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THE RANDIĆ ENERGY OF GENERALIZED DOUBLE SUN

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Abstract. We show that the family of trees defined as generalized double sun of odd order satisfies the conjecture for the Randić energy proposed by I. Gutman, B. Furtula, S. B. Bozkurt (2014).

Keywords: graph; Randić matrix; Randić energy

MSC 2020: 05C50, 05C09, 05C92

1. Introduction

Let G be a graph of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $i = 1, 2, \ldots, n$, denote by $d_G(v_i)$ ($d(v_i)$ for short) the degree of the vertex v_i in G.

The *Randić matrix* $R(G) = (r_{ij})_{n\times n}$ of G is defined as (see [3], [4], [7])

$$r_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_G(u_i)d_G(v_j)}} & \text{if } v_iv_j \in E(G),\\ 0 & \text{otherwise.}\end{cases}$$

The eigenvalues of $R(G)$, denoted by $\varrho_1(G), \varrho_2(G), \ldots, \varrho_n(G)$, are called the *Randić eigenvalues* of G. The *Randić energy* of G is defined as (see [4], [7])

$$\mathcal{E}_R(G) = \sum_{i=1}^{n} |\varrho_i(G)|.$$

There are some results on $\mathcal{E}_R(G)$, see [3], [4], [5], [6], [7], [8].

For each $p \geqslant 0$, the *p-sun*, denoted by Su_p, depicted in Figure 1, is the tree of order $n = 2p + 1$ formed by taking the star on $p + 1$ vertices and subdividing each edge.

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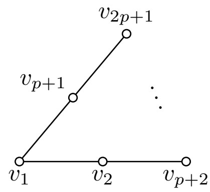

Figure 1. The p-sun Su_p.

For $p, q \geqslant 0$, the (p, q)-*double sun*, denoted by $DSu_{p,q}$, depicted in Figure 2, is the tree of order $n = 2(p+q+1)$ obtained by connecting the centers of DSu_p and DSu_q with an edge.

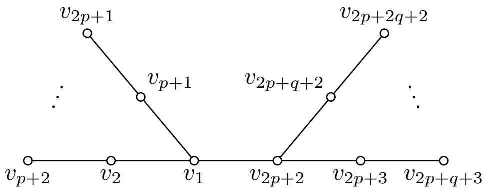

Figure 2. The (p, q)-double sun $DSu_{p,q}$.

The tree with exactly two vertices of degree greater than 2 is called a *generalized double sun*. The vertex of degree greater than 2 is called a *branched vertex*. Let T be a generalized double sun with branched vertices u and v. We call the path centered at u (or v) a *pendant path*.

Conjecture 1.1 ([7]). *Let T be a tree of order n. If n is odd, then the maximum $\mathcal{E}_R(T)$ is achieved for T being the $(\frac{1}{2}(n-1))$-sun. If n is even, then the maximum $\mathcal{E}_R(T)$ is achieved for T being the $(\lceil \frac{1}{4}(n-2) \rceil, \lfloor \frac{1}{4}(n-2) \rfloor)$-double sun.*

In [1], [2], the authors present some families of graphs that satisfy Conjecture 1.1. Motivated by them, in this work we show that the generalized double suns of odd order satisfy Conjecture 1.1.

In Section 2, we give some lemmas. In Section 3, we present a few operations. In Section 4, we show that generalized double suns of odd order satisfy Conjecture 1.1.

2. Preliminaries

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. Then its *Randić index* is given by

$$R_{-1}(G) = \sum_{uv\in E(G)} \frac{1}{d(u)d(v)}.$$

Theorem 2.1 ([2]). *Let $p \geqslant 3$, and Su_p be the p-sun of order $n = 2p+1$ as depicted in Figure 1. Then $\mathcal{E}_R(Su_p) = 2 + (p-1)\sqrt{2} = (n-3)\frac{1}{2}\sqrt{2} + 2$.*

Lemma 2.2 ([2]). *Let G be a connected graph with the Randić matrix R. Then*

$$\operatorname{tr}(R^2) = 2R_{-1}(G).$$

Lemma 2.3 ([2]). *Let G be a graph with the Randić matrix R. Then*

$$\mathcal{E}_R(G) \leqslant \sqrt{(n-1-\operatorname{null}(R))(\operatorname{tr}(R^2)-1)} + 1,$$

where $\operatorname{null}(R)$ *is the nullity of the matrix R. Furthermore, if G is bipartite, then*

$$\mathcal{E}_R(G) \leqslant \sqrt{(n-2-\operatorname{null}(R))(\operatorname{tr}(R^2)-2)} + 2.$$

Lemma 2.4. *Let T be a generalized double sun of order n with branched vertices u and v.*

(1) *If $d(u,v) \geqslant 2$, then $R_{-1}(T) \leqslant \frac{1}{4}(n+1)$.*
(2) *If $d(u,v) = 1$, then $R_{-1}(T) < \frac{1}{4}(n+2)$. In particular, if T has at least one pendant vertex centered at u (or v), then $R_{-1}(T) < \frac{1}{4}(n+1)$.*

Proof. Denote $d(u) = p+1$, $d(v) = q+1$, and there are s and t pendant paths centered at u and v, respectively, see Figure 3.

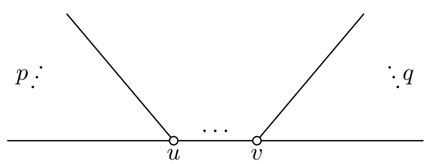

Figure 3. Tree T.

(1) If $d(u,v) \geqslant 2$, then

$$\begin{aligned} R_{-1}(T) &= \sum_{v_i v_j \in E(T)} \frac{1}{d_T(v_i) d_T(v_j)} \\ &= \frac{s}{p+1} + \frac{p-s+1}{2(p+1)} + \frac{p-s}{2} + \frac{t}{q+1} + \frac{q-t+1}{2(q+1)} \\ &\quad + \frac{q-t}{2} + \frac{n-1-(2p-s+1)-(2q-t+1)}{4} \\ &= \frac{n+1}{4} - s\frac{p-1}{4(p+1)} - t\frac{q-1}{4(q+1)} \leqslant \frac{n+1}{4}. \end{aligned}$$

(2) If $d(u,v) = 1$, then

$$\begin{aligned} R_{-1}(T) &= \sum_{v_i v_j \in E(T)} \frac{1}{d_T(v_i) d_T(v_j)} \\ &= \frac{s}{p+1} + \frac{p-s}{2(p+1)} + \frac{p-s}{2} + \frac{t}{q+1} + \frac{q-t}{2(q+1)} + \frac{q-t}{2} \\ &\quad + \frac{1}{(p+1)(q+1)} + \frac{n-1-(2p-s)-(2q-t)-1}{4} \\ &= \frac{n}{4} - s\frac{p-1}{4(p+1)} - t\frac{q-1}{4(q+1)} + \frac{pq+1}{2(p+1)(q+1)} \\ &\leqslant \frac{n}{4} + \frac{pq+1}{2(p+1)(q+1)} < \frac{n}{4} + \frac{1}{2} = \frac{n+2}{4}. \end{aligned}$$

In particular, if T has at least one pendant path centered at u (or v), that is, $s \geqslant 1$ (or $t \geqslant 1$), then

$$\begin{aligned} R_{-1}(T) &= \frac{n}{4} - s\frac{p-1}{4(p+1)} - t\frac{q-1}{4(q+1)} + \frac{pq+1}{2(p+1)(q+1)} \\ &\leqslant \frac{n}{4} - \frac{p-1}{4(p+1)} + \frac{pq+1}{2(p+1)(q+1)} \\ &= \frac{n}{4} + \frac{1}{4} - \frac{p-1}{2(p+1)(q+1)} < \frac{n+1}{4}. \end{aligned}$$

This completes the proof. $\square$

3. Some operations

For a tree T and $e = uv \in E(T)$, we denote $R_T(e) = R_T(uv) = 1/(d_T(u)d_T(v))$, and we say that $R_T(e)$ is the *Randić value* of the edge e. If $\alpha_k = \{e_1, e_2, \ldots, e_k\}$ is a k-matching of T, we say that $\prod_{i=1}^{k} R_T(e_i)$ is the *Randić value of the matching* α_k, and write $R_T(\alpha_k) = \prod_{i=1}^{k} R_T(e_i)$.

