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HYPER ZAGREB INDICES AND ITS COINDICES OF GRAPHS

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Abstract. For a (molecular) graph, the hyper Zagreb index is defined as $HM(G) = \sum\limits_{uv \in E(G)} (d_G(u) + d_G(v))^2$ and the hyper Zagreb coindex is defined as $\overline{HM}(G) = \sum\limits_{uv \notin E(G)} (d_G(u)+d_G(v))^2$. In this paper, the hyper Zagreb indices and its coindices of edge corona product graph, double graph and Mycielskian graph are obtained.

1. Introduction

All the graphs considered in this paper are connected and simple. For vertex $u \in V(G)$, the degree of the vertex u in G, denoted by $d_G(u)$, is the number of edges incident to u in G. A *topological index* of a graph is a parameter related to the graph; it does not depend on labeling or pictorial representation of the graph. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [**2**]. Several types of such indices exist, especially those based on vertex and edge distances. One of the most intensively studied topological indices is the Wiener index. Two of these topological indices are known under various names, the most commonly used ones are the first and second Zagreb indices.

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The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [**3**]. They are defined as

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

Note that the first Zagreb index may also written as $M_1(G) = \sum\limits_{uv \in E(G)} (d_G(u) + d_G(v))$. The Zagreb indices are found to have appilications in QSPR and QSAR studies as well, see [**1**].

The *hyper Zagreb index* is defined as $HM(G) = \sum\limits_{uv \in E(G)} (d_G(u) + d_G(v))^2$ and the *hyper Zagreb coindex* is defined as $\overline{HM}(G) = \sum\limits_{uv \notin E(G)} (d_G(u) + d_G(v))^2$.

For the survey on theory and application of Zagreb indices see [**6**]. Feng et al.[**4**] have given a sharp bounds for the Zagreb indices of graphs with a given matching number. Khalifeh et al. [**5**] have obtained the Zagreb indices of the Cartesian product, composition, join, disjunction and symmetric difference of graphs. Ashrafi et al. [**8**] determined the extremal values of Zagreb coindices over some special class of graphs. Hua and Zhang [**10**] have given some relations between Zagreb coindices and some other topolodical indices. Ashrafi et al. [**7**] have obtained the Zagreb indices of the Cartesian product, composition, join, disjunction and symmetric difference of graphs. Shirdel et al [**11**], have obtained the hyper-Zagreb indices of the Cartesian product, composition, join and disjunction of graphs. The hyper Zagreb indices of some classes of chemical graphs are obtained in [**11, 13, 14**]. In this paper, we obtain the hyper Zagreb indices and its coindices of the edge corona product graph, double graph and Mycielskian graph are obtained.

2. Main results

In this section, we compute the hyper Zagreb indices and its coindices of edge corona product graph, double graph and Mycielskian graph.

2.1. Edge corona product. Let G and H be two graphs on disjoint sets of n and m vertices, p and q edges, respectively. 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. Now we compute the hyper Zagreb index and its coindex of edge corona product of two given graphs.

THEOREM 2.1. *Let G and H be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then* $HM(G \bullet H) = (n_2+1)^3 HM(G) + m_2 HM(H) + 4(n_2+1)(n_2+m_2)M_1(G) + (8m_2+m_1)M_1(H) + 16m_2^2 + 4m_1(n_2+2m_2)$.

PROOF. By the definition of edge corona product, for each vertex $x \in V(G)$, we have $d_{G\bullet H}(x) = d_G(x)(|V(H)|+1)$ and for each vertex $y \in V(H_i)$, $d_{G\bullet H}(y) =$

$d_H(y)+2$. Clearly, $|V(G\bullet H)| = |V(G)| + |E(G)|\,|V(H)|$.

