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SOME RESULTS ON THE DIFFERENCE OF THE ZAGREB INDICES OF A GRAPH

MINGQIANG AN✉ and LIMING XIONG

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Abstract

The classical first and second Zagreb indices of a graph G are defined as $M_1(G) = \sum_{v\in V(G)} d(v)^2$ and $M_2(G) = \sum_{e=uv\in E(G)} d(u)d(v)$, where $d(v)$ is the degree of the vertex v of G. Recently, Furtula *et al.* ['On difference of Zagreb indices', *Discrete Appl. Math.* **178** (2014), 83–88] studied the difference of M_1 and M_2, and showed that this difference is closely related to the vertex-degree-based invariant $RM_2(G) = \sum_{e=uv\in E(G)}[d(u) - 1][d(v) - 1]$, the reduced second Zagreb index. In this paper, we present sharp bounds for the reduced second Zagreb index, given the matching number, independence number and vertex connectivity, and we also completely determine the extremal graphs.

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1. Introduction

All graphs considered in this paper are finite undirected simple connected graphs. Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. Let $d_G(v)$ be the degree of a vertex v in G. When the graph is clear from the context, we will omit the subscript G from the notation. For graph theoretical terms that are not defined here, we refer to [3].

For a given graph G, its first and second Zagreb indices are defined as follows:

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

and

$$M_2(G) = \sum_{e=uv\in E(G)} d(u)d(v). \tag{1.1}$$

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The first Zagreb index can also be expressed as a sum over edges of G [6],

$$M_1(G) = \sum_{e=uv\in E(G)} [d(u) + d(v)]. \tag{1.2}$$

In 1972, the quantities M_1 and M_2 were discovered in certain approximate expressions for the total π-electron energy [12]. In 1975, these graph invariants were proposed as measures of branching of the carbon atom skeleton [11]. The name 'Zagreb index' (or, more accurately, 'Zagreb group index') seems to be first used in the review article [1] and after that became standard. For a survey of mathematical properties and chemical applications of the Zagreb indices, we refer to [6, 8, 9, 16]. What we call here the 'first Zagreb index' was independently studied in the mathematical literature under other names [2, 4, 5, 17].

Although the fact that the two Zagreb indices were introduced simultaneously [11, 12] and analysed together, the relations between them were not considered until relatively recently. Given the extensive research on the two Zagreb indices, it is somewhat astonishing that these indices were not directly compared. In particular, their difference $M_2 - M_1$ seems to have been studied only to a limited extent [10, 15].

Recently, Furtula *et al.* [7] considered this problem, and showed that the difference of M_1 and M_2 is closely related to the vertex-degree-based invariant named the *reduced second Zagreb index*, which is defined as

$$RM_2(G) = \sum_{e=uv\in E(G)} [d(u) - 1][d(v) - 1].$$

In mathematical chemistry, this invariant is often referred to as the 'Wiener polarity index'. A few basic properties of RM_2 were determined [7]. If the graph G is a tree, then $RM_2(G)$ is equal to the number of pairs of vertices at distance 3 [19].

In this paper, we present sharp bounds for the reduced second Zagreb indices with given matching number, independence number and vertex connectivity, and we also completely determine the extremal graphs.

2. Preliminaries

Let us first introduce some notation and terminology. We denote by K_n and S_n the complete graph and the star graph on n vertices, respectively. For two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, the *union* $G_1 \cup G_2$ is defined to be $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. The *join* $G_1 \vee G_2$ of G_1 and G_2 is obtained from $G_1 \cup G_2$ by connecting each vertex of G_1 with each vertex of G_2 by an edge. We write $G - e$ for the graph formed from G by deleting the edge $e \in E(G)$ and $G + e$ for the graph obtained from G by adding the edge e, provided that $e \notin E(G)$.

The addition of new edges in the graph increases some vertex degrees.

