G)}(d_G(v_i)+1)\cdot(2d_G(v_j))\\ &= 2\sum_{v_iv_j\notin E(G)} d_G(v_i)d_G(v_j)+2\sum_{v_iv_j\notin E(G)} d_G(v_j)\\ &= 2\overline{M}_2(G)+2\sum_{v_k\in V(G)} d_G(v_k)-2(n-1)\|n-1\|_G\\ &= 2\overline{M}_2(G)+4m-2(n-1)\|n-1\|_G.\end{aligned}$$

The total contribution of nonadjacent vertex pairs of type 5 to $\overline{M}_1(\mu(G))$ and $\overline{M}_2(\mu(G))$ are, respectively, given by

$$\begin{aligned}\sum_{v_iw\notin E(\mu(G))}(d_{\mu(G)}(v_i)+d_{\mu(G)}(w)) &= \sum_{v_i\in V(G)}(2d_G(v_i)+n+1)\\ &= 4m+n(n+1)\end{aligned}$$

and

$$\begin{aligned}\sum_{v_iw\notin E(\mu(G))} d_{\mu(G)}(v_i)d_{\mu(G)}(w) &= \sum_{v_i\in V(G)}(2d_G(v_i))(n+1)\\ &= 4m(n+1).\end{aligned}$$

Summarizing the total contributions of five types of nonadjacent vertex pairs, we can obtain the desired result. This completes the proof. □

Hou and Shiu [11] introduced a kind of new graph operation, named edge corona, as introduced in the following definition. In [11], the adjacency spectrum and Laplacian spectrum of edge corona of G_1 and G_2 were presented in terms of the spectrum and Laplacian spectrum of G_1 and G_2, respectively.

Definition 2.6. *Let G_1 and G_2 be two graphs on disjoint sets of n_1 and n_2 vertices, m_1 and m_2 edges, respectively. The* **edge corona** *$G_1 \diamond G_2$ of G_1 and G_2 is defined as the graph obtained by taking one copy of G_1 and m_1 copies of G_2, and then joining two end-vertices of the i-th edge of G_1 to every vertex in the i-th copy of G_2.*

Ashrafi et al. [2] obtained explicit formulas for Zagreb coindices of vertex corona of two graphs. In the following theorem, we will give explicit formulas for Zagreb coindices of edge corona of two graphs.

Theorem 2.7. *Let G_1 and G_2 be two graphs on disjoint sets of n_1 and n_2 vertices, m_1 and m_2 edges, respectively. Then*

(i) $\overline{M}_1(G_1 \diamond G_2) = m_1\overline{M}_1(G_2) + (n_2+1)\overline{M}_1(G_1) - n_2(n_2+1)M_1(G_1) + 2m_1n_2(m_1+1)(m_2+n_2) + 2n_1^2(m_2+n_2) - 4m_1(2m_2+n_2)$;

(ii) $\overline{M}_2(G_1 \diamond G_2) = m_1\overline{M}_2(G_2) + 2m_1\overline{M}_1(G_2) + (n_2+1)^2\overline{M}_2(G_1) - 2(m_2+n_2)(n_2+1)M_1(G_1) + 2m_1n_2^2(m_1+2n_1) + 2m_1m_2(m_1m_2 + 2m_1n_2 + 2n_1n_2 + 2n_1 - 2n_2 - m_2 - 2) + 2m_1n_2(2n_1 - 1)$.

Proof. We let x_{ij} be the j-th vertex in the i-th copy of G_2, where $i = 1, \dots, m_1$, $j = 1, \dots, n_2$, and let y_k be the k-th in G_1, $k = 1, \dots, n_1$. Also, we let x_j be the j-th vertex in G_2.

By the definition of edge corona, for each vertex x_{ij}, we have $d_{G_1\diamond G_2}(x_{ij}) = d_{G_2}(x_j) + 2$, and for every vertex y_k in G_1, $d_{G_1\diamond G_2}(y_k) = d_{G_1}(y_k)\cdot n_2 + d_{G_1}(y_k) = (n_2+1)d_{G_1}(y_k)$.