$$\begin{aligned}
HM(G\bullet H) &= \sum_{xy\in E(G\bullet H)} \Big(d_{G\bullet H}(x)+d_{G\bullet H}(y)\Big)^2 \\
&= \sum_{xy\in E(G)} \Big((n_2+1)d_G(x)+(n_2+1)d_G(y)\Big)^2 \\
&\quad +\sum_{i=1}^{m_2}\sum_{xy\in E(H)} \Big((d_H(x)+2)+(d_H(y)+2)\Big)^2 \\
&\quad +\sum_{xy\in E(G)}\sum_{u\in V(H)} \Big((n_2+1)(d_G(x)+d_G(y))+(d_H(u)+2)\Big)^2 \\
&= (n_2+1)^2\sum_{xy\in E(G)} (d_G(x)+d_G(y))^2 \\
&\quad +\sum_{i=1}^{m_2}\sum_{xy\in E(H)} \Big((d_H(x)+d_H(y))^2+16+8(d_H(x)+d_H(y)\Big) \\
&\quad +\sum_{xy\in E(G)}\sum_{u\in V(H)} \Big((n_2+1)(d_G(x)+d_G(y))+d_H(u)+2\Big)^2 \\
&= (n_2+1)^3HM(G)+m_2HM(H)+4(n_2+1)(n_2+m_2)M_1(G) \\
&\quad +(8m_2+m_1)M_1(H)+16m_2^2+4m_1(n_2+2m_2).
\end{aligned}$$

$\square$

THEOREM 2.2. *Let G and H be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then* $\overline{HM}(G\bullet H) = \Big(m_1+(n_2+1)^2\Big)\overline{HM}(G)+8m_1\overline{M}_1(H)+\Big(n_1^2-2m_1+n_2m_1(m_1-1)\Big)M_1(H)+(n_2+1)(n_1n_2(n_2+1)-4n_2-4m_2)M_1(G)-n_2(n_2+1)^2F(G)+8(n_2+1)n_1m_1(n_2+m_2)-32m_1m_2-8m_1n_2(n_2-2)+4n_1^2(2m_2+n_2)+m_1(m_1-1)(4m^2+8n_2^2+16n_2m_2)$.

PROOF. Let x_{ij} be the jth vertex in the ith copy of H, $i=1,2,\ldots,m_1$,$j=1,2,\ldots,n_2$, and let y_k be the kth in G,$k=1,2,\ldots,n_1$. Also let x_j be the jth 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, $d_{G\bullet H}(y_k) = d_G(y_k)n_2+d_G(y_k) = (n_2+1)d_G(y_k)$.

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

Case 1: The nonadjacent vertex pairs $\{x_{ij};x_{ih}\}$, $1\leqslant i\leqslant m_1$,$1\leqslant j<h\leqslant n_2$, and

it is assumed that $x_jx_h \notin E(H)$.

$$\begin{aligned}
& \sum_{i=1}^{m_1} \sum_{x_{ij}x_{ih} \notin E(G\bullet H)} \Big(d_{G\bullet H}(x_{ij}) + d_{G\bullet H}(x_{ih})\Big)^2 \\
= & \sum_{i=1}^{m_1} \sum_{x_jx_h \notin E(H)} \Big(d_H(x_j) + d_H(x_h) + 4\Big)^2 \\
= & \sum_{i=1}^{m_1} \sum_{x_jx_h \notin E(H)} \Big((d_H(x_j) + d_H(x_h))^2 + 8(d_H(x_j) + d_H(x_h)) + 16\Big) \\
= & \sum_{i=1}^{m_1} \Big(\overline{HM}(H) + 16\Big(\frac{n_2(n_2-1)}{2} - m_2\Big) + 8\overline{M_1}(H)\Big) \\
= & \ m_1\overline{HM}(H) + 8m_1\overline{M_1}(H) + 8m_1n_2(n_2-1) - 16m_1m_2.
\end{aligned}$$