LEMMA 2.1. *Let G be a connected graph of order at least three.*

(a) *If G is not isomorphic to K_n, then $RM_2(G) < RM_2(G + e)$ for any $e \in E(\overline{G})$.*

(b) *If G has an edge e not being a cut edge, then $RM_2(G) > RM_2(G - e)$.*

By Lemma 2.1, we can characterise the connected graphs with maximum RM_2-value. More precisely, we arrive at the following result.

THEOREM 2.2. *Among all connected graphs of order n, the complete graph K_n has maximum RM_2.*

PROOF. If G is not the complete graph, then we can repeatedly add edges into G until we obtain $G = K_n$. By Lemma 2.1, $RM_2(G) \leq RM_2(K_n)$, with equality if and only if $G \cong K_n$. □

A *matching* of a graph G is a set of edges with no shared end points. The *matching number* $\beta(G)$ of the graph G is the number of edges in a maximum matching. Obviously, $\beta(G) = 0$ if and only if G is an empty graph (with no edges). For a connected graph G with $n \geq 2$ vertices, $\beta(G) = 1$ if and only if $G = S_n$ or $G = K_3$. If $\beta(G) = n/2$, then the graph G has a perfect matching.

The following lemma, known as the Tutte–Berge formula, is an important tool to characterise the matching number.

LEMMA 2.3 [14, 18]. *Suppose that G is a graph of order n with matching number β. Let $o(H)$ denote the number of odd components (that is, components of odd cardinality) of a graph H. Then*

$$n - 2\beta = \max\{o(G - X) - |X| : X \subset V(G)\}.$$

We also need the following result.

LEMMA 2.4. *Let G be a connected graph of size m. Then*

$$M_2(G) - M_1(G) = RM_2(G) - m.$$

PROOF. By (1.1) and (1.2), noting that the set $E(G)$ has m elements,

$$\begin{aligned} M_2(G) - M_1(G) &= \sum_{e=uv\in E(G)} [d(u)d(v) - d(u) - d(v)] \\ &= \sum_{e=uv\in E(G)} [(d(u) - 1)(d(v) - 1) - 1] \\ &= RM_2(G) - m. \end{aligned}$$

□

3. Main results

In this section, we shall establish various bounds for RM_2 in terms of other graph parameters including the matching number, independence number and vertex connectivity. First we present the following auxiliary result.

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Lemma 3.1 [13]. *The four roots of the quartic $ax^4 + bx^3 + cx^2 + dx + e = 0$ $(a \neq 0)$ with real coefficients are given by*

$$\begin{aligned}
x_1 &= -\frac{b}{4a} - \Psi(A,B,C) + \Phi(A,B),\\
x_2 &= -\frac{b}{4a} + \Psi(A,B,C) + \Phi(A,B),\\
x_3 &= -\frac{b}{4a} + \Psi'(A,B,C) - \Phi(A,B),\\
x_4 &= -\frac{b}{4a} - \Psi'(A,B,C) - \Phi(A,B),
\end{aligned}$$

where

$$\begin{aligned}
\Psi(A,B,C) &= \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} + \frac{C}{8a^3\Phi(A,B)}},\\
\Psi'(A,B,C) &= \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} - \frac{C}{8a^3\Phi(A,B)}},\\
\Phi(A,B) &= \frac{1}{2}\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}}
\end{aligned}$$

and $A = c^2 - 3bd + 12ae$, $B = \sqrt[3]{D + \sqrt{-4A^3 + D^2}}$, $C = -b^3 + 4abc - 8a^2d$ *and* $D = 2c^3 - 9bcd + 27ad^2 + 27b^2e - 72ace$.

