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On Randić Energy of Coral Trees*

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Abstract

Let G be a simple and connected graph. A vertex v_i is said to be pendent if $d_G(v_i) = 1$, and its adjacent vertex is called a quasi-pendent vertex. Let $\mathcal{T}(n)$ be a set of trees of order n with at most two quasi-pendent vertices of degree less than 4. We name $\mathcal{T}(n)$ the set of coral trees.

The Randić matrix of G, denoted by $R(G)$, is an $n \times n$ matrix whose (i, j)-entry is equal to $\frac{1}{\sqrt{d_G(v_i)d_G(v_j)}}$ if $v_iv_j \in E(G)$, and 0 otherwise. The Randić energy of G is defined as

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

where $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$ are the eigenvalues of $R(G)$.

In [*I. Gutman, B. Furtula, S. B. Bozkurt, On Randić energy, Linear Algebra Appl. 442 (2014) 50–57*], the authors conjectured that for a tree T of order n, if n is odd, then the maximum $\mathcal{E}_R(T)$ is achieved for T being the $(\frac{n-1}{2})$-sun; if n is even, then the maximum $\mathcal{E}_R(T)$ is achieved for T being the $(\lceil\frac{n-2}{4}\rceil, \lfloor\frac{n-2}{4}\rfloor)$-double sun.

In this work, we get the following results.

(1) For $T \in \mathcal{T}(n)$, $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.

(2) For a graph G, if $\mathcal{E}_R(G) \leq \mathcal{E}_R(P_n)$, then G satisfies the conjecture.

(3) $\mathcal{T}(n)$ is a family of trees that satisfies the conjecture.

1 Introduction

Let G be a simple and connected 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 $d_G(v_i)$ the degree of the vertex v_i in G.

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A vertex $v_i \in V(G)$ is said to be pendent if $d_G(v_i) = 1$, and its adjacent vertex is called a quasi-pendent vertex of G. If a quasi-pendent vertex has degree less than 4, then we call it a small quasi-pendent vertex.

Let $\mathcal{T}(n)$ be the set of trees of order n with at most two small quasi-pendent vertices. For each $T \in \mathcal{T}(n)$, we name it coral tree and say that $\mathcal{T}(n)$ is the set of coral trees.

The Randić index of a graph G is defined as ([13])

$$\chi(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_G(v_i)d_G(v_j)}}.$$

The Randić matrix of G, denoted by $R(G)$ ([3,4,11]), is an $n \times n$ matrix whose (i,j)-entry is equal to $\frac{1}{\sqrt{d_G(v_i)d_G(v_j)}}$ if $v_iv_j \in E(G)$, and 0 otherwise. The Randić energy of G is defined as ([4])

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

where $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$ are the eigenvalues of $R(G)$.

Let $p \geq 0$. The tree Su_p of order $n = 2p+1$, containing with p pendent vertices, each attached to a vertex of degree 2, and a vertex of degree p, is called the p-sun. Let $p, q \geq 0$. The tree $DSu_{p,q}$ of order $n = 2(p+q+1)$, obtained from a p-sun and a q-sun, by connecting their central vertices, is called a (p,q)-double sun.

In [11], the authors proved that the star S_n is the unique tree with minimal Randić energy over all trees, pointed out that for $n \geq 7$, the path P_n is not the connected n-vertex graph with maximal Randić energy. They also presented the following conjecture about the trees with maximal $\mathcal{E}_R(T)$.

Conjecture 1.1 ([11]) *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 $(\frac{n-1}{2})$-sun. If n is even, then the maximum $\mathcal{E}_R(T)$ is achieved for T being the $(\lceil\frac{n-2}{4}\rceil, \lfloor\frac{n-2}{4}\rfloor)$-double sun.*

In [9], the authors got the minimal Randić energy of trees with given diameter. In [8], the author showed that the generalized double suns of odd order satisfy Conjecture 1.1. In [1,2], the authors presented some families of graphs that satisfy Conjecture 1.1. For more related research results, we refer to [3,4,6,7,9,11,12].

In this paper, we get the following results.

(1) For $T \in \mathcal{T}(n)$, $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.

(2) For a graph G, if $\mathcal{E}_R(G) \leq \mathcal{E}_R(P_n)$, then G satisfies Conjecture 1.1.

(3) $\mathcal{T}(n)$ is a family of trees that satisfies Conjecture 1.1.

2 Preliminaries

For a tree T, we use $\mathcal{M}_k(T)$ to denote the set of all k-matchings of T. If $e = v_iv_j \in E(T)$ and $\alpha_k = \{e_1, e_2, \dots, e_k\} \in \mathcal{M}_k(T)$, then we denote $R_T(e) = R_T(v_iv_j) = \frac{1}{d_G(v_i)d_G(v_j)}$ and $R_T(\alpha_k) = \prod_{i=1}^{k} R_T(e_i)$, respectively.