Now, we need only to consider the following four types of nonadjacent vertex pairs in $G_1 \diamond G_2$, namely,

• Type 1: The nonadjacent vertex pairs $\{x_{ij}, x_{ih}\}$, where $1 \le i \le m_1$, $1 \le j < h \le n_2$, and it is assumed that $x_jx_h \notin E(G_2)$;

• Type 2: The nonadjacent vertex pairs $\{y_k, y_s\}$, where $1 \le k < s \le n_1$ and it is assumed that $y_ky_s \notin E(G_1)$;

• Type 3: The nonadjacent vertex pairs $\{x_{ij}, y_k\}$, where $1 \le i \le m_1$, $1 \le j \le n_2$, $1 \le k \le n_1$, and it is assumed that the i-th edge e_i $(1 \le i \le m_1)$ in G_1 does not pass through y_k;

• Type 4: The nonadjacent vertex pairs $\{x_{ij}, x_{lh}\}$, where $1 \le i < l \le m_1$, $1 \le j, h \le n_2$.

The total contribution of nonadjacent vertex pairs of type 1 to $\overline{M}_1(G_1 \diamond G_2)$ and $\overline{M}_2(G_1 \diamond G_2)$ are given by

$$\begin{aligned}\sum_{i=1}^{m_1}\sum_{x_{ij}x_{ih}\notin E(G_1\diamond G_2)}(d_{G_1\diamond G_2}(x_{ij}) + d_{G_1\diamond G_2}(x_{ih})) &= \sum_{i=1}^{m_1}\sum_{x_jx_h\notin E(G_2)}(d_{G_2}(x_j) + d_{G_2}(x_h) + 4)\\ &= \sum_{i=1}^{m_1}\left\{\overline{M}_1(G_2) + 4\left[\binom{n_2}{2} - m_2\right]\right\}\\ &= m_1\overline{M}_1(G_2) + 2m_1n_2(n_2-1) - 4m_1m_2\end{aligned}$$

and

$$\begin{aligned}\sum_{i=1}^{m_1}\sum_{x_{ij}x_{ih}\notin E(G_1\diamond G_2)} d_{G_1\diamond G_2}(x_{ij})d_{G_1\diamond G_2}(x_{ih}) &= \sum_{i=1}^{m_1}\sum_{x_jx_h\notin E(G_2)}(d_{G_2}(x_j)+2)(d_{G_2}(x_h)+2)\\ &= \sum_{i=1}^{m_1}\left\{\overline{M}_2(G_2) + 2\overline{M}_1(G_2) + 4\left[\binom{n_2}{2} - m_2\right]\right\}\\ &= m_1\overline{M}_2(G_2) + 2m_1\overline{M}_1(G_2) + 2m_1n_2(n_2-1) -\\ &\quad 4m_1m_2,\end{aligned}$$

respectively.

The total contribution of nonadjacent vertex pairs of type 2 to $\overline{M}_1(G_1 \diamond G_2)$ and $\overline{M}_2(G_1 \diamond G_2)$ are given by

$$\begin{aligned}\sum_{y_ky_s\notin E(G_1\diamond G_2)}(d_{G_1\diamond G_2}(y_k) + d_{G_1\diamond G_2}(y_s)) &= \sum_{y_ky_s\notin E(G_1)}(n_2+1)(d_{G_1}(y_k) + d_{G_1}(y_s))\\ &= (n_2+1)\overline{M}_1(G_1)\end{aligned}$$

and

$$\begin{aligned}\sum_{y_ky_s\notin E(G_1\diamond G_2)} d_{G_1\diamond G_2}(y_k)d_{G_1\diamond G_2}(y_s) &= \sum_{y_ky_s\notin E(G_1)}(n_2+1)^2 d_{G_1}(y_k)d_{G_1}(y_s)\\ &= (n_2+1)^2\overline{M}_2(G_1),\end{aligned}$$

respectively.

