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# Maximizing the Zagreb Indices of $(n,m)$-Graphs[1]

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**Abstract**

For a (molecular) graph, the first and second Zagreb indices ($M_1$ and $M_2$) are two well-known topological indices in chemical graph theory introduced in 1972 by Gutman and Trinajstić. Let $\mathcal{G}_{n,m}$ be the set of connected graphs of order $n$ and with $m$ edges. In this paper we characterize the extremal graphs from $\mathcal{G}_{n,m}$ with $n+2 \leq m \leq 2n-4$ with maximal first Zagreb index and from $\mathcal{G}_{n,m}$ with $m-n = \binom{k}{2} - k$ for $k \geq 4$ with maximal second Zagreb index, respectively. Finally a related conjecture has been proposed to the extremal graphs with respect to second Zagreb index.

## 1 Introduction

We only consider finite, undirected and simple graphs throughout this paper. Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The cardinality of $E(G)$ is usually denoted by $m(G)$. The *degree* of $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices in $G$ adjacent to $v$. In particular, $\Delta(G)$ denotes the maximum degree of vertices in $G$, and $\Delta_2(G)$ is the second maximum degree of vertices in $G$. For each $v \in V(G)$ , the set of neighbors of the vertex $v$ is denoted by $N_G(v)$. For a subset $W$ of $V(G)$, let $G-W$ be the

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subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them. Similarly, for a subset $E'$ of $E(G)$, we denote by $G - E'$ the subgraph of $G$ obtained by deleting the edges of $E'$. If $W = \{v\}$ and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v$ and $G - xy$ for short, respectively. For any two nonadjacent vertices $x$ and $y$ of graph $G$, we let $G + xy$ be the graph obtained from $G$ by adding an edge $xy$. In the following we always denote by $K_{1,n-1}$ the star graph of order $n$, and by $K_n$ the complete graph of order $n$. Other undefined notations and terminology on the graph theory can be found in [4].

A graphical invariant is a number related to a graph which is a structural invariant, in other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also known as the topological indices. Two of the oldest graph invariants are the well-known Zagreb indices first introduced in [16] where Gutman and Trinajstić examined the dependence of total $\pi$-electron energy on molecular structure and elaborated in [17]. For a (molecular) graph $G$, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined as follows:

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

Alternatively, the first Zagreb index $M_1$ can be also rewritten as the following useful form:

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)) \tag{1}$$

These two classical topological indices reflect the extent of branching of the molecular carbon-atom skeleton [3, 23]. The main properties of $M_1$ and $M_2$ were summarized in [5, 6, 8, 9, 11, 12, 14, 18, 21, 26, 30]. In particular, Deng [9] gave a unified approach to determine extremal values of Zagreb indices for trees, unicyclic, and bicyclic graphs, respectively. In recent years, some novel variants of ordinary Zagreb indices have been introduced and studied, such as Zagreb coindices [1, 2], multiplicative Zagreb indices [13, 24, 29], multiplicative sum Zagreb index [10, 27] and multiplicative Zagreb coindices [28]. Especially the first and second Zagreb coindices of graph $G$ are defined [1] in the following:

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

Let $\mathcal{G}_{n,m}$ be the set of connected graphs of order $n$ and with $m$ edges. In this paper we characterized the extremal graphs from $\mathcal{G}_{n,m}$ where $n-1 \leq m \leq 2n-3$ maximizing the first Zagreb index and from $\mathcal{G}_{n,m}$ where $m-n = \binom{k}{2} - k$ with $k \geq 4$ with maximal second Zagreb index, respectively. Finally a related conjecture has been proposed with to the extremal graphs with respect to second Zagreb index.

## 2 Main results

Before stating our main results, we will list or prove some lemmas as preliminaries, which will play an important role in the next proofs.