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

$$\begin{aligned}
& \sum_{y_ky_s \notin E(G\bullet H)} \Big(d_{G\bullet H}(y_k) + d_{G\bullet H}(y_s)\Big)^2 \\
= & \sum_{y_ky_s \notin E(G)} \Big((n_2+1)d_G(y_k) + (n_2+1)d_G(y_s)\Big)^2 \\
= & \ (n_2+1)^2 \sum_{y_ky_s \notin E(G)} \Big(d_G(y_k) + d_G(y_s)\Big)^2 \\
= & \ (n_2+1)^2\overline{HM}(G).
\end{aligned}$$

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

$$\begin{aligned}
& \sum_{j=1}^{n_2} \Big(d_H(x_j) + 2 + (n_2+1)d_G(y_k)\Big)^2 \\
= & \sum_{j=1}^{n_2} \Big(d_H^2(x_j) + (n_2+1)^2d_G^2(y_k) + 4d_H(x_j) \\
& +4(n_2+1)d_G(y_k) + 2(n_2+1)d_H(x_j)d_G(y_k) + 4\Big) \\
= & \ M_1(H) + 8m_2 + 4n_2 + n_2(n_2+1)^2d_G^2(y_k) \\
& +(4n_2(n_2+1) + 4m_2(n_2+1))d_G(y_k).
\end{aligned}$$

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

$$\begin{aligned}
&\sum_{k=1}^{n_1}(n_1 - d_G(y_k))\sum_{j=1}^{n_2}\Big(d_H(x_j) + 2 + (n_2+1)d_G(y_k)\Big)^2 \\
= \;& n_1\Big(n_1 M_1(H) + n_1(8m_2 + 4n_2)\Big) \\
& + \Big(4n_1(n_2+1)(n_2+m_2) - M_1(H) - 8m_2 - 4n_2\Big)\sum_{k=1}^{n_1} d_G(y_k) \\
& + (n_2+1)\Big(n_1 n_2(n_2+1) - 4n_2 - 4m_2\Big)\sum_{k=1}^{n_1} d_G^2(y_k) - n_2(n_2+1)^2\sum_{k=1}^{n_1} d_G^3(y_k) \\
= \;& (n_1^2 - 2m_1)M_1(H) + (n_2+1)(n_1 n_2(n_2+1) - 4n_2 - 4m_2)M_1(G) - n_2(n_2+1)^2 \\
& F(G) + 4n_1^2(2m_2 + n_2) - 16m_1m_2 - 8n_2m_1 + 8n_1m_1(n_2+1)(n_2+m_2).
\end{aligned}$$

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

$$\begin{aligned}
&\sum_{x_{ij}x_{\ell h} \notin E(G\bullet H)} \Big(d_{G\bullet H}(x_{ij}) + d_{G\bullet H}(x_{\ell h})\Big)^2 \\
= \;& \frac{m_1(m_1-1)}{2}\sum_{j=1}^{n_2}\sum_{h=1}^{n_2}\Big(d_H(x_j) + d_H(x_h) + 4\Big)^2 \\
= \;& \frac{m_1(m_1-1)}{2}\sum_{j=1}^{n_2}\sum_{h=1}^{n_2}\Big(d_H^2(x_j) + d_H^2(x_h) + 2d_H(x_j)d_H(x_h) + 8d_H(x_j) \\
& +8d_H(x_h) + 16\Big) \\
= \;& \frac{m_1(m_1-1)}{2}\sum_{j=1}^{n_2}\Big(n_2 d_H^2(x_j) + M_1(H) + 4m_2 d_H(x_j) + 8n_2 d_H(x_j) \\
& +16m_2 + 16n_2\Big) \\
= \;& m_1(m_1-1)\Big(n_2 M_1(H) + 16n_2m_2 + 8n_2^2 + 4m_2^2\Big).
\end{aligned}$$

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

2.2. Double graph. Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. The vertices of the double graph G^* are given by the two sets $X = \{x_1, x_2, \ldots, x_n\}$ and $Y = \{y_1, y_2, \ldots, y_n\}$. 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 $v_iv_j \in E(G)$, two more edges x_iy_j and x_jy_i are added. For a given vertex v in G, let $D_G(v) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v))$. Now we compute the hyper Zagreb index and its coindex for double of a given graph.