Let T be a tree of order n. We use $\mathcal{M}_k(T)$ to denote the set of all k-matchings of T for $1 \leqslant k \leqslant \lfloor \frac{1}{2}n \rfloor$. Then the Randić characteristic polynomial of T can be written as

$$\varphi_R(T, x) = |xI - R(T)| = \sum_{k=0}^{\lfloor \frac{1}{2}n \rfloor} (-1)^k b(R(T), k) x^{n-2k},$$

where $b(R(T), 0) = 1$ and $b(R(T), k) = \sum_{\alpha_k \in \mathcal{M}_k(T)} R_T(\alpha_k)$ for $1 \leqslant k \leqslant \lfloor \frac{1}{2}n \rfloor$.

It has been pointed out in paper (see [7]) that the $\mathcal{E}_R(T)$ of a tree T of order n can be directly computed from its Randić characteristic polynomial by means of the Coulson integral formula:

$$\mathcal{E}_R(T) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \ln\left[1 + \sum_{k=1}^{\lfloor \frac{1}{2}n \rfloor} b(R(T), k) x^{2k}\right] \mathrm{d}x.$$

It implies that $\mathcal{E}_R(T)$ is a strictly monotonically increasing function of $b(R(T), k)$, $k = 1, 2, \ldots, \lfloor \frac{1}{2}n \rfloor$. So the following lemma is clear.

Theorem 3.1. *Let T_1 and T_2 be two trees of order n, and let their Randić characteristic polynomials be*

$$\varphi_R(T_1) = \sum_{k=0}^{\lfloor \frac{1}{2}n \rfloor} (-1)^k b(R(T_1), k) x^{n-2k},$$

$$\varphi_R(T_2) = \sum_{k=0}^{\lfloor \frac{1}{2}n \rfloor} (-1)^k b(R(T_2), k) x^{n-2k},$$

respectively. If $b(R(T_1), k) \geqslant b(R(T_2), k)$ for all $k \geqslant 1$, then $\mathcal{E}_R(T_1) \geqslant \mathcal{E}_R(T_2)$. Furthermore, if there is an integer number k such that $b(R(T_1), k) > b(R(T_2), k)$, then $\mathcal{E}_R(T_1) > \mathcal{E}_R(T_2)$.

Lemma 3.2. *Let T and T' be trees as depicted in Figure 4, where T_1 is a subtree of T with $v_1 \in V(T_1)$, $d_{T'}(v_1) = d_T(v_1) + 1 \geqslant 3$. Let l be a positive integer number, and let a and b be real numbers. Denote $N_{T_1}(v_1) = \{u_1, \ldots, u_s\}$. Then*

$$\sum_{\alpha_l \in \mathcal{M}_l(T_1)} (aR_{T'}(\alpha_l) - bR_T(\alpha_l)) = (a-b) \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_1)} R_T(\alpha_l) + \sum_{i=1}^{s} \frac{(a-b)s + a - 2b}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{l-1} \in \mathcal{M}_{l-1}(T_1 - v_1 - u_i)} R_T(\alpha_{l-1}).$$

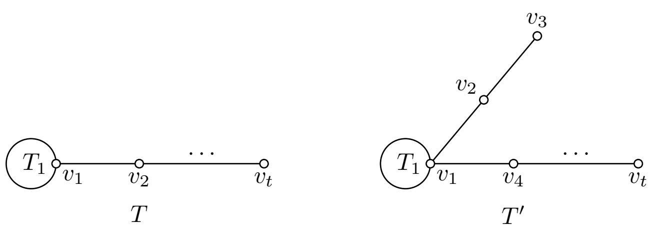

Figure 4. Trees T and T'.

P r o o f. Note that

$$\begin{aligned}\sum_{\alpha_l \in \mathcal{M}_l(T_1)} R_T(\alpha_l) &= \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_1)} R_T(\alpha_l) + \sum_{i=1}^{s} R_T(v_1 u_i) \sum_{\alpha_{l-1} \in \mathcal{M}_{l-1}(T_1 - v_1 - u_i)} R_T(\alpha_{l-1}) \\ &= \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_1)} R_T(\alpha_l) + \sum_{i=1}^{s} \frac{1}{(s+1)d_T(u_i)} \sum_{\alpha_{l-1} \in \mathcal{M}_{l-1}(T_1 - v_1 - u_i)} R_T(\alpha_{l-1}),\end{aligned}$$

$$\begin{aligned}\sum_{\alpha_l \in \mathcal{M}_l(T_1)} R_{T'}(\alpha_l) &= \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_1)} R_{T'}(\alpha_l) + \sum_{i=1}^{s} R_{T'}(v_1 u_i) \sum_{\alpha_{l-1} \in \mathcal{M}_{l-1}(T_1 - v_1 - u_i)} R_{T'}(\alpha_{l-1}) \\ &= \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_1)} R_T(\alpha_l) + \sum_{i=1}^{s} \frac{1}{(s+2)d_T(u_i)} \sum_{\alpha_{l-1} \in \mathcal{M}_{l-1}(T_1 - v_1 - u_i)} R_T(\alpha_{l-1}).\end{aligned}$$

It is easy to see that the lemma holds. □

In Lemma 3.2, if we denote $P = v_5v_6\dots v_t$ with $t \geqslant 5$, then similarly to the proof of Lemma 3.2, for any positive integer number l and real numbers a and b, we have

$$\begin{aligned}(3.1)\qquad &\sum_{\alpha_l\in\mathcal{M}_l(T_1\cup P)}(aR_{T'}(\alpha_l)-bR_T(\alpha_l))\\ &\quad=(a-b)\sum_{\alpha_l\in\mathcal{M}_l((T_1-v_1)\cup P)}R_T(\alpha_l)\\ &\quad\quad+\sum_{i=1}^{s}\frac{(a-b)s+a-2b}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{l-1}\in\mathcal{M}_{l-1}((T_1-v_1-u_i)\cup P)}R_T(\alpha_{l-1}),\end{aligned}$$

and

$$\begin{aligned}(3.2)\qquad &\sum_{\alpha_l\in\mathcal{M}_l(T_1\cup(P-v_5))}(aR_{T'}(\alpha_l)-bR_T(\alpha_l))\\ &\quad=(a-b)\sum_{\alpha_l\in\mathcal{M}_l((T_1-v_1)\cup(P-v_5))}R_T(\alpha_l)\\ &\quad\quad+\sum_{i=1}^{s}\frac{(a-b)s+a-2b}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{l-1}\in\mathcal{M}_{l-1}((T_1-v_1-u_i)\cup(P-v_5))}R_T(\alpha_{l-1}).\end{aligned}$$

Lemma 3.3. *Let T and T' be trees of order n as depicted in Figure 5, where $d_T(v_1)\geqslant 3$, $N_T(v_1)$ has no pendant paths, and T_1 is a subtree of T with $v_1\in V(T_1)$. Then $\mathcal{E}_R(T)\leqslant\mathcal{E}_R(T')$.*

P r o o f. Denote $N_T(v_1)=\{v_2,u_1,\dots,u_s\}$, where $s\geqslant 2$. Then

$$\begin{aligned}&b(R(T'),1)-b(R(T),1)\\ &\quad=\sum_{e\in E(T')}R_{T'}(e)-\sum_{e\in E(T)}R_T(e)\\ &\quad=\sum_{i=1}^{s}R_{T'}(v_1u_i)+R_{T'}(v_1v_2)+R_{T'}(v_1v_4)+R_{T'}(v_2v_3)+R_{T'}(v_4v_5)\\ &\quad\quad-\sum_{i=1}^{s}R_T(v_1u_i)-R_T(v_1v_2)-R_T(v_2v_3)-R_T(v_3v_4)-R_T(v_4v_5)\\ &\quad=\sum_{i=1}^{s}\frac{1}{(s+2)d_T(u_i)}+\frac{2}{2(s+2)}+1-\sum_{i=1}^{s}\frac{1}{(s+1)d_T(u_i)}-\frac{1}{2(s+1)}-1\\ &\quad=-\sum_{i=1}^{s}\frac{1}{(s+1)(s+2)d_T(u_i)}+\frac{s}{2(s+1)(s+2)}\\ &\quad=\frac{1}{(s+1)(s+2)}\Big(\frac{s}{2}-\sum_{i=1}^{s}\frac{1}{d_T(u_i)}\Big).\end{aligned}$$

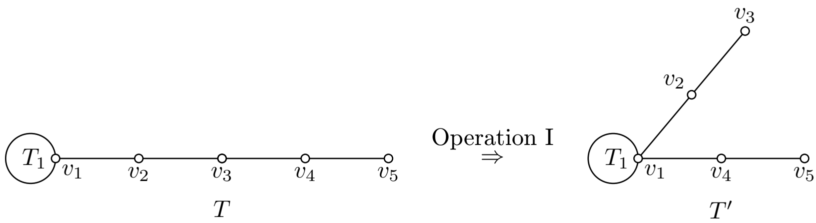

Figure 5. Trees T and T'.