**Lemma 2.1.** *Let $G \in \mathcal{G}_{n,m}$ with maximum Zagreb index $M_i$ for $i = 1, 2$. Then we have $\Delta(G) = n-1$.*

*Proof.* If $\Delta(G) = n-1$, our result in this lemma holds immediately. If not, we choose a vertex $u$ in the graph $G$ with maximum degree and another vertex $v \in V(G)$. So we have $d_G(u) \geq d_G(v)$. Assume that $N_G(v) \setminus N_G(u) = \{v_1, v_2, \cdots, v_s\}$. Note that $N_G(v) \setminus N_G(u) \neq \emptyset$ because of the fact that $d_G(u) < n-1$. Now we construct a new graph $G'$, which is called the *neighbor-change transformation* of $G$ on the vertices $u, v$ (or, exactly, from vertex $v$ to vertex $u$), in the following way:

$$G' = G - \{vv_1, vv_2, \cdots, vv_s\} + \{uv_1, uv_2, \cdots, uv_s\}.$$

Next we will show that $M_i(G') > M_i(G)$ for $i = 1, 2$. For convenience, we set $A_i = M_i(G') - M_i(G)$ for $i = 1, 2$. By the definition of first Zagreb index ($M_1$), we have

$$\begin{aligned} A_1 &= (d(u)+s)^2 + (d(v)-s)^2 - d(u)^2 - d(v)^2 \\ &= 2s(d(u)-d(v)) + 2s^2 \\ &> 0. \end{aligned}$$

Note that, for the edges not incident with $u$ or $v$, the corresponding parts in $M_2(G)$

and $M_2(G')$ are identical. It follows that

$$\begin{aligned}
A_2 &= \sum_{x\in N_G(u)\setminus N_G(v)} (d(u)+s)d(x) + \sum_{i=1}^{s}(d(u)+s)d(v_i) \\
&\quad + \sum_{y\in N_G(u)\cap N_G(v)} (d(u)+s+d(v)-s)d(y) - \sum_{x\in N_G(u)\setminus N_G(v)} d(u)d(x) - \sum_{i=1}^{s} d(v)d(v_i) \\
&\quad - \sum_{y\in N_G(u)\cap N_G(v)} (d(u)+d(v))d(y) \\
&= \sum_{x\in N_G(u)\setminus N_G(v)} sd(x) + \sum_{i=1}^{s}(s+d(u)-d(v))d(v_i) > 0.
\end{aligned}$$

Therefore $M_i(G') > M_i(G)$ for $i = 1, 2$ as claimed above. Thus we find that $G' \in \mathcal{G}_{n,m}$ with a larger Zagreb index ($M_1$ or $M_2$) than that of $G$. This is a contradiction to the choice of $G$, which finishes the proof of this lemma. $\square$

**Lemma 2.2.** *Let $G$ be a connected graph with two non-adjacent vertices $u, v \in V(G)$ and $G' = G + uv$. Then we have $M_1(G') = M_1(G) + 2 + 2(d_G(u) + d_G(v))$.*

*Proof.* By the definition of first Zagreb index, we have

$$\begin{aligned}
M_1(G') - M_1(G) &= d_{G'}(u)^2 - d_G(u)^2 + d_{G'}(v)^2 - d_G(v)^2 \\
&= (d_G(u)+1)^2 - d_G(u)^2 + (d_G(v)+1)^2 - d_G^2(v) \\
&= 2 + 2(d_G(u) + d_G(v)),
\end{aligned}$$

which completes the proof. $\square$

**Lemma 2.3.** *Let $G$ be a connected graph with two non-adjacent vertices $u, v \in V(G)$ and $N_G(v) = \{v_1, v_2, \cdots, v_\alpha\}$ and $N_G(u) = \{u_1, u_2, \cdots, u_\beta\}$. Suppose that $G' = G+uv$. Then $M_2(G') = M_2(G) - [(d_G(u)+1)(d_G(v)+1) + d_G(v_1) + \cdots + d_G(v_\alpha) + d_G(u_1) + \cdots + d_G(u_\beta)]$.*

*Proof.* From the definition of second Zagreb index, we have

$$\begin{aligned}
M_2(G') - M_2(G) &= (d_G(v)+1)[d_G(v_1)+\cdots+d_G(v_\alpha)] + (d_G(u)+1)[d_G(u_1)+\cdots+d_G(u_\beta)] \\
&\quad - [d_G(v)(d_G(v_1)+\cdots+d_G(v_\alpha)) + d_G(u)(d_G(u_1)+\cdots+d_G(u_\beta))] \\
&\quad + (d_G(u)+1)(d_G(v)+1) \\
&= [(d_G(u)+1)(d_G(v)+1) + d_G(v_1)+\cdots+d_G(v_\alpha) + d_G(u_1)+\cdots+d_G(u_\beta)].
\end{aligned}$$

Thus we complete the proof of this lemma. $\square$

**Lemma 2.4.** ( [1,2]) *Let $G$ be a connected graph of order $n$ and with $m$ edges. Then*

(*i*) $\overline{M}_1(G) = 2m(n-1) - M_1(G)$;

(ii) $\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$.

