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UPPER BOUNDS FOR THE REDUCED SECOND ZAGREB INDEX OF GRAPHS

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Abstract. The graph invariant RM_2, known under the name reduced second Zagreb index, is defined as $RM_2(G) = \sum_{uv\in E(G)}(d_G(u)-1)(d_G(v)-1)$, where $d_G(v)$ is the degree of the vertex v of the graph G. In this paper, we give a tight upper bound of RM_2 for the class of graphs of order n and size m with at least one dominating vertex. Also, we obtain sharp upper bounds on RM_2 for all graphs of order n with k dominating vertices and for all graphs of order n with k pendant vertices. Finally, we give a sharp upper bound on RM_2 for all k-apex trees of order n. Moreover, the corresponding extremal graphs are characterized.

1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $d_G(u)$, the degree of the vertex u of G. If $d_G(u) = 1$ then vertex u is called a pendant vertex and if $d_G(u) = |V(G)| - 1$ then vertex u is called a dominating vertex of G. For a subset X of $E(G)$, we denote by $G - X$ the subgraph of G obtained by deleting the edges in X. Similarly, the graph obtained from G by adding a set of edges X is denoted by $G + X$. If $X = \{e\}$, we write $G - e$ and $G + e$. For a subset A of $V(G)$, the subgraph obtained from G by deleting the vertices in A together with their incident edges is denoted by $G - A$. If $A = \{v\}$ then we write $G - v$. For any positive integer k with $k \geq 1$, a graph G is called a k-apex tree if there exists a subset A of $V(G)$ such that $G - A$ is a tree and $|A| = k$,

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while for any $B \subseteq V(G)$ with $\mid B \mid < k$, $G - B$ is not a tree. A vertex of A is called a k-apex vertex. The join $G \oplus H$ of disjoint graphs G and H is the graph obtained from $G + H$ by joining each vertex of G to each vertex of H.

A topological index of a graph is a quantity which is invariant under automorphism of the graph. The most studied and well-known topological indices are the first Zagreb index M_1 and second Zagreb index M_2 of a graph G and they are defined as

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2$$

and

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

These indices were first found to occur within certain approximate expressions for the total π-electron energy [16]. For more details of the mathematical studies and chemical applications of M_1 and M_2, we refer the reader to [5, 7, 22, 25, 26, 32] and references quoted therein. For the last ten years, much attention is being paid to the relation of M_1 and M_2 of graph G, for details see [18]. Direct comparisons were obtained on the Zagreb indices for trees [12, 30] and cyclic graphs [21, 23, 29].

Furtula, Gutman and Ediz [13] studied the difference between Zagreb indices and showed that this difference is closely related to the vertex-degree-based invariant named the reduced second Zagreb index, which is defined as

$$RM_2(G) = \sum_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1).$$

Note that $RM_2(G) = M_2(G) - M_1(G) + m$ where m is the number of edges of G and if the graph G is a tree, then $RM_2(G)$ is the number of unordered pairs of vertices u and v in G such that the distance between u and v is equal to three.

Gutman, Furtula, Elphick [15] showed that if G is a graph with t triangles, then $RM_2(G) = p + 3t$ where p is the number of subgraphs of G isomorphic to P_4. An and Xiong [3] presented sharp bounds for the reduced second Zagreb indices with a given matching number, independence number and vertex connectivity, and they also determined the extremal graphs. In [8] and [19], the graphs having extremal value of RM_2 were determined for some special classes of graphs. He, Li and Zhao [17] presented sharp upper and lower bounds on RM_2 of connected cyclic graphs of given order with a given number of cut vertices. Recently, Gao and Xu [14] determined the extremal graphs among all connected graphs of order n and with $n(n-1)/2 - m$ edges with respect to RM_2, and obtain the first ten largest RM_2 for connected graphs of order n. Moreover, they obtained the sharp upper bound on RM_2 for all connected bipartite graphs with given connectivity k and determined the extremal graphs with respect to RM_2 for all connected bipartite graphs with given matching number q.