Theorem 3.2. *Let G be a connected graph of order $n \geq 4$ with matching number β, $2 \leq \beta \leq \lfloor n/2 \rfloor$. Let $\sigma_1, \sigma_2, \sigma_3$ and σ_4 be the four roots of the equation*

$$8x^4 + (n-30)x^3 - (\tfrac{3}{2}n^2 - 7n - 28)x^2 + (\tfrac{3}{2}n^2 - 10n - 6)x + 2n = 0.$$

(1) *If $\beta = \lfloor n/2 \rfloor$, then $RM_2(G) \leq \frac{1}{2}n(n-1)(n-2)^2$, with equality if and only if $G \cong K_n$.*

(2) *If $\beta \in (\sigma_2, \sigma_3) \cup (\sigma_4, \lfloor n/2 \rfloor - 1)$, then $RM_2(G) \leq 8\beta^4 - 28\beta^3 + (4n+28)\beta^2 - (6n+8)\beta + 2n$, with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

(3) *If $\beta = \sigma_i$ $(i = 2,3,4)$, then $RM_2(G) \leq 8\beta^4 - 28\beta^3 + (4n+28)\beta^2 - (6n+8)\beta + 2n = (2-n)\beta^3 + (\frac{3}{2}n^2 - 3n)\beta^2 - (\frac{3}{2}n^2 - 4n + 2)\beta$, with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$ or $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

(4) *If $\beta \in [2, \sigma_2] \cup [\sigma_3, \sigma_4]$, then $RM_2(G) \leq (2-n)\beta^3 + (\frac{3}{2}n^2 - 3n)\beta^2 - (\frac{3}{2}n^2 - 4n + 2)\beta$, with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

Proof. Let G_0 be a graph having maximum reduced second Zagreb index among all connected graphs of order n with matching number β. By Lemma 2.3, there is a vertex subset $X_0 \subset V(G_0)$ such that

$$n - 2\beta = \max\{o(G_0 - X) - |X| : X \subset V(G_0)\} = o(G_0 - X_0) - |X_0|.$$

For convenience, let $|X_0| = s$ and $o(G_0 - X_0) = t$. Then $n - 2\beta = t - s$.

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Suppose that $s = 0$. Then $G_0 - X_0 = G_0$ and $n - 2\beta = t \leq 1$. If $t = 0$ then $\beta = n/2$ and if $t = 1$ then $\beta = (n-1)/2$. In both cases, by Lemma 2.1, $G_0 = K_n$ and $RM_2(G) = \frac{1}{2}n(n-1)(n-2)^2$.

Assume in the following that $s \geq 1$ and consequently $t \geq 1$. Let $G_1, G_2, \ldots, G_t$ be all the odd components of $G_0 - X_0$. If $G_0 - X_0$ has an even component, then, by adding an edge in G_0 between a vertex of an even component and a vertex of an odd component of $G_0 - X_0$, we obtain a graph G' for which $n - 2\beta(G') \geq o(G' - X_0) - |X_0| = o(G_0 - X_0) - |X_0|$. It follows that $\beta(G') = \beta$ and, by Lemma 2.1, G' has larger reduced second Zagreb index than G_0, which is a contradiction. Thus, $G_0 - X_0$ does not have an even component. Similarly, $G_1, G_2, \ldots, G_t$ and the subgraph induced by X_0 are all complete and any vertex of $G_1, G_2, \ldots, G_t$ is adjacent to every vertex in X_0. Let $n_i = |V(G_i)|$ for $i = 1, 2, \ldots, t$. Then

$$G_0 = K_s \vee (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_t}).$$

Assume that $n_1 \leq n_2 \leq \cdots \leq n_t$. If $3 \leq n_i \leq n_j$, let

$$G_0' = K_s \vee (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_i - 2} \cup \cdots \cup K_{n_j + 2} \cup \cdots \cup K_{n_t}).$$

Define $f(x) = \binom{x}{2}(x + s - 2)^2 + sx(n-2)(x + s - 2)$ as a function of x on the interval $[2, +\infty)$ so that

$$RM_2(G_0) - RM_2(G_0') = f(n_i) + f(n_j) - f(n_i - 2) - f(n_j + 2).$$

Denote $F(x) = f(x) - f(x-2)$ so that $RM_2(G_0) - RM_2(G_0') = F(n_i) - F(n_j + 2)$. Note $F(x) = 4x^3 + (6s - 27)x^2 + (2s^2 - 32s + 4ns + 62)x - 7s^2 + 40s + 2ns^2 - 8ns - 48$. By taking the derivative,