In the next step we start to deal with the extremal graphs with maximal Zagreb indices. First we focus on the case when $m$ is small. As two examples, two graphs $B_n^{(1)}$ and $B_n^{(2)}$ in $\mathcal{G}_{n,n+1}$ are shown in Fig. 1. Based on Lemma 2.1, we can obtain easily the following result.

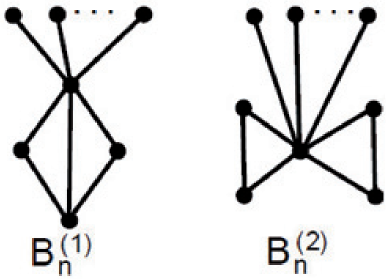


Figure 1: Two graphs $B_n^{(1)}$ and $B_n^{(2)}$

**Theorem 2.5.** ( [9]) *Let $n-1 \le m \le n+1$ and $G_i \in \mathcal{G}_{n,m}$ with maximum Zagreb index $M_i$ for $i = 1, 2$. Then we have*

*(i) $G_1 = G_2 \cong K_{1,n-1}$ for $m = n-1$;*

*(ii) $G_1 = G_2 \cong K_{1,n-1} + e$ for $m = n$ where $e = uv$ with $u, v$ as two pendent vertices in $K_{1,n-1}$;*

*(iii) $G_1 = G_2 \cong B_n^{(1)}$ for $m = n+1$ where $B_n^{(1)}$ is shown in Fig. 1.*

*Proof.* From Lemma 2.1 and the definition of the set $\mathcal{G}_{n,m}$, the results in $(i)$ and $(ii)$ holds immediately. Now we turn the proof for $(iii)$. Thanks to Lemma 2.1, again, we find that the extremal graph from $\mathcal{G}_{n,m}$ with $m = n+1$ maximizing the first and second Zagreb indices must be graph obtained by adding two new edges into the star $S_n$, that is, one of graphs $B_n^{(1)}$ and $B_n^{(2)}$ as shown in Fig. 1. By some simple calculation of $M_i(B_n^{(1)})$ and $M_i(B_n^{(2)})$ for $i = 1, 2$, our result in $(iii)$ follows immediately. □

From Theorem 2.5 we notice that, in $\mathcal{G}_{n,m}$ with $n-1 \le m \le n+1$, the graphs with maximal first Zagreb index are the same as the graphs with maximal second Zagreb index. By Lemma 2.4, the following corollary can be easily obtained.

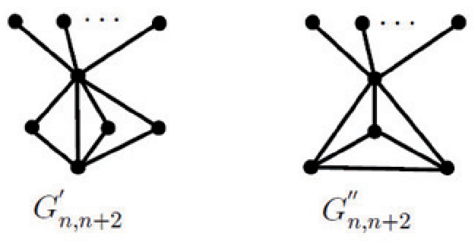


Figure 2: Two graphs $G'_{n,n+2}$ and $G''_{n,n+2}$ in $\mathcal{G}_{n,n+2}$

**Corollary 2.6.** ( [2]) *Let* $n-1 \leq m \leq n+1$ *and* $H_i \in \mathcal{G}_{n,m}$ *with minimum Zagreb coindex* $\overline{M}_i$ *for* $i = 1, 2$. *Then we have*

(*i*) $H_1 = H_2 \cong K_{1,n-1}$ *for* $m = n-1$;

(*ii*) $H_1 = H_2 \cong K_{1,n-1} + e$ *for* $m = n$ *where* $e = uv$ *with* $u, v$ *as two pendent vertices in* $K_{1,n-1}$;

(*iii*) $H_1 = H_2 \cong B_n^{(1)}$ *for* $m = n+1$ *where* $B_n^{(1)}$ *is shown in Fig. 1.*

In the next theorem we will determine the graphs from $\mathcal{G}_{n,n+2}$ maximizing the Zagreb indices ($M_1$ and $M_2$). Before doing it, we first give two graphs $G'_{n,n+2}$ and $G''_{n,n+2}$ in $\mathcal{G}_{n,n+2}$ as shown in Fig. 2.