THEOREM 2.3. *The hyper-Zagreb index of the double graph G^* of a graph G is given by $HM(G^*) = 16\,HM(G)$.*

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

$$\begin{aligned}
HM(G^*) &= \sum_{uv \in E(G^*)} (d_{G^*}(u) + d_{G^*}(v))^2 \\
&= \sum_{x_ix_j \in E(G^*)} (d_{G^*}(x_i) + d_{G^*}(x_j))^2 + \sum_{y_iy_j \in E(G^*)} (d_{G^*}(y_i) + d_{G^*}(y_j))^2 \\
&\quad + \sum_{x_iy_j \in E(G^*)} (d_{G^*}(x_i) + d_{G^*}(y_j))^2 + \sum_{x_jy_i \in E(G^*)} (d_{G^*}(x_j) + d_{G^*}(y_i))^2 \\
&= 4 \sum_{v_iv_j \in E(G)} (2d_G(v_i) + 2d_G(v_j))^2 = 16\,HM(G).
\end{aligned}$$

□

THEOREM 2.4. *Let G be a connected graph with n vertices and m edges. Then $\overline{HM}(G^*) = 16\overline{HM}(G) + 16M_1(G)$.*

PROOF. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$. Suppose that x_i and y_i are the corresponding clone vertices, in G^*, of v_i for each $i = 1, 2, \ldots, n$. 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 $v_iv_j \notin E(G)$, then $x_ix_j \notin E(G)$,$y_iy_j \notin E(G)$,$x_iy_j \notin E(G)$and $y_ix_j \notin E(G)$.

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

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

$$\begin{aligned}
\sum_{y_iy_j \notin E(G^*)} \Big(d_{G^*}(y_i) + d_{G^*}(y_j)\Big)^2 &= \sum_{x_ix_j \notin E(G^*)} \Big(d_{G^*}(x_i) + d_{G^*}(x_j)\Big)^2 \\
&= \sum_{v_iv_j \notin E(G)} \Big(2d_G(v_i) + 2d_Gv_j)\Big)^2 \\
&= 4\overline{HM}(G).
\end{aligned}$$

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

$$\begin{aligned}
\sum_{i=1}^{n} \Big(d_{G^*}(x_i) + d_{G^*}(y_i)\Big)^2 &= \sum_{i=1}^{n} \Big(2d_G(v_i) + 2d_G(v_i)\Big)^2 \\
&= 16 \sum_{i=1}^{n} d_G^2(v_i) \\
&= 16M_1(G).
\end{aligned}$$

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

For each x_i, there exist $n-1-d_G(v_i)$ vertices in the set $\{y_1, y_2, \ldots, y_n\}$, 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 $\overline{HM}(G^*)$ is

$$\begin{aligned}\sum_{x_iy_j \notin E(G^*)} \Big(d_{G^*}(x_i) + d_{G^*}(y_j)\Big)^2 &= \sum_{v_iv_j \notin E(G^*)} \Big(2d_G(v_i) + 2d_G(v_j)\Big)^2 \\ &= 4D_G(v_i).\end{aligned}$$

Hence

$$\begin{aligned}\sum_{i\neq j,\ x_iy_j \notin E(G^*)} \Big(d_{G^*}(x_i) + d_{G^*}(y_j)\Big)^2 &= \sum_{i=1}^{n} 4D_G(v_i) \\ &= 8\overline{HM}(G).\end{aligned}$$

Hence

$$\begin{aligned}\overline{HM}(G^*) &= \sum_{x_ix_j \notin E(G^*)} \Big(d_{G^*}(x_i) + d_{G^*}(x_j)\Big)^2 + \sum_{y_iy_j \notin E(G^*)} \Big(d_{G^*}(y_i) + d_{G^*}(y_j)\Big)^2 \\ &\quad + \sum_{i=1}^{n} \Big(d_{G^*}(x_i) + d_{G^*}(y_i)\Big)^2 + \sum_{i\neq j,\ x_iy_j \notin E(G^*)} \Big(d_{G^*}(x_i) + d_{G^*}(y_j)\Big)^2 \\ &= 16\overline{HM}(G) + 16M_1(G).\end{aligned}$$

□

EXAMPLE 2.1. Let $G = H_{2n}$, where H_{2n} is the double graph of the star S_n, see Figure 1. The hyper Zagreb coindices of H_{2n} is $\overline{HM}(H_{2n}) = 16n(n-1)(n+1)$.