Note that $s \geqslant 2$, and $N_T(v_1)$ has no pendant paths. Then $d_T(u_i) \geqslant 2$ for $i = 1, \ldots, s$. So $b(R(T'),1) - b(R(T),1) \geqslant 0$, that is, $b(R(T'),1) \geqslant b(R(T),1)$.

For $2 \leqslant k \leqslant \lfloor \frac{1}{2}n \rfloor$,

$$\begin{aligned} b(R(T),k) = & \sum_{\alpha_k \in \mathcal{M}_k(T)} R_T(\alpha_k) \\ = & \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_T(\alpha_k) + R_T(v_1v_2) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1)} R_T(\alpha_{k-1}) \\ & + (R_T(v_2v_3) + R_T(v_3v_4) + R_T(v_4v_5)) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1)} R_T(\alpha_{k-1}) \\ & + R_T(v_1v_2)(R_T(v_3v_4) + R_T(v_4v_5)) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_T(\alpha_{k-2}) \\ & + R_T(v_2v_3)R_T(v_4v_5) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1)} R_T(\alpha_{k-2}) \\ = & \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_T(\alpha_k) + \frac{1}{2(s+1)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1)} R_T(\alpha_{k-1}) \\ & + \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1)} R_T(\alpha_{k-1}) + \frac{3}{8(s+1)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_T(\alpha_{k-2}) \\ & + \frac{1}{8} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1)} R_T(\alpha_{k-2}), \end{aligned}$$

and

$$\begin{aligned} b(R(T'),k) = & \sum_{\alpha_k \in \mathcal{M}_k(T')} R_{T'}(\alpha_k) = \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_{T'}(\alpha_k) \\ & + (R_{T'}(v_1v_2) + R_{T'}(v_1v_4)) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1)} R_{T'}(\alpha_{k-1}) \\ & + (R_{T'}(v_2v_3) + R_{T'}(v_4v_5)) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1}) \\ & + (R_{T'}(v_1v_2)R_{T'}(v_4v_5) + R_{T'}(v_1v_4)R_{T'}(v_2v_3)) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_{T'}(\alpha_{k-2}) \end{aligned}$$

$$+ R_{T'}(v_2v_3)R_{T'}(v_4v_5) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2})$$

$$= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_{T'}(\alpha_k) + \frac{1}{s+2} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})$$

$$+ \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1}) + \frac{1}{2(s+2)} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})$$

$$+ \frac{1}{4} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2}).$$

So

$$b(R(T'),k) - b(R(T),k)$$
$$= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} (R_{T'}(\alpha_k) - R_T(\alpha_k)) + \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} (R_{T'}(\alpha_{k-1}) - R_T(\alpha_{k-1}))$$
$$+ \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} \Big(\frac{1}{4}R_{T'}(\alpha_{k-2}) - \frac{1}{8}R_T(\alpha_{k-2})\Big)$$
$$+ \frac{s}{2(s+1)(s+2)} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})$$
$$+ \frac{s-2}{8(s+1)(s+2)} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2}).$$

Applying Lemma 3.2 to the first three terms, respectively, we have

$$b(R(T'),k) - b(R(T),k)$$
$$= \sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1-u_i)} R_T(\alpha_{k-1})$$
$$+ \sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1-u_i)} R_T(\alpha_{k-2})$$
$$+ \frac{1}{8} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})$$
$$+ \sum_{i=1}^{s} \frac{s}{8(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{x-3}\in\mathcal{M}_{k-3}(T_1-v_1-u_i)} R_T(\alpha_{k-3})$$
$$+ \frac{s}{2(s+1)(s+2)} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})$$
$$+ \frac{s-2}{8(s+1)(s+2)} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2}).$$

Since $d_T(u_i) \geqslant 2$ for $i = 1, \ldots, s$, we have

$$\sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1 - u_i)} R_T(\alpha_{k-1}) \geqslant \frac{-s}{2(s+1)(s+2)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1)} R_T(\alpha_{k-1}),$$

$$\sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1 - u_i)} R_T(\alpha_{k-2}) \geqslant \frac{-s}{2(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_T(\alpha_{k-2}).$$

Note that

$$\sum_{i=1}^{s} \frac{s}{8(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{x-3} \in \mathcal{M}_{k-3}(T_1 - v_1 - u_i)} R_T(\alpha_{k-3}) \geqslant 0.$$

Then

$$\begin{aligned} b(R(T'), k) - b(R(T), k) &\geqslant \Big(\frac{s}{2(s+1)(s+2)} - \frac{s}{2(s+1)(s+2)}\Big) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_1)} R_{T'}(\alpha_{k-1}) \\ &\quad + \Big(\frac{s-2}{8(s+1)(s+2)} - \frac{s}{2(s+1)(s+2)} + \frac{1}{8}\Big) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_T(\alpha_{k-2}) \\ &= \frac{s^2}{8(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 - v_1)} R_T(\alpha_{k-2}) \geqslant 0. \end{aligned}$$

The lemma follows by Theorem 3.1. □

Lemma 3.4. *Let T and T' be trees of order n as depicted in Figure 6, where $d_T(v_1) \geqslant 3$, $N_T(v_1)$ has no pendant paths, and T_1 is a subtree of T with $v_1 \in V(T_1)$. Then $\mathcal{E}_R(T) \leqslant \mathcal{E}_R(T')$.*

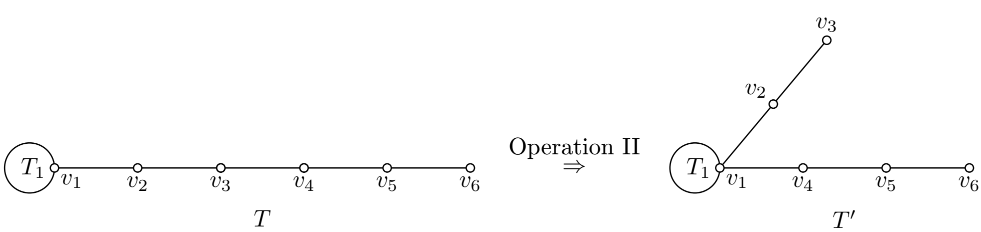

Figure 6. Trees T and T'.