**Theorem 2.7.** *Let* $G \in \mathcal{G}_{n,n+2}$. *Then we have*

(*i*) $M_1(G) \leq n^2 - n + 24$ *with equality holding if and only if* $G \cong G'_{n,n+2}$ *or* $G \cong G''_{n,n+2}$;

(*ii*) $M_2(G) \leq n^2 + 4n + 22$ *with equality holding if and only if* $G \cong G''_{n,n+2}$.

*Proof.* Note that any graph in $\mathcal{G}_{n,n+2}$ can be obtained by adding a new edge to a graph in $\mathcal{G}_{n,n+1}$. By the respective definitions of first and second Zagreb indices, we have

$$M_1(B_n^{(1)}) = n^2 - n + 14, \tag{2}$$

$$M_2(B_n^{(1)}) = n^2 + 2n + 9. \tag{3}$$

Assume that $G \in \mathcal{G}_{n,n+2}$ with $M_1(G)$ as large as possible. In view of Lemma 2.1, we claim that $\Delta(G) = n-1$. Therefore there exists a graph $G_0 \in \mathcal{G}_{n,n+1}$ with $\Delta(G_0) = n-1$ such that $G = G_0 + uv$. Combining the fact that $\Delta(G_0) = n-1$ and $G_0 \in \mathcal{G}_{n,n+1}$, we conclude that, for any non-adjacent vertices $u, v \in V(G_0)$, $d_{G_0}(u) + d_{G_0}(v) \leq 4$. Moreover, the second maximum vertex degree in $G_0$ is at most 3 and the case occurs only when there is a single vertex with degree 3 in $G_0$.

Firstly we prove the result in $(i)$. By Lemma 2.2 and Theorem 2.5 $(iii)$, considering the equality (2), we have

$$\begin{aligned} M_1(G) &= M_1(G_0) + 2 + 2(d_{G_0}(u) + d_{G_0}(v)) \\ &\leq n^2 - n + 14 + 2 + 2 \times 4 \\ &= n^2 - n + 24. \end{aligned}$$

The above equality holds if and only if $G_0 \cong B_n^{(1)}$ and $d_{G_0}(u) + d_{G_0}(v) = 4$, that is, $(d_{G_0}(u), d_{G_0}(v)) = (1,3)$ *or* $(2,2)$ in $G_0 \cong B_n^{(1)}$. Equivalently, we have $G \cong G'_{n,n+2}$ or $G \cong G''_{n,n+2}$, finishing the proof of (1).

Next we turn to the proof of the result in $(ii)$. Assume that $N_{G_0}(v) = \{v_1, v_2, \cdots, v_\alpha\}$ with $d_{G_0}(v_1) \geq d_{G_0}(v_2) \geq \cdots \geq d_{G_0}(v_\alpha)$ and $N_{G_0}(u) = \{u_1, u_2, \cdots, u_\beta\}$ with $d_{G_0}(u_1) \geq d_{G_0}(u_2) \geq \cdots \geq d_{G_0}(u_\beta)$. By the above argument we claim that $d_{G_0}(v_1) = n-1 = d_{G_0}(u_1)$, $\alpha \leq 2$ and $\beta \leq 2$. From Lemma 2.3, Theorem 2.5 $(iii)$ and the equality (3), we arrive at

$$\begin{aligned} M_2(G) &= M_2(G_0) + (d_{G_0}(u)+1)(d_{G_0}(v)+1) \\ &\quad + [d_{G_0}(v_1) + \cdots + d_{G_0}(v_\alpha) + d_{G_0}(u_1) + \cdots + d_{G_0}(u_\beta)] \\ &\leq n^2 + 2n + 9 + (2+1) \times (2+1) + [(n-1) + 3 + (n-1) + 3] \\ &= n^2 + 4n + 22. \end{aligned}$$

The above equality holds if and only if $G_0 \cong B_n^{(1)}$, $d_{G_0}(u) = d_{G_0}(v) = 2$ and $d_{G_0}(v_2) = d_{G_0}(u_2) = 3$ with $v_2 = u_2$ in $G_0$, that is to say, $G \cong G''_{n,n+2}$, which completes the proof. $\square$

In view of the formulas in Lemma 2.4, we have $\overline{M}_1(G'_{n,n+2}) = \overline{M}_1(G''_{n,n+2}) = n^2 + 3n - 28$ and $\overline{M}_2(G''_{n,n+2}) = \frac{1}{2}n^2 + \frac{9}{2}n - 26$. Thanks to Lemma 2.4, again, the following is an immediate result.