Ahlswede and Katona [2] showed that the maximum value of M_1 is achieved on the quasi-complete or quasi-star graphs. In 2009, Ábrego, Fernández-Merchant, Neubauer and Watkins [1] determined all other graphs for which the maximum value of M_1 is attained. Also the problem of maximizing the second Zagreb index M_2 for general graphs of given order and size was studied in 1999 by Bollobás, Erdős and Sarkar [6]. Xu, Das and Balachandran studied this problem for connected graphs and posed a conjecture which is still open [31]. However, there are vast researches on bounds of Zagreb indices for various classes of graphs [4, 9, 10, 11, 20, 24, 27].

The paper is organized as follows. In section 2, we give a tight upper bound of RM_2 for the class of graphs of order n and size m with at least one dominating vertex. Interestingly, the extremal graph corresponding to our obtained bound is isomorphic to the extremal graph for the conjecture of Xu et al. [31]. However, we show that it does not hold in general. In section 3, we obtain a sharp upper bound on RM_2 in terms of order and the number of dominating vertices and determine the graphs for which the bound is attained. In section 4, we give a sharp upper bound on RM_2 in terms of order and the number of pendant vertices and determine the graphs for which the bound is attained. Finally, we determine the graphs having maximum RM_2 in the class of k-apex trees of order n.

2. Upper bound on RM_2 of graphs of order n and size m with at least one dominating vertex

Let n and m be given positive integers. Then, for m, there uniquely exist two integers k and r such that $m = \binom{k}{2} + r$ and $0 < r \leq k$. A quasi-complete graph $QC(n, m)$ is a graph of order n and size m consisting of a complete subgraph of order k and at least $n-k-1$ isolated vertices, with the remaining vertex connected to r vertices of the complete subgraph. Then we have

$$M_2(QC(n,m)) = \binom{r}{2}k^2 + \binom{k-r}{2}(k-1)^2 + rk(k-r)(k-1) + r^2k. \tag{2.1}$$

Bollobás, Erdős and Sarkar [6] proved that if $\binom{k}{2} < m \leq \binom{k+1}{2}$ then the maximum value of M_2 is attained on the graph $QC(k+1, m)$. From the definition of M_2, we have $M_2(QC(k+1, m) = M_2(QC(n, m))$. Hence the above result can be reformulated as follows.

Lemma 2.1. [6] *Let G be a graph of order n and size m. Then $M_2(G) \leq M_2(QC(n, m))$.*

Now we give the following a tight upper bound of RM_2 by using the above result.

Theorem 2.2. *Let G be a graph of order n and size m that has at least one dominating vertex. Let k and r be positive integers such that $m - n + 1 = \binom{k}{2} + r$ and $0 < r \leq k$. Then*

$$RM_2(G) \leq \binom{r}{2}k^2 + \binom{k-r}{2}(k-1)^2 + rk(k-r)(k-1) + r^2k + 2(n-2)(m-n+1)$$

the bound is tight and is attained if G is isomorphic to $QC(n-1, m-n+1) \oplus K_1$.

Proof. Let x be a dominating vertex of G. Then we have

$$\begin{aligned} RM_2(G) &= \sum_{uv\in E(G)} (d_G(u)-1)(d_G(v)-1) \\ &= \sum_{uv\in E(G-x)} d_{G-x}(u)d_{G-x}(v) + (d_G(x)-1)\sum_{u\in V(G-x)} d_{G-x}(u) \\ &= M_2(G-x) + 2(n-2)|E(G-x)| \\ &= M_2(G-x) + 2(n-2)(m-n+1). \qquad (2.2) \end{aligned}$$

Clearly we have $|V(G-x)| = n-1$ and $|E(G-x)| = m-n+1$. Consider the quasi-complete graph $QC(n-1, m-n+1)$. Then since k and r are integers such that $m-n+1 = \binom{k}{2} + r$ and $0 < r \leq k$, we have

$$M_2(QC(n-1, m-n+1)) = \binom{r}{2}k^2 + \binom{k-r}{2}(k-1)^2 + rk(k-r)(k-1) + r^2k. \qquad (2.3)$$

On the other hand, we have

$$M_2(G-x) \leq M_2(QC(n-1, m-n+1)) \qquad (2.4)$$

by Lemma 2.1.