Now, we consider the total contribution of nonadjacent vertex pairs of type 3 to $\overline{M}_1(G)$ and $\overline{M}_2(G)$, respectively. Note that each y_k is adjacent to all vertices of $d_{G_1}(y_k)$ copies of G_2, or equivalently, each y_k is not adjacent to any vertex of $m_1 - d_{G_1}(y_k)$ copies of G_2.

Then the total contribution of nonadjacent vertex pairs of type 3 to $\overline{M}_1(G_1 \diamond G_2)$ and $\overline{M}_2(G_1 \diamond G_2)$ are given by

$$\sum_{k=1}^{n_1}(n_1 - d_{G_1}(y_k)) \sum_{j=1}^{n_2}[d_{G_2}(x_j) + 2 + (n_2+1)d_{G_1}(y_k)]$$

$$= \sum_{k=1}^{n_1}(n_1 - d_{G_1}(y_k))[2m_2 + 2n_2 + n_2(n_2+1)d_{G_1}(y_k)]$$
$$= 2n_1^2(m_2+n_2) - 4m_1(m_2+n_2) + 2m_1n_1n_2(n_2+1) - n_2(n_2+1)M_1(G_1)$$

and

$$\sum_{k=1}^{n_1}(n_1 - d_{G_1}(y_k)) \sum_{j=1}^{n_2}(d_{G_2}(x_j) + 2)(n_2+1)d_{G_1}(y_k)$$

$$= 2(m_2+n_2)(n_2+1)\sum_{k=1}^{n_1} d_{G_1}(y_k)(n_1 - d_{G_1}(y_k))$$
$$= 2(m_2+n_2)(n_2+1)(2m_1n_1 - M_1(G_1)),$$

respectively.

The total contribution of nonadjacent vertex pairs of type 4 to $\overline{M}_1(G_1 \diamond G_2)$ and $\overline{M}_2(G_1 \diamond G_2)$ are given by

$$\begin{aligned}
\sum_{x_{ij}x_{lh} \notin E(G_1 \diamond G_2)} (d_{G_1 \diamond G_2}(x_{ij}) + d_{G_1 \diamond G_2}(x_{lh})) &= \binom{m_1}{2} \cdot \sum_{j=1}^{n_2}\sum_{h=1}^{n_2}(d_{G_2}(x_j) + d_{G_2}(x_h) + 4) \\
&= \binom{m_1}{2} \cdot \sum_{j=1}^{n_2}(n_2 d_{G_2}(x_j) + 2m_2 + 4n_2) \\
&= \binom{m_1}{2}(4m_2n_2 + 4n_2^2) \\
&= 2m_1n_2(m_1-1)(m_2+n_2)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{x_{ij}x_{lh} \notin E(G_1 \diamond G_2)} d_{G_1 \diamond G_2}(x_{ij}) d_{G_1 \diamond G_2}(x_{lh}) &= \binom{m_1}{2} \cdot \sum_{j=1}^{n_2}\sum_{h=1}^{n_2}(d_{G_2}(x_j) + 2)(d_{G_2}(x_h) + 2) \\
&= \binom{m_1}{2} \cdot \sum_{j=1}^{n_2}(d_{G_2}(x_j) + 2)(2m_2 + 2n_2) \\
&= 4\binom{m_1}{2}(m_2+n_2)^2 \\
&= 2m_1(m_1-1)(m_2+n_2)^2,
\end{aligned}$$

respectively.

Summarizing the total contributions of four types of nonadjacent vertex pairs, we can obtain the desired result. This completes the proof. □

3. Two estimations on Zagreb coindices

In this section, we build two estimations on Zagreb coindices of connected graphs involving the number of pendent vertices and the Merrifield-Simmons index, respectively.

Theorem 3.1. *Let G be a connected graph of order n and p pendent vertices. Then*
(i)$\overline{M}_1(G) \geq -2p^2 + 3pn - 4p$;
(ii)$\overline{M}_2(G) \geq -\frac{3}{2}p^2 - \frac{5}{2}p + 2pn$.