**Corollary 2.8.** *Let $H \in \mathcal{G}_{n,n+2}$. Then we have*

*(i) $\overline{M}_1(H) \geq n^2 + 3n - 28$ with equality holding if and only if $H \cong G'_{n,n+2}$ or $H \cong G''_{n,n+2}$;*

*(ii) $\overline{M}_2(H) \geq \frac{1}{2}n^2 + \frac{9}{2}n - 26$ with equality holding if and only if $H \cong G''_{n,n+2}$.*

The following result is very similar to Theorem 3.7 [5], we omit its proof.

**Lemma 2.9.** *Let $G$ be a graph of order $n$ with $m$ edges* $(1 \le m \le n-1)$. *Then*

$$M_1(G) \le m(m+1) \tag{4}$$

*with equality holding if and only if* $G \cong K_{1,m} \cup (n-m-1)K_1$.

For any integer $m$ satisfying $n+3 \le m \le 2n-4$, we denote by $N_{n,m}^{n-1,\,m-n+2}$ a graph of order $n$ and with $m$ edges in which maximum degree is $n-1$ and the second maximum degree is $m-n+2$. The structure of graph $N_{n,m}^{n-1,\,m-n+2}$ can be seen in Fig. 3.

**Theorem 2.10.** *For any graph* $G \in \mathcal{G}_{n,m}$ *where* $n+3 \le m \le 2n-4$, *we have*

$$M_1(G) \le n(n-1) + (m-n+1)(m-n+6) \tag{5}$$

*with equality holding if and only if* $G \cong N_{n,m}^{n-1,\,m-n+2}$.

*Proof.* Assume that $G \in \mathcal{G}_{n,m}$ with $M_1(G)$ as large as possible. By Lemma 2.1, we find that the graph $G$ contains a star $K_{1,n-1}$ as a subgraph. Therefore $G$ can be viewed as a graph obtained by adding $m-n+1$ new edges to the star $S_n$. Then we can construct a new graph $G'$ of order $n-1$ with $m-n+1$ edges $(n+3 \le m \le 2n-4)$, obtained from $G$ by deleting the vertex of maximum degree and the incident edges with it. Let the degree sequence of $G$ be $\pi(G) = (d_1, d_2, d_3, \dots, d_n)$ and also let the degree sequence of $G'$ be $\pi(G') = (d'_1, d'_2, \dots, d'_{n-1})$. Then we have $d_1 = n-1$, $d_{i+1} = d'_i + 1$, $i = 1, 2, \dots, n-1$, and

$$\begin{aligned}
M_1(G) &= \sum_{i=1}^{n} d_i^2 = (n-1)^2 + \sum_{i=1}^{n-1} \left(d'_i + 1\right)^2 \\
&= (n-1)^2 + (n-1) + \sum_{i=1}^{n-1} d_i'^2 + 2\sum_{i=1}^{n-1} d'_i \\
&\le n(n-1) + (m-n+1)(m-n+2) + 4(m-n+1) \quad \text{by Lemma 2.9} \quad (6) \\
&= n(n-1) + (m-n+1)(m-n+6).
\end{aligned}$$

Moreover, the equality holds in (5) if and only if the equality holds in (6), that is to say, $G' \cong K_{1,\,m-n+1} \cup (2n-m-3)K_1$ by Lemma 2.9. Thus we conclude that $\Delta_2(G) = m-n+2$ and $G \cong N_{n,m}^{n-1,\,m-n+2}$, finishing the proof of this theorem. $\square$

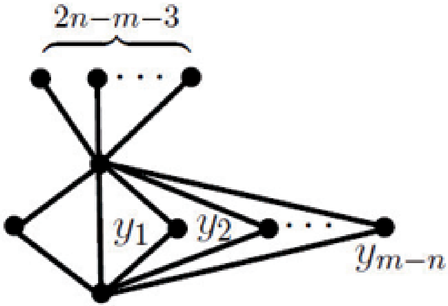


Figure 3: The graph $N_{n,m}^{n-1,\,m-n+2}$

To characterize the extremal graphs from $\mathcal{G}_{n,m}$ where $m \geq n+3$ with maximum second Zagreb index, we need introduce some new notations. Denote by $K_k^{n-k}$ the graph obtained by attaching $n-k$ pendent vertices to one vertex of $K_k$. For any positive integer $t < k$, let $K_k^{n-k}(t)$ be a graph obtained by adding $t$ new edges between one pendent vertex in $K_k^{n-k}$ and $t$ vertices with degree $k-1$ in it. In particular, the graph $G''_{n,n+2}$ defined before is just $K_4^{n-4}$. For a graph $G$, we define $M^*(G) = \sum_{uv \in E(G)} (d_G(u)+1)(d_G(v)+1)$.