P r o o f. Denote $N_T(v_1)=\{v_2,u_1,\ldots,u_s\}$, where $s\geqslant 2$. Then

$$\begin{aligned}
&b(R(T'),1)-b(R(T),1)\\
&=\sum_{e\in E(T')}R_{T'}(e)-\sum_{e\in E(T)}R_T(e)\\
&=\sum_{i=1}^{s}R_{T'}(v_1u_i)+R_{T'}(v_1v_2)+R_{T'}(v_1v_4)+R_{T'}(v_2v_3)+R_{T'}(v_4v_5)+R_{T'}(v_5v_6)\\
&\quad-\sum_{i=1}^{s}R_T(v_1u_i)-R_T(v_1v_2)-R_T(v_2v_3)-R_T(v_3v_4)-R_T(v_4v_5)-R_T(v_5v_6)\\
&=\sum_{i=1}^{s}\frac{1}{(s+2)d_T(u_i)}+\frac{2}{2(s+2)}+\frac{5}{4}-\sum_{i=1}^{s}\frac{1}{(s+1)d_T(u_i)}-\frac{1}{2(s+1)}-\frac{5}{4}\\
&=\frac{1}{(s+1)(s+2)}\left(\frac{s}{2}-\sum_{i=1}^{s}\frac{1}{d_T(u_i)}\right).
\end{aligned}$$

Note that $s\geqslant 2$, and $N_T(v_1)$ has no pendant paths. Then $d_T(u_i)\geqslant 2$ for $i=1,\ldots,s$. So $b(R(T'),1)-b(R(T),1)\geqslant 0$, that is, $b(R(T'),1)\geqslant b(R(T),1)$.

For $2\leqslant k\leqslant\lfloor\frac{1}{2}n\rfloor$,

$$\begin{aligned}
&b(R(T),k)\\
&=\sum_{\alpha_k\in\mathcal{M}_k(T_1)}R_T(\alpha_k)+R_T(v_1v_2)\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)}R_T(\alpha_{k-1})\\
&\quad+(R_T(v_2v_3)+R_T(v_3v_4)+R_T(v_4v_5)+R_T(v_5v_6))\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)}R_T(\alpha_{k-1})\\
&\quad+R_T(v_1v_2)(R_T(v_3v_4)+R_T(v_4v_5)+R_T(v_5v_6))\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\quad+R_T(v_2v_3)(R_T(v_4v_5)+R_T(v_5v_6))\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)}R_T(\alpha_{k-2})\\
&\quad+R_T(v_3v_4)R_T(v_5v_6)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)}R_T(\alpha_{k-2})\\
&\quad+R_T(v_1v_2)R_T(v_3v_4)R_T(v_5v_6)\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3})\\
&=\sum_{\alpha_k\in\mathcal{M}_k(T_1)}R_T(\alpha_k)+\frac{1}{2(s+1)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)}R_T(\alpha_{k-1})\\
&\quad+\frac{5}{4}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)}R_T(\alpha_{k-1})+\frac{1}{2(s+1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\quad+\frac{5}{16}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)}R_T(\alpha_{k-2})+\frac{1}{16(s+1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}),
\end{aligned}$$

and

$$
\begin{aligned}
&b(R(T'),k)\\
&= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_{T'}(\alpha_k) + (R_{T'}(v_1v_2)+R_{T'}(v_1v_4)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_{T'}(\alpha_{k-1})\\
&\quad + (R_{T'}(v_2v_3)+R_{T'}(v_4v_5)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1})\\
&\quad + R_{T'}(v_1v_4)(R_{T'}(v_2v_3)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_{T'}(\alpha_{k-2})\\
&\quad + R_{T'}(v_1v_2)(R_{T'}(v_4v_5)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_{T'}(\alpha_{k-2})\\
&\quad + R_{T'}(v_2v_3)(R_{T'}(v_4v_5)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2})\\
&\quad + R_{T'}(v_1v_4)R_{T'}(v_2v_3)R_{T'}(v_5v_6) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_{T'}(\alpha_{k-3})\\
&= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_{T'}(\alpha_k) + \frac{1}{s+2} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})\\
&\quad + \frac{5}{4} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1}) + \frac{7}{8(s+2)} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})\\
&\quad + \frac{3}{8} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2}) + \frac{1}{8(s+2)} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3}).
\end{aligned}
$$

So

$$
\begin{aligned}
&b(R(T'),k)-b(R(T),k)\\
&\qquad = \sum_{\alpha_k\in\mathcal{M}_k(T_1)} (R_{T'}(\alpha_k)-R_T(\alpha_k))\\
&\qquad\quad + \frac{5}{4} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} (R_{T'}(\alpha_{k-1})-R_T(\alpha_{k-1}))\\
&\qquad\quad + \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} \Big(\frac{3}{8}R_{T'}(\alpha_{k-2}) - \frac{5}{16}R_T(\alpha_{k-2})\Big)\\
&\qquad\quad + \Big(\frac{1}{s+2} - \frac{1}{2(s+1)}\Big) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})\\
&\qquad\quad + \Big(\frac{7}{8(s+2)} - \frac{1}{2(s+1)}\Big) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})\\
&\qquad\quad + \Big(\frac{1}{8(s+2)} - \frac{1}{16(s+1)}\Big) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3}).
\end{aligned}
$$

Applying Lemma 3.2 to the first three terms, respectively, we have

$$\begin{aligned}
&b(R(T'),k)-b(R(T),k)\\
&\quad=\sum_{i=1}^{s}\frac{-1}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1-u_i)}R_T(\alpha_{k-1})\\
&\qquad+\frac{5}{4}\sum_{i=1}^{s}\frac{-1}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1-u_i)}R_T(\alpha_{k-2})\\
&\qquad+\Big(\frac{3}{8}-\frac{5}{16}\Big)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\qquad+\sum_{i=1}^{s}\frac{s-4}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1-u_i)}R_T(\alpha_{k-3})\\
&\qquad+\Big(\frac{1}{s+2}-\frac{1}{2(s+1)}\Big)\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)}R_T(\alpha_{k-1})\\
&\qquad+\Big(\frac{7}{8(s+2)}-\frac{1}{2(s+1)}\Big)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\qquad+\Big(\frac{1}{8(s+2)}-\frac{1}{16(s+1)}\Big)\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}).
\end{aligned}$$

Note that $d_T(u_i)\geqslant 2$ for $i=1,\ldots,s$. So

$$\begin{aligned}
&\sum_{i=1}^{s}\frac{-1}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1-u_i)}R_T(\alpha_{k-1})\\
&\qquad\geqslant\frac{-s}{2(s+1)(s+2)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)}R_T(\alpha_{k-1}),\\
&\sum_{i=1}^{s}\frac{-1}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1-u_i)}R_T(\alpha_{k-2})\\
&\qquad\geqslant\frac{-s}{2(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2}),\\
&\sum_{i=1}^{s}\frac{s-4}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1-u_i)}R_T(\alpha_{k-3})\\
&\qquad\geqslant\begin{cases}0 & \text{if } s\geqslant 4,\\ \dfrac{s(s-4)}{32(s+1)(s+2)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}) & \text{if } 2\leqslant s\leqslant 3.\end{cases}
\end{aligned}$$

Then

$$
\begin{aligned}
&b(R(T'),k)-b(R(T),k)\\
&\quad\geqslant\Big(\frac{1}{s+2}-\frac{1}{2(s+1)}-\frac{s}{2(s+1)(s+2)}\Big)\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)}R_T(\alpha_{k-1})\\
&\qquad+\Big(\frac{7}{8(s+2)}-\frac{1}{2(s+1)}-\frac{5}{4}\cdot\frac{s}{2(s+1)(s+2)}+\frac{3}{8}-\frac{5}{16}\Big)\\
&\qquad\quad\times\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\qquad+\Big(\frac{1}{8(s+2)}-\frac{1}{16(s+1)}\Big)\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3})\\
&\qquad+\begin{cases}0 & \text{if } s\geqslant 4,\\ \dfrac{s(s-4)}{32(s+1)(s+2)}\sum\limits_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}) & \text{if } 2\leqslant s\leqslant 3\end{cases}\\
&\quad=\frac{s^2-s}{16(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)}R_T(\alpha_{k-2})\\
&\qquad+\begin{cases}\dfrac{s}{16(s+1)(s+2)}\sum\limits_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}) & \text{if } s\geqslant 4,\\ \dfrac{s(s-2)}{32(s+1)(s+2)}\sum\limits_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)}R_T(\alpha_{k-3}) & \text{if } 2\leqslant s\leqslant 3\end{cases}\\
&\quad\geqslant 0.
\end{aligned}
$$

The lemma follows by Theorem 3.1. □

Lemma 3.5. *Let T and T' be trees of order n as depicted in Figure 7, where $t\geqslant 7$, $d_T(v_1)\geqslant 3$, $N_T(v_1)$ has no pendant paths, and T_1 is a subtree of T with $v_1\in V(T_1)$. Then $\mathcal{E}_R(T)\leqslant\mathcal{E}_R(T')$.*

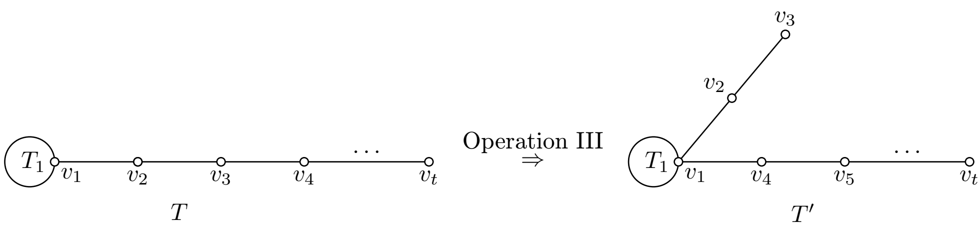

Figure 7. Trees T and T'.