Therefore, using (2.3) and (2.4) in (2.2), we get the required inequality. One can easily see that the bound is tight and is attained if G is isomorphic to $QC(n-1, m-n+1) \oplus K_1$. This completes the proof. □

Xu, Das and Balachandran [31] conjectured that the graph $QC(n-1, m-n+1) \oplus K_1$ has the maximum value of M_2 in the class of connected graphs of order n and size m. We have proved that this graph also has the maximum value of RM_2 in the class of graphs of order n and size m with at least one dominating vertex. But the following remark tells us that the graph $QC(n-1, m-n+1) \oplus K_1$ does not have maximum value of RM_2 in the class of connected graphs of order n and size m.

G_1 G_2

Figure 1. $RM_2(G_1) = 204$ and $RM_2(G_2) = 81$

Remark 2.3. In general, $RM_2(QC(n-1, m-n+1) \oplus K_1)$ is not maximum in the class of connected graphs of order n and size m. If $n = 9$ and $m = 16$ then $RM_2(QC(8, 8) \oplus K_1) = 201$, but we have $RM_2(G_1) = 204$. Also if $n = 9$ and $m = 12$ then $RM_2(QC(8, 4) \oplus K_1) = 75$ and $RM_2(G_2) = 81$ (see Figure 1).

3. Sharp upper bound on RM_2 of graphs of order n with k dominating vertices

A matching in a graph G is a set of edges without common vertices. Let M be a matching in G. Then a vertex v of G is said to be M-saturated, if some edge of M is incident with v, otherwise, v is M-unsaturated. If every vertex of G is M-saturated, then M is called perfect. A maximum matching in G is a matching that contains the largest possible number of edges. Let A be any subset of $V(G)$. Then the induced subgraph $G[A]$ is the graph whose vertex set is A and edge set consists of all of the edges in $E(G)$ that have both end vertices in A.

Theorem 3.1. *Let G be a graph of order n with k dominating vertices.*
(i) If $n-k$ is even then

$$RM_2(G) \leq \left(\binom{n-k}{2} - \frac{n-k}{2}\right)(n-3)^2 + \binom{k}{2}(n-2)^2 + k(n-k)(n-2)(n-3) \tag{3.1}$$

with equality holding if and only if G is isomorphic to $(K_{n-k}-M)\oplus K_k$, where M is a perfect matching in K_{n-k}.
(ii) If $n-k$ is odd then

$$\begin{aligned} RM_2(G) \quad \leq \quad & \binom{n-k-1}{2}(n-3)^2 + \binom{k}{2}(n-2)^2 + \frac{(n-3)(n-5)(n-k-3)}{2} \\ & + k(n-2)\left((n-k)(n-3)-1\right) \end{aligned} \tag{3.2}$$

with equality holding if and only if G is isomorphic to $(K_{n-k}-M-e)\oplus K_k$, where M is a maximum matching in K_{n-k} and e is an edge of K_{n-k} such that one end vertex of e is M-unsaturated.

Proof. Let A and B be disjoint subsets of $V(G)$. Then denote by $E_G(A,B)$ the set of edges connecting a vertex in A to a vertex in B. Let us denote by A the set of all dominating vertices of G and $B=V(G)\setminus A$. Then, we have $d_G(u)=n-1$ for all $u\in A$ and

$$|E(G[A])| = \binom{k}{2}$$

since $|A|=k$. Hence by the definition of the reduced second Zagreb index, we get

$$\begin{aligned} RM_2(G) \quad = \quad & \sum_{uv\in E(G[B])}(d_G(u)-1)(d_G(v)-1) + \sum_{uv\in E(G[A])}(d_G(u)-1)(d_G(v)-1) \\ & + \sum_{uv\in E_G(A,B)}(d_G(u)-1)(d_G(v)-1) \\ = \quad & \sum_{uv\in E(G[B])}(d_G(u)-1)(d_G(v)-1) + \binom{k}{2}(n-2)^2 + k(n-2)\sum_{v\in B}(d_G(v)-1). \end{aligned} \tag{3.3}$$