Before turning to my main result, we first prove a preliminary lemma as follows.

**Lemma 2.11.** *Let $G$ be a graph of order $n$ and with $\binom{k}{2}$ edges where $4 \leq k \leq n-1$. Then we have*

$$M^*(G) \leq \frac{(k-1)k^3}{2}$$

*with equality holding if and only if $G \cong K_k \cup (n-k)K_1$.*

*Proof.* By the definition of $M^*(G)$, considering the equality (1), we have

$$\begin{aligned}
M^*(G) &= \sum_{uv \in E(G)} (d_G(u)+1)(d_G(v)+1) \\
&\leq \frac{1}{2} \sum_{uv \in E(G)} [(d_G(u)+1)^2 + (d_G(v)+1)^2] \qquad (7) \\
&= \frac{1}{2} \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2 + 2(d_G(u)+d_G(v)) + 2] \\
&= \frac{1}{2} \sum_{u \in V(G)} [d_G(u)^3 + 2d_G(v)^2 + d_G(u)] \\
&= \frac{1}{2} \sum_{u \in V(G)} [d_G(u)^3 + 2d_G(u)^2] + \binom{k}{2}.
\end{aligned}$$

Note that the above equality (7) holds if and only if $d_G(u) = d_G(v)$ for any edge $uv \in E(G)$. Now it suffices to determine the maximum of $A(G) \triangleq \sum_{u \in V(G)} [d_G(u)^3 + 2d_G(u)^2]$. Next we will distinguish the following two cases.

**Case 1.** All $\binom{k}{2}$ edges in $G$ form exactly one nontrivial connected component in it.

In this case, we find that the equality (7) holds if and only if $G \cong G^* \cup (n-s)K_1$ where $G^*$ is a connected regular graph of order $s$. Moreover, $A(G^*) = A(G)$. Now we conclude that all vertices in $G^*$ have degree $\frac{k(k-1)}{s}$, and

$$\begin{aligned} A(G^*) &= s\left[ (\frac{k(k-1)}{s})^3 + 2(\frac{k(k-1)}{s})^2 \right] \\ &= \frac{(k(k-1))^3}{s^2} + 2\frac{(k(k-1))^2}{s}. \end{aligned}$$

Clearly $A(G^*)$ will reach its maximum when $s$ is as small as possible. Taking into account the fact the simple graph $G^*$ is a regular one with $\binom{k}{2}$ edges, we find that the minimum value of $s$ is $k$. Thus we have

$$\begin{aligned} A(G^*) &= \frac{(k(k-1))^3}{s^2} + 2\frac{(k(k-1))^2}{s} \\ &\le \frac{(k(k-1))^3}{k^2} + 2\frac{(k(k-1))^2}{k} \\ &= (k-1)^2 k(k+1). \end{aligned}$$

The above equality holds if and only if $s = k$, that is to say, $G^* \cong K_k \cup (n-k)K_1$. This finishes the proof of "Only if" part in this case.

**Case 2.** All $\binom{k}{2}$ edges in $G$ form more than one nontrivial connected components in it.

From the above argument (before Case 1), these $\binom{k}{2}$ edges form a regular subgraph in $G$ and with $t \ge 2$ nontrivial connected components when $M^*(G)$ reaches its maximum. Assume that $G = G_0 \cup (n-s)K_1$ where $G_0 = G_{s_1}^{(p_1)} \cup G_{s_2}^{(p_2)} \cdots G_{s_t}^{(p_t)}$ denotes a union of some connected or disconnected regular graphs with $G_{s_i}^{(p_i)}$ being an $p_i$-regular graph of order $s_i$ and with $m_i$ edges for $p_i \in \{1, 2, \cdots, t\}$ with $1 \le t \le k-2$ such that $\sum_{i=1}^{t} m_i = \binom{k}{2}$. Then we have $s_i = \frac{2m_i}{p_i}$. Therefore in this case we only need to prove the following inequality:

$$\sum_{i=1}^{t} \frac{2m_i}{p_i}(p_i^3 + 2p_i^2) \quad < \quad (k-1)^2 k(k+1),$$

which is just

$$\sum_{i=1}^{t} (p_i^2 + 2p_i)m_i < (k^2-1) \sum_{i=1}^{t} m_i \qquad (8)$$

We claim that the inequality (8) holds immediately from the fact that $p_i^2+2p_i < k^2-1$ for $p_i \in \{1,2,\cdots,t\}$ with $1 \leq t \leq k-2$. This completes the proof of "only if" part in this case.