P r o o f. Denote $N_T(v_1) = \{v_2, u_1, \ldots, u_s\}$, where $s \geqslant 2$. Note that $t \geqslant 7$, $d_T(u_i) \geqslant 2$ for $i = 1, \ldots, s$, $d_T(v_t) = 1$, and $d_T(v_i) = 2$ for $i = 2, \ldots, t-1$. Then

$$\begin{aligned}
b(R(T'),1) - b(R(T),1) &= \sum_{e \in E(T')} R_{T'}(e) - \sum_{e \in E(T)} R_T(e) \\
&= \sum_{i=1}^{s} R_{T'}(v_1 u_i) + R_{T'}(v_1 v_2) + R_{T'}(v_1 v_4) + R_{T'}(v_2 v_3) \\
&\quad + \sum_{i=4}^{t-1} R_{T'}(v_i v_{i+1}) - \sum_{i=1}^{s} R_T(v_1 u_i) - \sum_{i=1}^{t-1} R_T(v_i v_{i+1}) \\
&= \sum_{i=1}^{s} \frac{1}{(s+2) d_T(u_i)} + \frac{1}{s+2} + 1 + \frac{t-5}{4} \\
&\quad - \sum_{i=1}^{s} \frac{1}{(s+1) d_T(u_i)} - \frac{1}{2(s+1)} - \frac{t-3}{4} - \frac{1}{2} \\
&= \frac{1}{(s+1)(s+2)} \Big(\frac{s}{2} - \sum_{i=1}^{s} \frac{1}{d_T(u_i)} \Big) \geqslant 0,
\end{aligned}$$

that is, $b(R(T'),1) \geqslant b(R(T),1)$.

To prove that $b(R(T'),k) \geqslant b(R(T),k)$ for $2 \leqslant k \leqslant \lfloor \frac{1}{2} n \rfloor$, we denote $P = v_5 \ldots v_{t-1} v_t$. Then for $2 \leqslant k \leqslant \lfloor \frac{1}{2} n \rfloor$,

$$\begin{aligned}
b(R(T),k) = &\sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) + R_T(v_1 v_2) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1 - v_1) \cup P)} R_T(\alpha_{k-1}) \\
&+ (R_T(v_2 v_3) + R_T(v_3 v_4)) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) \\
&+ R_T(v_4 v_5) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P - v_5))} R_T(\alpha_{k-1}) \\
&+ R_T(v_1 v_2) R_T(v_3 v_4) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup P)} R_T(\alpha_{k-2}) \\
&+ R_T(v_1 v_2) R_T(v_4 v_5) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
&+ R_T(v_2 v_3) R_T(v_4 v_5) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup (P - v_5))} R_T(\alpha_{k-2}) \\
= &\sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) + \frac{1}{2(s+1)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1 - v_1) \cup P)} R_T(\alpha_{k-1}) \\
&+ \frac{1}{2} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) + \frac{1}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P - v_5))} R_T(\alpha_{k-1})
\end{aligned}$$

$$+\frac{1}{8(s+1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup P)} R_T(\alpha_{k-2})$$
$$+\frac{1}{8(s+1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))} R_T(\alpha_{k-2})$$
$$+\frac{1}{16}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_T(\alpha_{k-2}),$$

and

$$\begin{aligned}
b(R(T'),k) = & \sum_{\alpha_k\in\mathcal{M}_k(T_1\cup P)} R_{T'}(\alpha_k) \\
& + (R_{T'}(v_1v_4)+R_{T'}(v_1v_2))\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-v_1)\cup P)} R_{T'}(\alpha_{k-1}) \\
& + R_{T'}(v_2v_3)\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup P)} R_{T'}(\alpha_{k-1}) \\
& + R_{T'}(v_4v_5)\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-1}) \\
& + R_{T'}(v_1v_4)R_{T'}(v_2v_3)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup P)} R_{T'}(\alpha_{k-2}) \\
& + R_{T'}(v_1v_2)R_{T'}(v_4v_5)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))} R_{T'}(\alpha_{k-2}) \\
& + R_{T'}(v_2v_3)R_{T'}(v_4v_5)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-2}) \\
= & \sum_{\alpha_k\in\mathcal{M}_k(T_1\cup P)} R_{T'}(\alpha_k)+\frac{1}{s+2}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-v_1)\cup P)} R_T(\alpha_{k-1}) \\
& + \frac{1}{2}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup P)} R_{T'}(\alpha_{k-1}) \\
& + \frac{1}{4}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-1}) \\
& + \frac{1}{4(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup P)} R_T(\alpha_{k-2}) \\
& + \frac{1}{8(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))} R_T(\alpha_{k-2}) \\
& + \frac{1}{8}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-2}).
\end{aligned}$$

So

$$
\begin{aligned}
&b(R(T'),k) - b(R(T),k) \\
&\quad = \sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_{T'}(\alpha_k) - \sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) \\
&\qquad + \frac{s}{2(s+1)(s+2)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1 - v_1) \cup P)} R_T(\alpha_{k-1}) \\
&\qquad + \frac{1}{2} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_{T'}(\alpha_{k-1}) \\
&\qquad - \frac{1}{2} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) \\
&\qquad + \frac{1}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P - v_5))} R_{T'}(\alpha_{k-1}) \\
&\qquad - \frac{1}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P - v_5))} R_T(\alpha_{k-1}) \\
&\qquad + \frac{s}{8(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup P)} R_T(\alpha_{k-2}) \\
&\qquad - \frac{1}{8(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
&\qquad + \frac{1}{8} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup (P - v_5))} R_{T'}(\alpha_{k-2}) \\
&\qquad - \frac{1}{16} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup (P - v_5))} R_T(\alpha_{k-2}).
\end{aligned}
$$

Applying equation (3.1) to the first two terms and the fourth and fifth terms, respectively, we have

$$
\begin{aligned}
&\sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_{T'}(\alpha_k) - \sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) \\
&\qquad = \sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1 - v_1 - u_i) \cup P)} R_T(\alpha_{k-1}),
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{1}{2} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_{T'}(\alpha_{k-1}) - \frac{1}{2} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) \\
&\qquad = \sum_{i=1}^{s} \frac{-1}{2(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1 - u_i) \cup P)} R_T(\alpha_{k-2}).
\end{aligned}
$$

Applying equation (3.2) to the sixth and seventh terms, and the tenth and eleventh terms, respectively, we have

$$\begin{aligned}
&\frac{1}{4}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-1}) - \frac{1}{4}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup(P-v_5))} R_T(\alpha_{k-1})\\
&\quad=\sum_{i=1}^{s}\frac{-1}{4(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1-u_i)\cup(P-v_5))} R_T(\alpha_{k-2}),
\end{aligned}$$

and

$$\begin{aligned}
&\frac{1}{8}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_{T'}(\alpha_{k-2}) - \frac{1}{16}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_T(\alpha_{k-2})\\
&\quad=\frac{1}{16}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))} R_T(\alpha_{k-2})\\
&\qquad+\sum_{i=1}^{s}\frac{s}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1-u_i)\cup(P-v_5))} R_T(\alpha_{k-2}).
\end{aligned}$$