2.3. Mycielskian graph. The *Mycielskian 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 Mycielskian graph incudes two edges, u_iv_j and v_iu_j. Following lemma follows from the structure of the Mycielskian graph of a given graph.

LEMMA 2.1. *Let G be a connected graph on n vertices and m edges. Then for each $i = 1, 2, \ldots, n$, we have $d_{\mu(G)}(v_i) = 2d_G(v_i)$, $d_{\mu(G)}(u_i) = d_G(v_i) + 1$ and $d_{\mu(G)}(w) = n$.*

The maximum and minimum degree of the graph G are denoted by Δ and δ, respectively

THEOREM 2.5. *Let G be a graph on n vertices and m edges. Then* $2m(1+3\delta)^2 + n(n+\delta+1)^2 + 4HM(G) \leqslant HM(\mu(G)) \leqslant 2m(1+3\Delta)^2 + n(n+\Delta+1)^2 + 4HM(G)$.

PROOF. Let the edge set of $\mu E(G)$ can be partitioned into three subsets,

$$E_1 = \{xy \in E(\mu(G)) | x = u_i, y = v_j\},\ E_2 = \{xy \in E(\mu(G)) | x = w, y = u_i\} \text{ and } E_3 = \{xy \in E(\mu(G)) | x = v_i, y = v_j\}.$$

Case 1: If $x = u_i$ and $y = v_j$, then the contribution of the edges in E_1 is given by

$$\begin{aligned}
\sum_{u_iv_j \in E_1} \Big(d_{\mu(G)}(u_i) + d_{\mu(G)}(v_j)\Big)^2 &= \sum_{u_iv_j \in E_1} \Big(1 + d_G(v_i) + 2d_G(v_j)\Big)^2 \\
&= \sum_{i=1}^{n} \sum_{v_j \in N_G(v_i)} \Big(1 + d_G(v_i) + 2d_G(v_j)\Big)^2 \\
&\geqslant \sum_{i=1}^{n} \sum_{v_j \in N_G(v_i)} (1 + 3\delta)^2 \\
&= \sum_{i=1}^{n} d_G(v_i)(1 + 3\delta)^2 \\
&= 2m(1 + 3\delta)^2.
\end{aligned}$$

Case 2: If $x = w$ and $y = u_i$, then the contribution of the edges in E_2 is given by

$$\begin{aligned}
\sum_{wu_i \in E_2} \Big(d_{\mu(G)}(u_i) + d_{\mu(G)}(v_j)\Big)^2 &= \sum_{wu_i \in E_2} (n + 1 + d_G(v_i))^2 \\
&= \sum_{i=1}^{n} \Big(n + 1 + d_G(v_i)\Big)^2 \\
&\geqslant n(n + \delta + 1)^2.
\end{aligned}$$

Case 3: If $x = v_i$ and $y = v_j$, then the contribution of the edges in E_3 is given by

$$\begin{aligned}
\sum_{v_iv_j \in E_3} \Big(d_{\mu(G)}(v_i) + d_{\mu(G)}(v_j)\Big)^2 &= \sum_{v_iv_j \in E_3} \Big(2d_G(v_i) + 2d_G(v_j)\Big)^2 \\
&= 4HM(G).
\end{aligned}$$

Summarizing the total contributions of the above cases of edges in $\mu(G)$, we have

$2m(1 + 3\delta)^2 + n(n + \delta + 1)^2 + 4HM(G) \leqslant HM(\mu(G))$.