(i) Let $n-k$ be even. Since $|A|=k$ and there is no dominating vertex in B, we have

$$|B| = n-k \quad \text{and} \quad d_G(v)\leq n-2 \text{ for all } v\in B \tag{3.4}$$

and it follows that

$$|E(G[B])| = \frac{1}{2}\sum_{z\in V(G[B])} d_{G[B]}(z) \leq \binom{n-k}{2} - \frac{n-k}{2}. \tag{3.5}$$

Then using (3.4) and (3.5) in (3.3), we obtain

$$\begin{aligned} RM_2(G) &\leq \sum_{uv\in E(G[B])}(n-3)^2+\binom{k}{2}(n-2)^2+k(n-2)\sum_{v\in B}(n-3) \\ &\leq \left(\binom{n-k}{2}-\frac{n-k}{2}\right)(n-3)^2+\binom{k}{2}(n-2)^2+k(n-k)(n-2)(n-3), \end{aligned}$$

that is, the inequality (3.1).

Suppose now that equality holds in (3.1). Then, the equalities hold in (3.4) and (3.5). From the equality in (3.4), we have $d_G(v)=n-2$ for all $v\in B$. On the other hand, since $n-k$ is even, K_{n-k} has a perfect matching M. Therefore, the equalities in (3.4) and (3.5) hold if and only if the subgraph induced in G by B is isomorphic to $K_{n-k}-M$. From this, we conclude that G is isomorphic to $(K_{n-k}-M)\oplus K_k$.

(ii) Let $n-k$ be odd. Then since there is no dominating vertex in B, we have $d_{G[B]}(y)\leq n-k-2$ for all $y\in B$. But there exists a vertex $x\in B$ such that $d_{G[B]}(x)\leq n-k-3$ by the handshaking lemma. Hence, it follows that

$$2|E(G[B])|=\sum_{z\in V(G[B])}d_{G[B]}(z)\leq(n-k-1)(n-k-2)+d_{G[B]}(x) \tag{3.6}$$

and

$$d_G(x)\leq n-3,\quad d_G(y)\leq n-2 \text{ for all } y\in B\setminus\{x\}. \tag{3.7}$$

Therefore from (3.6) and (3.7), respectively, we have

$$|E(G[B\setminus\{x\}])|=|E(G[B])|-d_{G[B]}(x)\leq\binom{n-k-1}{2}-\frac{d_{G[B]}(x)}{2} \tag{3.8}$$

and

$$\sum_{v\in B}(d_G(v)-1)\leq(n-k-1)(n-3)+(n-4)=(n-k)(n-3)-1. \tag{3.9}$$

Let $n\leq 4$. Then since $n-k$ is odd, G is isomorphic to S_4 or S_4+e. In this case, we have $n=4$ and $k=1$. Hence, one can easily see that theorem holds.

Let now $n > 4$. Then from (3.7) and (3.8), we get

$$\begin{aligned}
&\sum_{uv\in E(G[B])}(d_G(u)-1)(d_G(v)-1)\\
= &\sum_{uv\in E([G(B\backslash\{x\}])}(d_G(u)-1)(d_G(v)-1)+(d_G(x)-1)\sum_{xv\in E(G[B])}(d_G(v)-1)\\
\leq &\sum_{uv\in E([G(B\backslash\{x\}])}(n-3)^2+(n-4)\sum_{xv\in E(G[B])}(n-3)\\
\leq &\left(\binom{n-k-1}{2}-\frac{d_{G[B]}(x)}{2}\right)(n-3)^2+d_{G[B]}(x)(n-3)(n-4)\\
= &\binom{n-k-1}{2}(n-3)^2+\frac{(n-3)(n-5)d_{G[B]}(x)}{2}\\
\leq &\binom{n-k-1}{2}(n-3)^2+\frac{(n-3)(n-5)(n-k-3)}{2}. \qquad (3.10)
\end{aligned}$$

Hence using (3.9) and (3.10) in (3.3), we obtain the required inequality (3.2).