Then

$$\begin{aligned}
&b(R(T'),k)-b(R(T),k)\\
&\quad=\sum_{i=1}^{s}\frac{-1}{(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-v_1-u_i)\cup P)} R_T(\alpha_{k-1})\\
&\qquad+\frac{s}{2(s+1)(s+2)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-v_1)\cup P)} R_T(\alpha_{k-1})\\
&\qquad+\sum_{i=1}^{s}\frac{-1}{2(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1-u_i)\cup P)} R_T(\alpha_{k-2})\\
&\qquad+\sum_{i=1}^{s}\frac{-1}{4(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1-u_i)\cup(P-v_5))} R_T(\alpha_{k-2})\\
&\qquad+\frac{s}{8(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup P)} R_T(\alpha_{k-2})\\
&\qquad+\Big(\frac{1}{16}-\frac{1}{8(s+1)(s+2)}\Big)\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))} R_T(\alpha_{k-2})\\
&\qquad+\sum_{i=1}^{s}\frac{s}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5))} R_T(\alpha_{k-3}).
\end{aligned}$$

Denote $b(R(T'),k) - b(R(T),k) = D_1(k) + D_2(k)$, where $D_1(k)$ expresses the algebraic sum of the first two terms and $D_2(k)$ the algebraic sum of the remaining terms. Note that $d_T(u_i) \geqslant 2$ for $i = 1, \ldots, s$. So

$$\sum_{i=1}^{s} \frac{-1}{(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1-v_1-u_i)\cup P)} R_T(\alpha_{k-1}) \geqslant \frac{-s}{2(s+1)(s+2)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1-v_1)\cup P)} R_T(\alpha_{k-1}).$$

Then $D_1(k) \geqslant 0$.

For $D_2(k)$, noting that

$$\begin{aligned}
\sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1-u_i)\cup P)} R_T(\alpha_{k-2})
&= \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1-u_i)\cup (P-v_5))} R_T(\alpha_{k-2}) \\
&\quad + R_T(v_5v_6) \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-v_1-u_i)\cup (P-v_5-v_6))} R_T(\alpha_{k-3}) \\
&= \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1-u_i)\cup (P-v_5))} R_T(\alpha_{k-2}) \\
&\quad + \frac{1}{4} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-v_1-u_i)\cup (P-v_5-v_6))} R_T(\alpha_{k-3})
\end{aligned}$$

and

$$\begin{aligned}
\sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1)\cup P)} R_T(\alpha_{k-2})
&= \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1)\cup (P-v_5))} R_T(\alpha_{k-2}) \\
&\quad + R_T(v_5v_6) \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-v_1)\cup (P-v_5-v_6))} R_T(\alpha_{k-3}) \\
&= \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-v_1)\cup (P-v_5))} R_T(\alpha_{k-2}) \\
&\quad + \frac{1}{4} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-v_1)\cup (P-v_5-v_6))} R_T(\alpha_{k-3}),
\end{aligned}$$

then

$$
\begin{aligned}
D_2(k) = & \sum_{i=1}^{s} \frac{-1}{2(s+1)(s+2)d_T(u_i)} \\
& \times \Bigg(\sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& \quad + \frac{1}{4} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1 - u_i) \cup (P - v_5 - v_6))} R_T(\alpha_{k-3}) \Bigg) \\
& + \sum_{i=1}^{s} \frac{-1}{4(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& + \frac{s}{8(s+1)(s+2)} \Bigg(\sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& \quad + \frac{1}{4} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1) \cup (P - v_5 - v_6))} R_T(\alpha_{k-3}) \Bigg) \\
& + \frac{s(s+3)}{16(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& + \sum_{i=1}^{s} \frac{s}{16(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-3}) \\
= & \sum_{i=1}^{s} \frac{-3}{4(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& + \frac{s(s+5)}{16(s+1)(s+2)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1) \cup (P - v_5))} R_T(\alpha_{k-2}) \\
& + \sum_{i=1}^{s} \frac{-1}{8(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1 - u_i) \cup (P - v_5 - v_6))} R_T(\alpha_{k-3}) \\
& + \frac{s}{32(s+1)(s+2)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1) \cup (P - v_5 - v_6))} R_T(\alpha_{k-3}) \\
& + \sum_{i=1}^{s} \frac{s}{16(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-3}).
\end{aligned}
$$

Dividing the third term into two terms, and noting that $s \geqslant 2$, and $d_T(u_i) \geqslant 2$ for $i = 1, \ldots, s$, we have

$$
D_2(k) = \sum_{i=1}^{s} \frac{-3}{4(s+1)(s+2)d_T(u_i)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1 - v_1 - u_i) \cup (P - v_5))} R_T(\alpha_{k-2})
$$

$$
\begin{aligned}
&+\frac{s(s+5)}{16(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))}R_T(\alpha_{k-2})\\
&+\sum_{i=1}^{s}\frac{-1}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})\\
&+\sum_{i=1}^{s}\frac{-1}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})\\
&+\frac{s}{32(s+1)(s+2)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})\\
&+\sum_{i=1}^{s}\frac{s}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5))}R_T(\alpha_{k-3})\\
\geqslant\ &\frac{-3s}{8(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))}R_T(\alpha_{k-2})\\
&+\frac{s(s+5)}{16(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))}R_T(\alpha_{k-2})\\
&+\frac{-s}{32(s+1)(s+2)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})\\
&+\sum_{i=1}^{s}\frac{-1}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5))}R_T(\alpha_{k-3})\\
&+\frac{s}{32(s+1)(s+2)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})\\
&+\sum_{i=1}^{s}\frac{s}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5))}R_T(\alpha_{k-3})\\
=\ &\frac{s(s-1)}{16(s+1)(s+2)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-v_1)\cup(P-v_5))}R_T(\alpha_{k-2})\\
&+\sum_{i=1}^{s}\frac{s-1}{16(s+1)(s+2)d_T(u_i)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-v_1-u_i)\cup(P-v_5))}R_T(\alpha_{k-3})\\
\geqslant\ &0.
\end{aligned}
$$

So far, we get that $b(R(T'),k)-b(R(T),k)=D_1(k)+D_2(k)\geqslant 0$ for $2\leqslant k\leqslant\lfloor\frac{1}{2}n\rfloor$. The lemma follows by Theorem 3.1. □

Lemma 3.6. *Let T and T' be trees of order n as depicted in Figure 8, where T_1 is a subtree of T with $v_1\in V(T_1)$, $d_T(v_1)\geqslant 3$, and $N_T(v_1)$ does not contain any pendant path. Then $\mathcal{E}_R(T)\leqslant\mathcal{E}_R(T')$.*

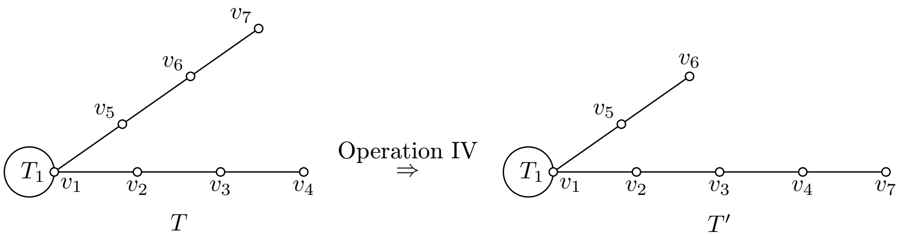

Figure 8. Trees T and T'.