$$\begin{aligned} F'(x) &= 12x^2 + 6(2s - 9)x + 2s^2 - 32s + 4ns + 62 \\ &= 6\Big(\sqrt{2}x - \frac{9}{2\sqrt{2}}\Big)^2 + 4s(n + 3x - 8) + 2s^2 + \frac{5}{4} > 0, \end{aligned}$$

since $x \geq 2$ and $n \geq 4$. This implies that $F(x)$ is a strictly increasing function on $[2, +\infty)$. Thus, $F(n_i) < F(n_j) < F(n_j + 2)$ and $RM_2(G_0) - RM_2(G_0') < 0$.

Therefore, $RM_2(G_0)$ attains its maximum if and only if $n_1 = n_2 = \cdots = n_{t-1} = 1$ and $n_t = n - s - t + 1 = 2\beta - 2s + 1$. It follows that

$$G_0 = K_s \vee (K_{2\beta - 2s + 1} \cup \overline{K_{n+s-2\beta-1}})$$

and

$$\begin{aligned} RM_2(G_0) = &\binom{s}{2}(n-2)^2 + \binom{2\beta - 2s + 1}{2}(2\beta - s - 1)^2 \\ &+ s(2\beta - 2s + 1)(n-2)(2\beta - s - 1) \\ &+ s(n + s - 2\beta - 1)(s-1)(n-2) \\ = &\,2s^4 + 3(n - 4\beta - 1)s^3 + \Big(\frac{3}{2}n^2 - 8n\beta - 5n + 26\beta^2 + 5\beta + 4\Big)s^2 \\ &- \Big(\frac{3}{2}n^2 - 4n + 24\beta^3 - 4\beta^2 + 2\beta - 4n\beta^2 - 2n\beta + 3\Big)s \\ &+ 8\beta^4 - 4\beta^3 - 2\beta^2 + \beta. \end{aligned}$$

We can consider the last expression as a function $\Phi(s)$. The second derivative of $\Phi(s)$ is

$$\Phi''(s) = 24s^2 + 18(n - 4\beta - 1)s + 3n^2 - 16n\beta - 10n + 52\beta^2 + 10\beta + 8.$$

Claim 1. $\Phi''(s) > 0$.

To prove our claim, recall that $1 \le s \le \beta \le n/2$. The discriminant of the quadratic equation $\Phi''(s) = 0$ is

$$\Delta_{\Phi''} = 192\beta^2 - (1056n - 1632)\beta + 36n^2 + 312n - 444.$$

Now consider the function

$$\Theta_1(\beta) = 192\beta^2 - (1056n - 1632)\beta + 36n^2 + 312n - 444.$$

The discriminant of $\Theta_1(\beta) = 0$ is $\Delta_{\Theta_1} = 1087488n^2 - 3686400n + 3004416$. Let us denote

$$\Theta_2(n) = 1087488n^2 - 3686400n + 3004416.$$

Since the discriminant of $\Theta_2(n) = 0$ is $\Delta_{\Theta_2} = 1.358954496 \times 10^{13} - 1.3069065388032 \times 10^{13} > 0$, the maximum positive root of the equation $\Theta_2(n) = 0$ is $n_* = (3686400 + \sqrt{\Delta_{\Theta_2}})/2174976$. Note that $\Delta_{\Theta_1} = \Theta_2(n) > 0$ when $n > n_*$. Therefore, the maximum positive root of the equation $\Theta_1(\beta) = 0$ is

$$\beta_* = \frac{1056n - 1632 + \sqrt{\Theta_2(n)}}{384} > \frac{1056n + \sqrt{147456n}}{384} > n > \left\lfloor \frac{n}{2} \right\rfloor - 1.$$

Since $\beta \in [2, \lfloor n/2 \rfloor - 1]$, we find that $\Delta_{\Phi''} = \Theta_1(\beta) < 0$, which completes the proof of Claim 1.