Suppose now that the equality holds in (3.2). Then, all inequalities in the above must be equalities. From the equality in (3.7), we have $d_G(x) = n-3$ and $d_G(y) = n-2$ for all $y \in B \setminus \{x\}$. Then the equalities in (3.9) and (3.10) hold. On the other hand, since $n-k$ is odd, K_{n-k} has a maximum matching M of size $(n-k-1)/2$. Let e be an edge of K_{n-k} such that one end vertex of e is M-unsaturated. Thus, one can easily see that the equalities in (3.9) and (3.10) hold if and only if the subgraph induced in G by B is isomorphic to $K_{n-k} - M - e$. From all above, we conclude that G is isomorphic to $(K_{n-k} - M - e) \oplus K_k$. □

4. Sharp upper bound on RM_2 of graphs of order n with k pendant vertices

Denote by $\mathcal{G}(n,k)$ the class of graphs of order n with k pendant vertices in which the removal of all pendant vertices and their incident edges results in a complete graph of order $n-k$. Let n and k be given positive integers with $k \leq n$. Also let $a_1, a_2, \dots, a_{n-k}$ be non-negative integers such that $a_1 \geq a_2 \geq \cdots \geq a_{n-k}$ and $a_1 + a_2 + \cdots + a_{n-k} = k$. Then, we denote by $G(a_1, a_2, \dots, a_{n-k})$ the graph obtained from complete graph K_{n-k} by attaching a_i edges to the vertex u_i of K_{n-k}, $i = 1, 2, \dots, n-k$.

Lemma 4.1. [19] *Let G be a connected graph and $xy \notin E(G)$. Consider the graph $G' = G + xy$. Then $RM_2(G') > RM_2(G)$.*

Let $(a_1, a_2, \dots, a_n)$ and $(b_1, b_2, \dots, b_n)$ be two sequences of real numbers. Then it is said that the sequence $(a_1, a_2, \dots, a_n)$ majorizes the sequence $(b_1, b_2, \dots, b_n)$ if the following conditions are satisfied

(i) $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$

(ii) $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ for all $1 \leq i \leq n-1$

(iii) $a_1 + a_2 + \cdots + a_n = b_1 + b_2 + \cdots + b_n$.

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Lemma 4.2. (Karamata's inequality) *Let $f\colon I \to \mathbb{R}$ be a convex function. If $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ are numbers in I such that $(a_1, a_2, \ldots, a_n)$ majorizes $(b_1, b_2, \ldots, b_n)$, then*

$$f(a_1) + f(a_2) + \cdots + f(x_n) \geq f(b_1) + f(b_2) + \cdots + f(b_n).$$

If f is a strictly convex function, then the above inequality holds with equality if and only if $a_i = b_i$ for all $1 \leq i \leq n$.

Theorem 4.3. *Let G be a graph of order n with k pendant vertices. Then*

$$\begin{aligned} RM_2(G) \quad \leq \quad & \frac{k(k-1)}{2} - \frac{1}{2}\left\lfloor \frac{k}{n-k} \right\rfloor \left(3k - n - (n-k)\left\lfloor \frac{k}{n-k} \right\rfloor\right) \\ & + (n-k-1)(n-k-2)\left(k + \frac{(n-k)(n-k-2)}{2}\right) \end{aligned} \tag{4.1}$$

with equality holding if and only if G is isomorphic to $G(\underbrace{q+1, \ldots, q+1}_{r}, \underbrace{q, \ldots, q}_{n-k-r})$, where q and r are positive integers such that $k = (n-k)q + r$ and $0 \leq r < n-k$.