P r o o f. Denote $d_T(v_1) = s$. It is easy to see that $b(R(T'),1) = b(R(T),1)$. For $2 \leqslant k \leqslant \lfloor \frac{1}{2}n \rfloor$,

$$\begin{aligned}
&b(R(T),k)\\
&= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_T(\alpha_k) + (R_T(v_1v_2)+R_T(v_1v_5)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})\\
&\quad + (R_T(v_2v_3)+R_T(v_3v_4)+R_T(v_5v_6)+R_T(v_6v_7)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_T(\alpha_{k-1})\\
&\quad + R_T(v_1v_2)(R_T(v_5v_6)+R_T(v_6v_7)+R_T(v_3v_4)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})\\
&\quad + R_T(v_1v_5)(R_T(v_2v_3)+R_T(v_3v_4)+R_T(v_6v_7)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})\\
&\quad + (R_T(v_2v_3)+R_T(v_3v_4))(R_T(v_5v_6)+R_T(v_6v_7)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_T(\alpha_{k-2})\\
&\quad + R_T(v_1v_2)R_T(v_3v_4)(R_T(v_5v_6)+R_T(v_6v_7)) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3})\\
&\quad + R_T(v_1v_5)R_T(v_6v_7)(R_T(v_2v_3)+R_T(v_3v_4)) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3})\\
&= \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_T(\alpha_k) + \frac{1}{s} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_T(\alpha_{k-1})\\
&\quad + \frac{3}{2} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_T(\alpha_{k-1})\\
&\quad + \frac{5}{4s} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2})\\
&\quad + \frac{9}{16} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_T(\alpha_{k-2})\\
&\quad + \frac{3}{8s} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3}),
\end{aligned}$$

and

$$
\begin{aligned}
& b(R(T'),k) \\
& \quad = \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_{T'}(\alpha_k) + (R_{T'}(v_1v_2)+R_{T'}(v_1v_5)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_{T'}(\alpha_{k-1}) \\
& \qquad + (R_{T'}(v_2v_3)+R_{T'}(v_3v_4)+R_{T'}(v_4v_7)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1}) \\
& \qquad + R_{T'}(v_1v_2)(R_{T'}(v_3v_4)+R_{T'}(v_4v_7)+R_{T'}(v_5v_6)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_{T'}(\alpha_{k-2}) \\
& \qquad + R_{T'}(v_1v_5)(R_{T'}(v_2v_3)+R_{T'}(v_3v_4)+R_{T'}(v_4v_7)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_{T'}(\alpha_{k-2}) \\
& \qquad + R_{T'}(v_5v_6)(R_{T'}(v_2v_3)+R_{T'}(v_3v_4)+R_{T'}(v_4v_7)) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2}) \\
& \qquad + R_{T'}(v_2v_3)R_{T'}(v_4v_7) \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2}) \\
& \qquad + R_{T'}(v_1v_2)R_{T'}(v_5v_6)(R_{T'}(v_3v_4)+R_{T'}(v_4v_7)) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_{T'}(\alpha_{k-3}) \\
& \qquad + R_{T'}(v_1v_5)R_{T'}(v_2v_3)R_{T'}(v_4v_7) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_{T'}(\alpha_{k-3}) \\
& \qquad + R_{T'}(v_5v_6)R_{T'}(v_2v_3)R_{T'}(v_4v_7) \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1)} R_{T'}(\alpha_{k-3}) \\
& \quad = \sum_{\alpha_k\in\mathcal{M}_k(T_1)} R_{T'}(\alpha_k) + \frac{1}{s} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1-v_1)} R_{T'}(\alpha_{k-1}) \\
& \qquad + \frac{3}{2} \sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1)} R_{T'}(\alpha_{k-1}) \\
& \qquad + \frac{9}{8s} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_{T'}(\alpha_{k-2}) + \frac{5}{8} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_{T'}(\alpha_{k-2}) \\
& \qquad + \frac{1}{4s} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_{T'}(\alpha_{k-3}) + \frac{1}{16} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1)} R_{T'}(\alpha_{k-3}).
\end{aligned}
$$

So

$$
\begin{aligned}
& b(R(T'),k) - b(R(T),k) \\
& \qquad = -\frac{1}{8s} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1-v_1)} R_T(\alpha_{k-2}) + \frac{1}{16} \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1)} R_T(\alpha_{k-2}) \\
& \qquad\quad -\frac{1}{8s} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1-v_1)} R_T(\alpha_{k-3}) + \frac{1}{16} \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1)} R_T(\alpha_{k-3}) \geqslant 0.
\end{aligned}
$$

The lemma follows by Theorem 3.1. □

4. Generalized double suns of odd order

In this section, we will show that generalized double suns of odd order satisfy Conjecture 1.1.

Theorem 4.1. *Let n be odd, and T be a generalized double sun of order n with branched vertices u and v. If one of the following conditions holds, then*

$$\mathcal{E}_R(T) \leqslant (n-3)\frac{\sqrt{2}}{2} + 2 = \mathcal{E}_R(Su_{(n+1)/2}).$$

(1) *$d(u, v) \geqslant 2$;*
(2) *$d(u, v) = 1$ and T has at least one pendant path centered at u (or v);*
(3) *$d(u, v) = 1$ and there are at least three pendant paths of odd $l \geqslant 3$ centered at the same branched vertex.*

Proof. If condition (1) or (2) holds, then by Lemmas 2.2 and 2.4, we have $R_{-1}(T) \leqslant \frac{1}{4}(n+1)$, and $\operatorname{tr}(R^2) = 2R_{-1}(T) \leqslant \frac{1}{2}(n+1)$. Since n is odd, we have $\operatorname{null}(R) \geqslant 1$. By Lemma 2.3,

$$\begin{aligned}\mathcal{E}_R(T) &\leqslant \sqrt{(n-2-\operatorname{null}(R))(\operatorname{tr}(R^2)-2)} + 2 \leqslant \sqrt{(n-3)\Big(\frac{n+1}{2}-2\Big)} + 2 \\ &= (n-3)\frac{\sqrt{2}}{2} + 2.\end{aligned}$$

If condition (3) holds, then by Lemmas 2.2 and 2.4, $R_{-1}(T) \leqslant \frac{1}{4}(n+2)$, and $\operatorname{tr}(R^2) = 2R_{-1}(T) \leqslant \frac{1}{2}(n+2)$. Since that n is odd and there are at least three pendant paths of odd length $l \geqslant 3$ centered at the same branched vertex, we have $\operatorname{null}(R) \geqslant 2$. By Lemma 2.3,

$$\begin{aligned}\mathcal{E}_R(T) &\leqslant \sqrt{(n-2-\operatorname{null}(R))(\operatorname{tr}(R^2)-2)} + 2 \leqslant \sqrt{(n-4)\Big(\frac{n+2}{2}-2\Big)} + 2 \\ &< (n-3)\frac{\sqrt{2}}{2} + 2.\end{aligned}$$

The theorem now follows. □

Theorem 4.2. *Let $p \geqslant 2$, $q \geqslant 2$, and T be a tree of order $n = 2p + 2q + 3$ as depicted in Figure 9. Then $\mathcal{E}_R(T) < 2 + (n-3)\frac{1}{2}\sqrt{2}$.*

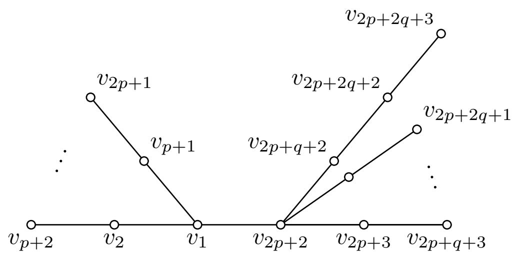

Figure 9. A tree T of order $2p+2q+3$.