By Claim 1, $\Phi(s)$ is a strictly convex function for $1 \le s \le \beta$ and the maximum value of $\Phi(s)$ is attained when $s = 1$ or $s = \beta$. Note that

$$\Phi(1) = 8\beta^4 - 28\beta^3 + (4n + 28)\beta^2 - (6n + 8)\beta + 2n,$$

$$\Phi(\beta) = (2 - n)\beta^3 + (\tfrac{3}{2}n^2 - 3n)\beta^2 - (\tfrac{3}{2}n^2 - 4n + 2)\beta.$$

After subtraction,

$$\Psi(\beta) = \Phi(1) - \Phi(\beta) = 8\beta^4 + (n - 30)\beta^3 - (\tfrac{3}{2}n^2 - 7n - 28)\beta^2 + (\tfrac{3}{2}n^2 - 10n - 6)\beta + 2n.$$

If $n > (6 + 2\sqrt{5})/2$, then $n^2 - 6n + 4 > 0$ and $\Psi(2) = -3(n^2 - 6n + 4) < 0$. Note that $\Psi(\beta)$ is continuous in the interval $[2, \lfloor n/2 \rfloor - 1]$. Further, by Lemma 3.1, $\Psi(\beta) < 0$ for $\beta \in [2, \sigma_2] \cup [\sigma_3, \sigma_4]$, while $\Psi(\beta) > 0$ for $\beta \in (\sigma_2, \sigma_3) \cup (\sigma_4, \lfloor n/2 \rfloor - 1)$. This completes the proof. □

Using Theorem 3.2 and Lemma 2.4, we have the following corollary.

COROLLARY 3.3. *Let G be a connected graph of order $n \ge 4$ and size m with matching number β, $2 \le \beta \le \lfloor n/2 \rfloor$. Let $\sigma_1, \sigma_2, \sigma_3$ and σ_4 be the four roots of the equation*

$$8x^4 + (n - 30)x^3 - (\tfrac{3}{2}n^2 - 7n - 28)x^2 + (\tfrac{3}{2}n^2 - 10n - 6)x + 2n = 0.$$

(1) *If* $\beta = \lfloor n/2 \rfloor$, *then* $M_2(G) - M_1(G) \le \frac{1}{2}n(n-1)(n-2)^2 - m$, *with equality if and only if* $G \cong K_n$.
(2) *If* $\beta \in (\sigma_2, \sigma_3) \cup (\sigma_4, \lfloor n/2 \rfloor - 1)$, *then* $M_2(G) - M_1(G) \le 8\beta^4 - 28\beta^3 + (4n+28)\beta^2 - (6n+8)\beta + 2n - m$, *with equality if and only if* $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.
(3) *If* $\beta = \sigma_i$ $(i = 2, 3, 4)$, *then* $M_2(G) - M_1(G) \le 8\beta^4 - 28\beta^3 + (4n+28)\beta^2 - (6n+8)\beta + 2n - m = (2-n)\beta^3 + (\frac{3}{2}n^2 - 3n)\beta^2 - (\frac{3}{2}n^2 - 4n + 2)\beta - m$, *with equality if and only if* $G \cong K_\beta \vee \overline{K_{n-\beta}}$ *or* $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.
(4) *If* $\beta \in [2, \sigma_2] \cup [\sigma_3, \sigma_4]$, *then* $M_2(G) - M_1(G) \le (2-n)\beta^3 + (\frac{3}{2}n^2 - 3n)\beta^2 - (\frac{3}{2}n^2 - 4n + 2)\beta - m$, *with equality if and only if* $G \cong K_\beta \vee \overline{K_{n-\beta}}$.

A vertex subset S of a graph G is said to be an *independent set* of G if the subgraph induced by S is an empty graph; $\beta = \max\{|S| : S$ is an independent set of $G\}$ is said to be the *independence number* of G.

THEOREM 3.4. *Let G be a connected graph of order $n \ge 4$ with independence number β. Then*

$$RM_2(G) \le \tfrac{1}{2}n^4 - \tfrac{5}{2}n^3 - (\tfrac{3}{2}\beta^2 - \tfrac{3}{2}\beta - 4)n^2 + (\beta^3 + 3\beta^2 - 4\beta - 2)n - 2\beta^3 + 2\beta,$$

with equality if and only if $G \cong \overline{K_\beta} \vee K_{n-\beta}$.