Proof. Let q and r be positive integers such that $k = (n-k)q + r$ and $0 \leq r < n-k$. For the convenience, we denote by $(b_1, b_2, \ldots, b_{n-k})$ the sequence

$$(\underbrace{q+1, \ldots, q+1}_{r}, \underbrace{q, \ldots, q}_{n-k-r}),$$

where $b_1 = \cdots = b_r = q+1$ and $b_{r+1} = \cdots = b_{n-k} = q$.

Suppose that G does not belong to $\mathcal{G}(n,k)$ and $RM_2(G)$ is maximum in the class of graphs of order n with k pendant vertices. Then there exist non-adjacent vertices u and v of degrees greater than one. Now consider the graph $G' = G + uv$. Then by Lemma 4.1, we have $RM_2(G') > RM_2(G)$ and a contradiction. Hence $G \in \mathcal{G}(n,k)$. Let $u_1, u_2, \ldots, u_{n-k}$ be the vertices of the clique K_{n-k} and a_i be the number of pendant vertices adjacent to vertex u_i in G. Then $d_G(u_i) = a_i + n - k - 1$ for $1 \leq i \leq n-k$ and $\sum_{i=1}^{n-k} a_i = k$. By definition of the reduced second Zagreb index, we get

$$\begin{aligned} RM_2(G) &= \sum_{i<j} (a_i + n - k - 2)(a_j + n - k - 2) \\ &= \sum_{i<j} a_i a_j + (n-k-2)\sum_{i<j}(a_i + a_j) + (n-k-2)^2 \binom{n-k}{2} \\ &= \frac{1}{2}\left(\sum_{i=1}^{n-k} a_i\right)^2 - \frac{1}{2}\sum_{i=1}^{n-k} a_i^2 + (n-k-1)(n-k-2)\left(k + \frac{(n-k)(n-k-2)}{2}\right) \\ &= \frac{k^2}{2} - \frac{1}{2}\sum_{i=1}^{n-k} a_i^2 + (n-k-1)(n-k-2)\left(k + \frac{(n-k)(n-k-2)}{2}\right). \end{aligned} \tag{4.2}$$

Assume that $a_1 \geq a_2 \geq \cdots \geq a_{n-k}$. Then there exists a positive integer t such that

$$a_1 \geq a_2 \geq \cdots \geq a_t \geq q+1 > q \geq a_{t+1} \geq \cdots \geq a_{n-k} \tag{4.3}$$

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because $\sum_{i=1}^{n-k} a_i = \sum_{i=1}^{n-k} b_i = k$. Then, clearly we have $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ for all $1 \leq i \leq t$. Suppose that

$$a_1 + a_2 + \cdots + a_j < b_1 + b_2 + \cdots + b_j \tag{4.4}$$

for some $t + 1 \leq j \leq n$. Then from (4.3) and $b_l \geq q$ for all l, it follows that

$$a_{j+1} + a_{j+2} + \cdots + a_{n-k} \leq q(n - k - j) \leq b_{j+1} + b_{j+2} + \cdots + b_{n-k}. \tag{4.5}$$

From (4.4) and (4.5), we have $\sum_{i=1}^{n-k} a_i < \sum_{i=1}^{n-k} b_i$ and a contradiction. Hence $(a_1, a_2, \ldots, a_{n-k})$ majorizes $(b_1, b_2, \ldots, b_{n-k})$. Obviously, the function $f(x) = x^2$ is strictly convex. Hence by Karamata's inequality, we obtain

$$\begin{aligned}
\sum_{i=1}^{n-k} a_i^2 &\geq r(q+1)^2 + (n-k-r)q^2 \\
&= 2rq + r + q^2(n-k) \\
&= k + q(3k - n - (n-k)q) \\
&= k + \left\lfloor \frac{k}{n-k} \right\rfloor \left(3k - n - (n-k)\left\lfloor \frac{k}{n-k} \right\rfloor\right) \qquad (4.6)
\end{aligned}$$

with equality holding if and only if $a_i = b_i$ for all $1 \leq i \leq n - k$.

Therefore from (4.2) and (4.6), we get the required result. □

5. Sharp upper bound on RM_2 of k-apex trees of order n

For positive integers $n \geq 3$ and $k \geq 1$, let $\mathbb{T}(n, k)$ denote the class of all k-apex trees of order n. The following bound was given in [28].