Proof. After some calculations, we have

$$\begin{aligned}
\left|xI-\sqrt{2}R(T)\right| &= \frac{\sqrt{2}}{2}\Big(x(x^2-1)^p-\frac{px}{p+1}(x^2-1)^{p-1}\Big)\\
&\quad\times\Big(\sqrt{2}x\Big(x(x^2-1)^{q-1}-\frac{(q-1)x}{q+1}(x^2-1)^{q-2}\Big)\Big(x^2-\frac{3}{2}\Big)\\
&\qquad-\frac{\sqrt{2}}{q+1}(x^2-1)^q\Big)\\
&\quad-\frac{2x}{(p+1)(q+1)}(x^2-1)^{p+q-1}\Big(x^2-\frac{3}{2}\Big)\\
&= x(x^2-2)(x^2-1)^{p+q-3}\\
&\quad\times\Big(x^6-\frac{7pq+5p+5q+7}{2(p+1)(q+1)}x^4+\frac{6pq+4p+3q+9}{2(p+1)(q+1)}x^2\\
&\qquad-\frac{p+2}{(p+1)(q+1)}\Big).
\end{aligned}$$

Denote

$$f(y)=y^3-\frac{7pq+5p+5q+7}{2(p+1)(q+1)}y^2+\frac{6pq+4p+3q+9}{2(p+1)(q+1)}y-\frac{p+2}{(p+1)(q+1)}.$$

Suppose the three roots of $f(y)$ are y_1, y_2, and y_3. Then the eigenvalues of $\sqrt{2}R(T)$ are

$$0,\pm\sqrt{2},\underbrace{\pm1,\ldots,\pm1}_{p+q-3},\pm\sqrt{y_1},\pm\sqrt{y_2},\pm\sqrt{y_3},$$

and the eigenvalues of $R(T)$ are

$$0,\pm1,\underbrace{\pm\sqrt{\frac{1}{2}},\ldots,\pm\sqrt{\frac{1}{2}}}_{p+q-3},\pm\sqrt{\frac{y_1}{2}},\pm\sqrt{\frac{y_2}{2}},\pm\sqrt{\frac{y_3}{2}}.$$

Note that $n=2p+2q+3$. Then

$$\mathcal{E}_R(T)=2+\sqrt{2}\big(p+q-3+\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3}\big)=2+\sqrt{2}\Big(\frac{n-9}{2}+\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3}\Big).$$

In the following, we will estimate the value of $\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3}$. Denote

$$Y=\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3},\quad A=y_1+y_2+y_3,\quad B=y_1y_2+y_2y_3+y_1y_3,\quad C=y_1y_2y_3.$$

From the relationship between roots and coefficients, we have

$$A=\frac{7pq+5p+5q+7}{2(p+1)(q+1)},\quad B=\frac{6pq+4p+3q+9}{2(p+1)(q+1)},\quad C=\frac{p+2}{(p+1)(q+1)}.$$

Note that

$$A=\frac{7pq+5p+5q+7}{2(p+1)(q+1)}<\frac{7}{2},\quad B=\frac{6pq+4p+3q+9}{2(p+1)(q+1)}<3,$$
$$C=\frac{p+2}{(p+1)(q+1)}\leqslant\frac{p+2}{3(p+1)}=\frac{1}{3}\Big(1+\frac{1}{p+1}\Big)\leqslant\frac{4}{9}.$$

We have

$$\begin{aligned}Y^2&=y_1+y_2+y_3+2\sqrt{y_1y_2}+2\sqrt{y_2y_3}+2\sqrt{y_1y_3}=A+2\big(\sqrt{y_1y_2}+\sqrt{y_2y_3}+\sqrt{y_1y_3}\big)\\&<\frac{7}{2}+2\big(\sqrt{y_1y_2}+\sqrt{y_2y_3}+\sqrt{y_1y_3}\big),\end{aligned}$$

and

$$\begin{aligned}\big(\sqrt{y_1y_2}+\sqrt{y_2y_3}+\sqrt{y_1y_3}\big)^2&=y_1y_2+y_2y_3+y_1y_3+2\sqrt{y_1y_2y_3}\big(\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3}\big)\\&=B+2\sqrt{C}Y<3+\frac{4}{3}Y.\end{aligned}$$

Then

$$Y^2<\frac{7}{2}+2\sqrt{3+\frac{4}{3}Y},\quad 12Y^4-84Y^2-64Y+3<0.$$

Denote

$$g(Y)=12Y^4-84Y^2-64Y+3.$$

Since

$$g'(Y)=48Y^3-168Y-64,$$

with the help of Matlab, it is easy to see that $Y_0\doteq 2.03818$ is the only positive zero of $g'(Y)$, and that $g'(Y)<0$ for $0<Y<Y_0$, and $g'(Y)>0$ for $Y>Y_0$. Note that $g(2.96)<0$, and $g(2.97)>0$. So $Y<2.97$, that is, $\sqrt{y_1}+\sqrt{y_2}+\sqrt{y_3}<2.97$. Thus

$$\mathcal{E}_R(T)<2+\sqrt{2}\Big(\frac{n-9}{2}+2.97\Big),$$

and so

$$2+\frac{\sqrt{2}}{2}(n-3)-\mathcal{E}_R(T)>\frac{3}{100}\sqrt{2}>0.$$

This completes the proof. □

Theorem 4.3. *Let n be odd, and T be a generalized double sun of order n. Then*

$$\mathcal{E}_R(T) \leqslant (n-3)\frac{\sqrt{2}}{2} + 2 = \mathcal{E}_R(Su_{(n+1)/2}).$$

P r o o f. Denote the two branched vertices of T by u and v. If one of the following conditions holds, then the result holds by Theorem 4.1.

(1) $d(u,v) \geqslant 2$;
(2) $d(u,v) = 1$ and T has at least one pendant path of length 1;
(3) $d(u,v) = 1$ and there are at least three pendant paths of odd $l \geqslant 3$ centered at the same branched vertex.

Now, suppose that $d(u,v) = 1$, T has no pendant path of length 1, and there are at most two pendant paths of odd $l \geqslant 3$ centered at the same branched vertex. Since n is odd, it is clear that the number of pendant paths of odd length is odd. By Lemmas 3.3, 3.4, 3.5, we have $\mathcal{E}_R(T) \leqslant \mathcal{E}_R(T^{(1)})$, or $\mathcal{E}_R(T) \leqslant \mathcal{E}_R(T^{(2)})$, where $T^{(1)}$ and $T^{(2)}$ are depicted in Figure 10.

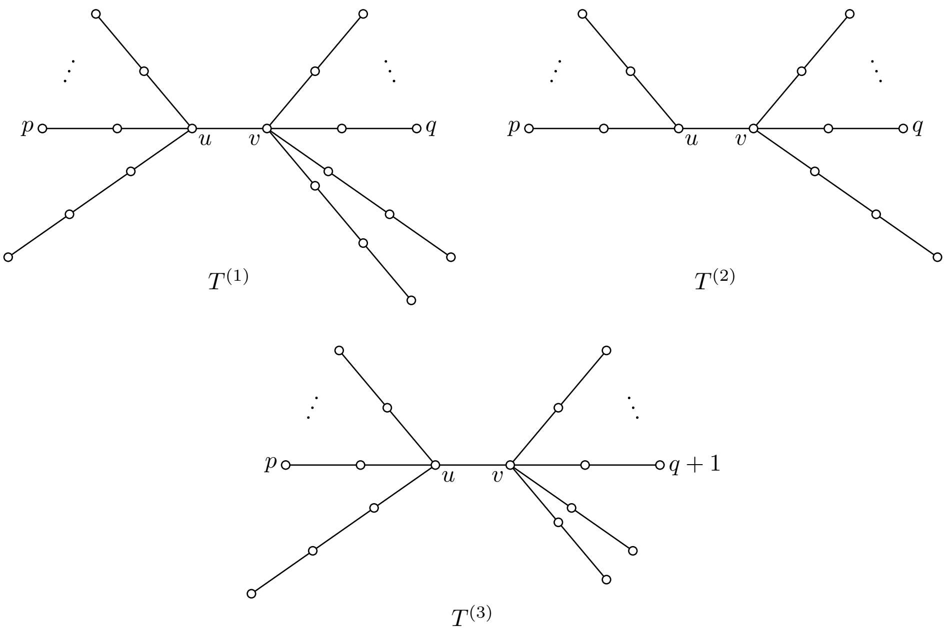

Figure 10. Three trees of order n for $d(u,v) = 1$.

By Lemmas 3.6, 3.3, and Theorem 4.2, $\mathcal{E}_R(T^{(1)}) \leqslant \mathcal{E}_R(T^{(3)}) < \mathcal{E}_R(Su_{(n+1)/2})$. By Theorem 4.2, $\mathcal{E}_R(T^{(2)}) < \mathcal{E}_R(Su_{(n+1)/2})$.

The theorem now follows. □

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