PROOF. Let $G_{\max}$ be a graph chosen among all n-vertex connected graphs with independence number β such that $G_{\max}$ has the largest RM_2. Let S be a maximal independent set in $G_{\max}$ with $|S| = \beta$. Since adding edges into a graph will increase its RM_2 by Lemma 2.1, each vertex x in S is adjacent to every vertex y in $G_{\max} - S$. Furthermore, the subgraph induced by vertices in $G_{\max} - S$ is a clique in $G_{\max}$. So, $G_{\max} \cong \overline{K_\beta} \vee K_{n-\beta}$.

An elementary calculation gives

$$\begin{aligned} RM_2(G) &= \binom{n-\beta}{2}(n-2)^2 + \beta(n-\beta)(n-\beta-1)(n-2) \\ &= \frac{1}{2}n^4 - \frac{5}{2}n^3 - \left(\frac{3}{2}\beta^2 - \frac{3}{2}\beta - 4\right)n^2 + (\beta^3 + 3\beta^2 - 4\beta - 2)n - 2\beta^3 + 2\beta. \quad \square \end{aligned}$$

The following result is an immediate consequence of Theorem 3.4 and Lemma 2.4.

COROLLARY 3.5. *Let G be a connected graph of order $n \ge 4$ and size m with independence number β. Then*

$$\begin{aligned} M_2(G) - M_1(G) \le \tfrac{1}{2}n^4 - \tfrac{5}{2}n^3 - (\tfrac{3}{2}\beta^2 - \tfrac{3}{2}\beta - 4)n^2 \\ + (\beta^3 + 3\beta^2 - 4\beta - 2)n - 2\beta^3 + 2\beta - m, \end{aligned}$$

with equality if and only if $G \cong \overline{K_\beta} \vee K_{n-\beta}$.

The *vertex connectivity* is the minimum number of vertices whose deletion from a connected graph disconnects it.

THEOREM 3.6. *Let G be a connected graph of order $n \geq 4$ with vertex connectivity k. Then*

$$RM_2(G) \leq \tfrac{1}{2}n^4 - \tfrac{9}{2}n^3 + (k + \tfrac{29}{2})n^2 + (k^2 - 6k - \tfrac{39}{2})n - \tfrac{3}{2}k^2 + \tfrac{15}{2}k + 9,$$

with equality if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

PROOF. We choose $G_{\max}$ to be a graph such that $G_{\max}$ has the largest RM_2 within all connected graphs of order n with vertex connectivity k. Let C be a vertex cut in $G_{\max}$ such that $|C| = k$ and let $G_{\max} - C = G_1 \cup G_2 \cup \cdots \cup G_t$ $(t \geq 2)$. By Lemma 2.1, we must have $t = 2$, for otherwise we can add edges between any two components, resulting in a new graph G' with vertex connectivity k and a strictly larger RM_2 than that of $G_{\max}$, in contradiction to our choice of $G_{\max}$.

The same reasoning shows that both G_1 and G_2 are cliques of $G_{\max}$, that the subgraph of $G_{\max}$ induced by C is a clique and that any vertex in $G_1 \cup G_2$ is adjacent to each vertex in C. Let n_i denote the order of G_i. Thus, we have $G_{\max} \cong K_k \vee (K_{n_1} \cup K_{n_2})$.