Conversely, we can easily find that $M^*(G) = \frac{(k-1)k^3}{2}$ if $G \cong K_k \cup (n-k)K_1$, ending the proof of this lemma. $\square$

**Theorem 2.12.** *Assume that* $m-n = \binom{k}{2} - k$ *with* $k \geq 4$*. Let* $G \in \mathcal{G}_{n,m}$ *with maximum second Zagreb index. Then we have* $G \cong K_k^{n-k}$ .

*Proof.* By Lemma 2.1, we conclude that there are at least one vertex of degree $n-1$. So we have

$$G = G^* \vee K_1 ,$$

where

$$|V(G^*)| = n-1, \quad \text{and} \quad m(G^*) = \frac{1}{2}(k-1)(k-2) .$$

Let $d_1 \geq d_2 \geq \cdots \geq d_{n-1} \geq d_n$ be the degree vertices of graph $G$ and also let $d_1^* \geq d_2^* \geq \cdots \geq d_{n-2}^* \geq d_{n-1}^*$ be the degree vertices of graph $G^*$. Thus we have $d_i = d_{i-1}^* + 1$, i=2, 3,. . . , n and $d_1 = n-1$. Then we have

$$\begin{aligned}
M_2(G) &= \sum_{v_iv_j \in E(G)} d_i\, d_j \\
&= \sum_{v_1v_j \in E(G)} d_1\, d_j + \sum_{v_iv_j \in E(G),\, 2 \leq i<j \leq n} d_i\, d_j \\
&= d_1 \sum_{i=2}^{n} d_i + \sum_{v_iv_j \in E(G^*)} (d_i^*+1)\,(d_j^*+1) \\
&= (n-1)\Big(k^2+n-3k+1\Big) + \sum_{v_iv_j \in E(G^*)} (d_i^*+1)\,(d_j^*+1) .
\end{aligned}$$

Now we have to find the maximum value of

$$\sum_{v_iv_j \in E(G^*)} (d_i^*+1)\,(d_j^*+1)$$

where

$$|V(G^*)| = n-1, \quad \text{and} \quad m(G^*) = \frac{1}{2}(k-1)(k-2) .$$

By Lemma 2.11, we have

$$\sum_{v_iv_j \in E(G^*)} (d_i^*+1)\,(d_j^*+1) \leq \frac{(k-1)(k-2)}{2}\,(k-1)^2 ,$$

with equality if and only if

$$G^* \cong K_{k-1} \cup (n-k)K_1 \,.$$

Therefore we arrive at $G = (K_{k-1} \cup (n-k)K_1) \vee K_1 \cong K_k^{n-k}$, completing the proof of this theorem. $\square$

Now we consider the extremal graph, which maximizes the second Zagreb index, from $\mathcal{G}_{n,m}$ with $m = n + \binom{k}{2} - k + t$ where $1 \leq t \leq k-1$. Note that the complement of graph $G$ of order $n$ and with $m = n + \binom{k}{2} - k + t$ edges where $1 \leq t \leq k-1$ is a forest of order $n$ and with $\binom{n}{2} - m = n - 2 - t$ edges. For the case when $m = n + \binom{k}{2} - k + t$ with $k = n-1$, we know, from Theorem 10 in [8], that the graph from $\mathcal{G}_{n,m}$ maximizing the second Zagreb index is obtained by joining one isolated vertex with complete graph $K_{n-1}$ by $t$ edges, which is just $K_1^{n-1}(t)$. But this problem is still open for the case when $4 \leq k \leq n-2$. Therefore we would like to end this paper with following conjecture.

**Conjecture 1.** Assume that $n + 3 \leq m$. Let $G \in \mathcal{G}_{n,m}$ with maximum second Zagreb index. Then $G \cong K_k^{n-k}(t)$ if $m - n = \binom{k}{2} - k + t$ with $1 \leq t \leq k-1$ and $4 \leq k \leq n-2$.

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