Lemma 5.1. [28] *Let $G \in \mathbb{T}(n, k)$. Then*

$$M_2(G) \leq \frac{1}{2}(n-1)(k+1)\Big(k(n-1) + 2(k+1)(n-k-1)\Big)$$

with equality if and only if G is isomorphic to $S_{n-k} \oplus K_k$.

Lemma 5.2. *Let $G \in \mathbb{T}(n, k)$ and x be an apex vertex of G. If $RM_2(G)$ is maximum in $\mathbb{T}(n, k)$, then x is the dominating vertex in G. i.e., $d_G(x) = n - 1$.*

Proof. Suppose that $d_G(x) < n - 1$ for any apex vertex x of G. Then there exists a vertex y in G such that $xy \notin E(G)$. We consider the graph $G' = G + xy$. Then we have $RM_2(G') > RM_2(G)$ by Lemma 4.1. But it contradicts to the fact that $RM_2(G)$ is maximum in $\mathbb{T}(n, k)$. □

Theorem 5.3. *Let $G \in \mathbb{T}(n, k)$. Then*

$$RM_2(G) \leq \frac{1}{2}(n-2)k(k+1)(3n - 2k - 4)$$

with equality holding if and only if G is isomorphic to $S_{n-k} \oplus K_k$.

Proof. Suppose that $RM_2(G)$ is maximum in $\mathbb{T}(n,k)$. Let x be an apex vertex in G. Then $d_G(x) = n-1$ by Lemma 5.2 and $d_G(u) = d_{G-x}(u) + 1$ for all $u \in V(G)$ with $u \neq x$. Therefore

$$\begin{aligned} RM_2(G) &= \sum_{uv \in E(G)} (d_G(u)-1)(d_G(v)-1) \\ &= \sum_{uv \in E(G-x)} d_{G-x}(u) d_{G-x}(v) + (d_G(x)-1) \sum_{u \in V(G-x)} d_{G-x}(u) \\ &= M_2(G-x) + 2(n-2)|E(G-x)|. \qquad (5.1) \end{aligned}$$

Let A with $|A| = k$ be the set of all k-apex vertices in G. Since $RM_2(G)$ is maximum in $\mathbb{T}(n,k)$, we have $d_G(x) = n-1$ for all $x \in A$ by Lemma 5.1. Hence the subgraph induced by A is a complete graph of order k and $G - A$ is a tree of order $n-k$. Thus

$$|E(G)| = \binom{k}{2} + k(n-k) + n - k - 1 = \frac{k(2n-k-3)}{2} + n - 1 \qquad (5.2)$$

and it follows that

$$|E(G-x)| = |E(G)| - n + 1 = \frac{k(2n-k-3)}{2} \qquad (5.3)$$

since $d_G(x) = n-1$. On the other hand by Lemma 5.1, we have

$$M_2(G-x) \leq \frac{1}{2}(n-2)k\Big((k-1)(n-2) + 2k(n-k-1)\Big) \qquad (5.4)$$

becuase $G - x$ is a $(k-1)$-apex tree of order $n-1$. Using the inequalities (5.3) and (5.4) in (5.1), we get

$$\begin{aligned} RM_2(G) &\leq \frac{1}{2}(n-2)k\Big((k-1)(n-2) + 2k(n-k-1) + 2(2n-k-3)\Big) \\ &= \frac{1}{2}(n-2)k\Big(3nk - 2k^2 - 6k + 3n - 4\Big) \\ &= \frac{1}{2}(n-2)k(k+1)(3n-2k-4). \qquad (5.5) \end{aligned}$$

By Lemma 5.1, the equality in (5.4) holds if and only if $G - x$ is isomorphic to $S_{n-k} \oplus K_{k-1}$. Thus since $d_G(x) = n-1$, it follows that the equality in (5.5) holds if and only if G is isomorphic to $S_{n-k} \oplus K_k$. □

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