Assume without loss of generality that $n_2 \geq n_1$. If $n_1 = 1$, then the result follows readily. Suppose now that $n_2 \geq n_1 \geq 2$. By the definition of RM_2,

$$\begin{aligned} RM_2(G_{\max}) &= \binom{n_1}{2}(n - n_2 - 2)^2 + \binom{n_2}{2}(n - n_1 - 2)^2 + \binom{k}{2}(n-2)^2 \\ &\quad + n_1 k(n - n_2 - 2)(n-2) + n_2 k(n - n_1 - 2)(n-2) \\ &= n_1^2 n_2^2 - \frac{1}{2}[4n^2 - (15 - 2k)n + 16 - 5k]n_1 n_2 + \frac{1}{2}n(n-1)(n-2)^2. \end{aligned}$$

Let $G' = K_k \vee (K_{n_1 - 1} \cup K_{n_2 + 1})$. Then

$$\begin{aligned} RM_2(G') - RM_2(G_{\max}) &= n_1^2 + n_2^2 + 2n_1^2 n_2 + 2n_2 + 1 - 2n_1 n_2^2 - 2n_1 - 4n_1 n_2 \\ &\quad - \tfrac{1}{2}[4n^2 - (15 - 2k)n + 16 - 5k](n_1 - n_2 - 1). \end{aligned}$$

Now we consider the function

$$\begin{aligned} F(x, y) &= x^2 + y^2 + 2x^2 y + 2y + 1 - 2xy^2 - 2x - 4xy \\ &\quad - \tfrac{1}{2}[4n^2 - (15 - 2k)n + 16 - 5k](x - y - 1), \end{aligned}$$

where $y \geq x \geq 2$. After simplification,

$$F(x, y) - F(y, x) = (x - y)[-4n^2 + (15 - 2k)n + 4xy + 5k - 20].$$

Set $\Phi(n) = -4n^2 + (15 - 2k)n + 4xy + 5k - 20$. The maximum positive root of the equation $\Phi(n) = 0$ is

$$n_{\max} = \frac{2k - 15 + \sqrt{4k^2 + 20k + 64xy - 95}}{-8}.$$

If $n > n_{\max}$, then $\Phi(n) < 0$ and $F(x, y) > F(y, x)$. This implies that

$$F(x, y) > F(x + 1, y - 1) > F(x + 2, y - 2) > \cdots > F(n - k - 2, 2). \tag{3.1}$$

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By direct calculation,

$$F(n-k-2,2) = -2n^3 + (k + \tfrac{45}{2})n^2 + (k^2 - 10k - \tfrac{167}{2})n + \tfrac{5}{2}k^2 + \tfrac{67}{2}k + 105.$$

It is easy to see that $F(n-k-2,2) > 0$ when $n > n_+$, where n_+ is the maximum root of the equation $F(n-k-2,2) = 0$. Thus, by (3.1), we have $F(x,y) > 0$. It follows that $RM_2(G') - RM_2(G_{\max}) = F(n_1,n_2) > 0$, in contradiction to our choice of $G_{\max}$.

Therefore, $G_{\max} \cong K_k \vee (K_1 \cup K_{n-k-1})$. An elementary calculation gives

$$\begin{aligned} RM_2(K_k \vee (K_1 \cup K_{n-k-1})) = {} & \tfrac{1}{2}n^4 - \tfrac{9}{2}n^3 + (k + \tfrac{29}{2})n^2 \\ & + (k^2 - 6k - \tfrac{39}{2})n - \tfrac{3}{2}k^2 + \tfrac{15}{2}k + 9, \end{aligned}$$

completing the proof. □

Combining Theorem 3.6 and Lemma 2.4, we can obtain the following result.

COROLLARY 3.7. *Let G be a connected graph of order $n \geq 4$ and size m with vertex connectivity k. Then*

$$M_2(G) - M_1(G) \leq \tfrac{1}{2}n^4 - \tfrac{9}{2}n^3 + (k + \tfrac{29}{2})n^2 + (k^2 - 6k - \tfrac{39}{2})n - \tfrac{3}{2}k^2 + \tfrac{15}{2}k + 9 - m,$$

with equality if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

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MINGQIANG AN, College of Science,
Tianjin University of Science and Technology, Tianjin 300457, PR China
e-mail: anmq@tust.edu.cn

LIMING XIONG, School of Mathematics and Statistics,
Beijing Institute of Technology, Beijing 100081, PR China
e-mail: lmxiong@bit.edu.cn