Proof. When $p = 0$, the result holds clearly, as $\overline{M}_i(G) \geq 0\,(i = 1, 2)$. Assume that $p \geq 1$.

Suppose first that G has exactly one pendent vertex, say v, and that u is the unique neighbor of v. Then

$$\begin{aligned}\overline{M}_1(G) &\geq \sum_{w\in V(G)\setminus\{u,v\}} (d_G(w) + 1)\\ &\geq \sum_{w\in V(G)\setminus\{u,v\}} 3\\ &= 3(n-2)\end{aligned}$$

and

$$\begin{aligned}\overline{M}_2(G) &\geq \sum_{w\in V(G)\setminus\{u,v\}} d_G(w)\\ &\geq \sum_{w\in V(G)\setminus\{u,v\}} 2\\ &= 2(n-2),\end{aligned}$$

as desired.

Now, we assume that $p \geq 2$. Clearly, each pair of pendent vertices contributes to $\overline{M}_1(G)$ and $\overline{M}_2(G)$ are 2 and 1, respectively. The total contribution of pendent vertices pairs to $\overline{M}_1(G)$ and $\overline{M}_2(G)$ are $2\binom{p}{2}$ and $\binom{p}{2}$, respectively.

Let v be a pendent vertex in G and let u be its unique neighbor. Then for any non-pendent vertex w in $V(G) \setminus \{u, v\}$, the contribution of vertex pairs $\{v, w\}$ to $\overline{M}_1(G)$ and $\overline{M}_2(G)$ are $1 + d_G(w)$ and $d_G(w)$, respectively. The total contribution of such vertex pairs $\{v, w\}$ to $\overline{M}_1(G)$ and $\overline{M}_2(G)$ are $(n - p - 1)\binom{p}{1}(1 + d_G(w))$ and $(n - p - 1)\binom{p}{1}d_G(w)$, respectively.

Since $d_G(w) \geq 2$ for any non-pendent vertex w in G, we have

$$\begin{aligned}\overline{M}_1(G) &\geq \binom{p}{2} \times (1+1) + (n-p-1)\binom{p}{1} \times (1+2)\\ &= -2p^2 + 3pn - 4p.\end{aligned}$$

Similarly,

$$\begin{aligned}\overline{M}_2(G) &\geq \binom{p}{2} \times (1\times 1) + (n-p-1)\binom{p}{1} \times (1\times 2)\\ &= -\frac{3}{2}p^2 - \frac{5}{2}p + 2pn.\end{aligned}$$

Since these two bounds are also valid for the case of $p = 1$, we have completed the proof. □

Remark 3.2. *Consider the sharpness of bounds in Theorem 3.1. When $p = 0$, both $-2p^2+3pn-4p$ and $-\frac{3}{2}p^2-\frac{5}{2}p+2pn$ equal to zero. Clearly, the complete graph K_n and $\overline{K}_n$ attain both bounds. When $p = 2$, the 4-vertex path P_4 attains both bounds in (i) and (ii). When $p \geq 3$, we fail to find the extremal graphs attaining bounds corresponding to each p.*

The *Merrifield-Simmons index* of a graph G (see [12, 13, 25]) is defined as

$$i(G) = \sum_{k\geq 0} i(G;k),$$

where $i(G;k)$ is the number of k-membered independent sets in G for $k \geq 1$, and $i(G;0) = 1$.

Theorem 3.3. *Let G be a connected graph of order n and maximum vertex degree $\triangle(G)$. Then*
(i) $\overline{M}_1(G) \leq 2\triangle(G)(i(G) - n - 1)$;
(ii) $\overline{M}_2(G) \leq (\triangle(G))^2(i(G) - n - 1)$.