Similarly, we can obtain $HM(\mu(G)) \leqslant 2m(1+3\Delta)^2+n(n+\Delta+1)^2+4HM(G)$. □

Let $\|n-1\|_G$ denote the number of vertices of degree $n-1$ in G. Now we compute the hyper Zagreb coindex of Mycielskian graph.

Theorem 2.6. *Let G be a graph on n vertices and m edges. Then* $\overline{HM}(\mu(G)) = \Big(\frac{n(n-1)-2m+10}{2}\Big)\overline{HM}(G) + mHM(G) + 2\Big(n(n-1) - 2m + 1\Big)\overline{M}_1(G) + 4\overline{M}_2(G) + 4(m+4)M_1(G) + \frac{n(n-1)}{2}\Big(2n(n-1) - 5m + 1\Big) + \Big(5m^2 + n^3 + 15m + n + 8mn\Big) - 5(n-1)\|n-1\|_G$.

PROOF. Let $v_1, v_2, \ldots, v_n$ be the vertices of G and let $V(\mu(G)) = \{v_1, \ldots, v_n, u_1, \ldots, u_n, w\}$. By the structure of Mycielski graph, if $v_iv_j \notin E(G)$, then $v_iu_j \notin E(G)$, and $v_ju_i \notin E(G)$.

Now we consider the following cases of nonadjacent vertex pairs in $\mu(G)$.

Case 1: The nonadjacent vertex pairs $\{v_i, v_j\}$ in $\mu(G)$.

$$\begin{aligned}
&\sum_{v_iv_j \notin E(\mu(G))} \Big(d_{\mu(G)}(v_i) + d_{\mu(G)}(v_j)\Big)^2 \\
&= \sum_{v_iv_j \notin E(G)} \Big(2d_G(v_i) + 2d_G(v_j)\Big)^2, \text{ by Lemma 2.1} \\
&= 4 \sum_{v_iv_j \notin E(G)} \Big(d_G(v_i) + d_G(v_j)\Big)^2 \\
&= 4\overline{HM}(G).
\end{aligned}$$

Case 2: The nonadjacent vertex pairs $\{u_i, u_j\}$ in $\mu(G)$.

Case 2.1: $u_iu_j \notin E(\mu(G))$ and $v_iv_j \notin E(G)$.

$$\begin{aligned}
&\sum_{u_iu_j \notin E(\mu(G))} \Big(d_{\mu(G)}(u_i) + d_{\mu(G)}(u_j)\Big)^2 \\
&= \sum_{v_iv_j \notin E(G)} \Big(d_G(v_i) + d_G(v_j) + 2\Big)^2, \text{ by Lemma 2.1} \\
&= \sum_{v_iv_j \notin E(G)} \Big((d_G(v_i) + d_G(v_j))^2 + 4(d_G(v_i) + d_G(v_j)) + 4\Big) \\
&= \overline{HM}(G) + 4\overline{M_1}(G) + 4\Big(\frac{n(n-1)}{2} - m\Big) \\
&= \overline{HM}(G) + 4\overline{M_1}(G) + 2n(n-1) - 4m.
\end{aligned}$$

Case 2.2: $u_iu_j \notin E(\mu(G))$ and $v_iv_j \in E(G)$.

$$\begin{aligned}
&\sum_{u_iu_j \notin E(\mu(G))} \Big(d_{\mu(G)}(u_i) + d_{\mu(G)}(u_j)\Big)^2 \\
&= \sum_{v_iv_j \in E(G)} \Big(d_G(v_i) + d_G(v_j) + 2\Big)^2, \text{ by Lemma 2.1} \\
&= \sum_{v_iv_j \in E(G)} \Big((d_G(v_i) + d_G(v_j))^2 + 4(d_G(v_i) + d_G(v_j)) + 4\Big) \\
&= HM(G) + 4M_1(G) + 4m.
\end{aligned}$$