Proof. It is obvious that the number of vertex pairs $\{u, v\}$ in G at distance greater than or equal to 2 is exactly $i(G;2)$. Moreover, we have

$$i(G) \geq 1 + n + i(G;2)$$

with equality if and only if the independence number of G is equal to 2. That is,

$$i(G;2) \leq i(G) - n - 1$$

with equality if and only if the independence number of G is equal to 2. Then

$$\begin{aligned}\overline{M}_1(G) &= \sum_{uv\notin E(G)} (d_G(u) + d_G(v)) \\ &\leq \sum_{uv\notin E(G)} 2\triangle(G) \\ &= 2\triangle(G)i(G;2) \\ &\leq 2\triangle(G)(i(G) - n - 1).\end{aligned}$$

Similarly, we have $\overline{M}_2(G) \leq (\triangle(G))^2(i(G) - n - 1)$. This proves theorem. □

Remark 3.4. *Consider the sharpness of bounds in Theorem 3.3. It is easy to see that both bounds in (i) and (ii) are attained if and only if G is a regular graph and the independence number of G is equal to 2. For example, the cycle C_4 or C_5 attains both bounds in (i) and (ii).*

4. Nordhaus-Gaddum type bounds for the first Zagreb coindex

Hossein-Zadeh et al. [10] obtained Nordhaus-Gaddum type bounds for the second Zagreb coindex by means of results in [26], but they left the case of the first Zagreb coindex untreated. In this section, we give several Nordhaus-Gaddum type (lower) bounds for the first Zagreb coindex by means of results in [27, 28].

Lemma 4.1. *([16]) Let G be a graph of order $n \geq 2$ and size m. Then*

$$M_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if $G \cong S_n$ or K_n.

Lemma 4.2. *([27]) Let G be a connected graph of order $n \geq 2$ and size m. If G is K_{r+1}-free, $2 \leq r \leq n-1$, then*

$$M_1(G) \leq \frac{2r-2}{r} mn$$

with equality if and only if G is a bipartite graph for $r = 2$, and regular complete r-partite graph for $r \geq 3$.

Let W_n be the graph obtained from the star S_n by adding $\lfloor \frac{n-1}{2} \rfloor$ independent edges. Let $even(n) = 1$ if n is even, and 0 otherwise.

Lemma 4.3. *([28]) Let G be a connected quadrangle-free graph graph of order $n \geq 2$ and size m. Then*

$$M_1(G) \leq n(n-1) + 2m - 2even(n)$$

with equality if and only if $G \cong W_n$.

Lemma 4.4. *([28]) Let G be a connected triangle- and a quadrangle-free graph of order $n \geq 2$. Then*

$$M_1(G) \leq n(n-1)$$

with equality if and only if $G \cong S_n$ or a Moore graph of diameter 2.

Theorem 4.5. (*i*) *If G is a graph of order $n \geq 2$ and size m, then*

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 2mn - \frac{4m^2}{n-1}$$

with equality if and only if $G \cong S_n$ or K_n.

(*ii*) *If G is a connected K_{r+1}-free graph, $2 \leq r \leq n-1$, then*

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 4m(\frac{n}{r} - 1)$$

with equality if and only if G is a bipartite graph for $r = 2$, and regular complete r-partite graph for $r \geq 3$.

(*iii*) *If G is a connected quadrangle-free graph, then*

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 4mn - 2n^2 + 2n - 8m + 4even(n)$$

with equality if and only if $G \cong W_n$.

(*iv*) *If G is a connected triangle- and a quadrangle-free graph, then*

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 2(n-1)(2m-n)$$

with equality if and only if $G \cong S_n$ or a Moore graph of diameter 2.

Proof. It follows from [2] that for any simple graph G, $\overline{M}_1(\overline{G}) = \overline{M}_1(G)$. Hence, $\overline{M}_1(G) + \overline{M}_1(\overline{G}) = 2\overline{M}_1(G)$.

From [2], we also have $\overline{M}_1(G) = 2m(n-1) - M_1(G)$ for any simple graph of order n and size m. So,

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) = 4m(n-1) - 2M_1(G). \quad (1)$$

By Lemmas 4.1–4.4 and Eq. (1), we have actually completed the proof. □

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