If $u_iu_j \notin E(\mu(G))$, then there are m edges $v_iv_j \in E(G)$ and $\frac{n(n-1)}{2} - m$ nonadjacent vertex pair $\{v_i, v_j\}$ in G as well as $\mu(G)$. By cases 2.1 and 2.2, we have the contribution of nonadjacent vertex pair of case 2 is given by

$\Big(\frac{n(n-1)}{2}-m\Big)\Big(\overline{HM}(G)+4\overline{M_1}(G)+2n(n-1)-4m\Big)+m\Big(HM(G)+4M_1(G)+4m\Big).$

Case 3: The nonadjacent vertex pairs $\{u_i, v_i\}$ in $\mu(G)$ for each $i = 1, 2, \ldots, n$.

$$\begin{aligned}\sum_{i=1}^{n}\Big(d_{\mu(G)}(u_i)+d_{\mu(G)}(v_i)\Big)^2 &= \sum_{i=1}^{n}\Big(3d_G(v_i)+1\Big)^2, \text{ by Lemma 2.1}\\ &= \sum_{i=1}^{n}\Big(9d_G^2(v_i)+6d_G(v_i)+1\Big)\\ &= 9M_1(G)+12m+n.\end{aligned}$$

Case 4: The nonadjacent vertex pairs $\{u_i, v_j\}$ in $\mu(G)$.

$$\begin{aligned}&\sum_{u_iv_j\notin E(\mu(G))}\Big(d_{\mu(G)}(u_i)+d_{\mu(G)}(v_j)\Big)\\ =&\sum_{v_iv_j\notin E(G)}\Big(d_G(v_i)+1+2d_G(v_j)\Big)^2, \text{ by Lemma 2.1}\\ =&\sum_{v_iv_j\notin E(G)}\Big(d_G^2(v_i)+4d_G^2(v_j)+2d_G(v_i)+4d_G(v_j)+4d_G(v_i)d_G(v_j)+1\Big)\\ =&\sum_{v_iv_j\notin E(G)}\Big(d_G^2(v_i)+d_G^2(v_j)\Big)+3\sum_{v_iv_j\notin E(G)}d_G^2(v_j)+2\sum_{v_iv_j\notin E(G)}(d_G(v_i)+d_G(v_i))\\ &+2\sum_{v_iv_j\notin E(G)}d_G(v_j)+4\sum_{v_iv_j\notin E(G)}d_G(v_i)d_G(v_j)+\Big(\frac{n(n-1)}{2}-m\Big)\\ =&\ \overline{HM}(G)+3\Big(\sum_{v_k\in V(G)}d_G^2(v_k)-(n-1)\left\|n-1\right\|_G\Big)+2\overline{M}_1(G)\\ &+2\Big(\sum_{v_k\in V(G)}d_G(v_k)-(n-1)\left\|n-1\right\|_G\Big)+4\overline{M}_2(G)+\frac{n(n-1)}{2}-m\\ =&\ \overline{HM}(G)+3M_1(G)+2\overline{M}_1(G)+4\overline{M}_2(G)+\frac{n(n-1)}{2}+3m-5(n-1)\left\|n-1\right\|_G.\end{aligned}$$

Case 5: The nonadjacent vertex pairs $\{w, v_i\}$ in $\mu(G)$ for each $i = 1, 2, \ldots, n$.

$$\begin{aligned}\sum_{v_iw\notin E(\mu(G))}\Big(d_{\mu(G)}(v_i)+d_{\mu(G)}(w)\Big)^2 &= \sum_{v_i\in V(G)}\Big(2d_G(v_i)+n\Big)^2, \text{ by Lemma 2.1}\\ &= \sum_{v_i\in V(G)}\Big(4d_G^2(v_i)+n^2+4nd_G(v_i)\Big)\\ &= 4M_1(G)+n^3+8mn.\end{aligned}$$

From the above five cases of nonadjacent vertex pairs, we can obtain the desired results. This completes the proof. □

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