Let T be a tree of order n with matrix $R(T)$. Then the Randić characteristic polynomial of T can be written as ([5])

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

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

Lemma 2.1 ([9]) *Let T_1 and T_2 be two trees of order n, and let their Randić characteristic polynomials be*

$$\phi_R(T_1, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T_1), k) x^{n-2k}, \quad \phi_R(T_2, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T_2), k) x^{n-2k},$$

respectively. If $b(R(T_1), k) \le b(R(T_2), k)$ for all $k \ge 0$, and there is a positive integer 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 2.2 ([10]) *Let T be a tree of order n. Then $|\mathcal{M}_k(T)| \le |\mathcal{M}_k(P_n)|$ for $1 \le k \le \lfloor \frac{n}{2} \rfloor$.*

3 Some operations

Let T be the tree as shown in Figure 1, where T_1 is a subtree of T with $v_0 \in V(T_1)$, $t \ge 2$, and $d_T(v_0) \ge 3$. Let $T' = T - \{v_0v_2, \dots, v_0v_t\} + v_1v_2 \dots v_t$. We say that T' is obtained from T by Operation I (as depicted in Figure 1).

Lemma 3.1 *Let T' be obtained from T by Operation I. Then $\mathcal{E}_R(T) < \mathcal{E}_R(T')$.*

Proof. Let the R-characteristic polynomials of T and T' be

$$\phi_R(T, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k}, \quad \phi_R(T', x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'), k) x^{n-2k},$$

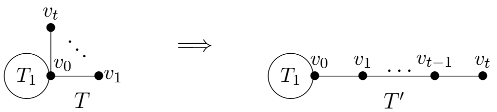

Figure 1. Operation I.

respectively, where $b(R(T), 0) = b(R(T'), 0) = 1$.

Denote $N_T(v_0) = \{v_1, \ldots, v_t, u_1, \ldots, u_s\}$, where $t \geq 2$, $s \geq 1$. Note that $d_T(v_0) = s+t$, $d_{T'}(v_0) = s+1$, and $d_T(u_i) = d_{T'}(u_i)$ for $i = 1, 2, \ldots, s$. Then

$$\begin{aligned}
& b(R(T'), 1) - b(R(T), 1) \\
= & \sum_{i=1}^{s} R_{T'}(v_0 u_i) + \sum_{j=0}^{t-1} R_{T'}(v_j u_{j+1}) - \sum_{i=1}^{s} R_T(v_0 u_i) - \sum_{j=1}^{t} R_T(v_0 v_j) \\
= & \sum_{i=1}^{s} \frac{t-1}{(s+1)(s+t) d_T(u_i)} + \frac{s(t-1)(t-2) + t(s^2+t-2)}{4(s+1)(s+t)} > 0.
\end{aligned}$$

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

$$\begin{aligned}
& b(R(T'), k) \\
\geq & \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_T(\alpha_k) + \sum_{i=0}^{t-1} R_{T'}(v_i v_{i+1}) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T - v_0)} R_{T'}(\alpha_{k-1}) \\
= & \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_T(\alpha_k) + \left(\frac{1}{2(s+1)} + \frac{t-2}{4} + \frac{1}{2} \right) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 - v_0)} R_T(\alpha_{k-1}),
\end{aligned}$$

$$\begin{aligned}
& b(R(T), k) \\
= & \sum_{\alpha_k \in \mathcal{M}_k(T_1)} R_T(\alpha_k) + \frac{t}{s+t} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T - v_0)} R_T(\alpha_{k-1}),
\end{aligned}$$

$$\begin{aligned}
& b(R(T'), k) - b(R(T), k) \\
\geq & \left(\frac{1}{2(s+1)} + \frac{t}{4} - \frac{t}{s+t} \right) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T - v_0)} R_T(\alpha_{k-1}) > 0.
\end{aligned}$$

By Lemma 2.1, the lemma holds. ■

Corollary 3.2 *Let $T \in \mathcal{T}(n)$ be a tree of order n (as depicted in Figure 2(a)), where T_1 is a subtree of T with $v_0, u_0 \in V(T_1)$, $t \geq 2$, $s \geq 2$. T' (as depicted in Figure 2(b)) is obtained from T by Operation I, and T'' (as depicted in Figure 2(c)) is obtained from T' by Operation I. Then*

$$\mathcal{E}_R(T) < \mathcal{E}_R(T') < \mathcal{E}_R(T'').$$

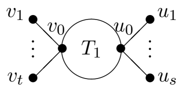

Figure 2(a). T

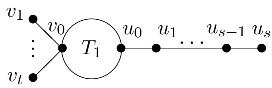

Figure 2(b). T'

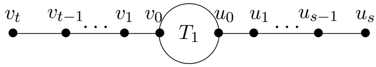

Figure 2(c). T''

By Corollary 3.2, the following result is clear.

Lemma 3.3 *Let $T \in \mathcal{T}(n)$ and u_0 be a quasi-pendent vertex of T. If $d(u_0) \geq 3$ and there are at least two pendent vertices in $N_T(u_0)$, then there is $T' \in \mathcal{T}(n)$ such that T' satisfies the following conditions.*

(1) u_0 is no longer a quasi-pendent vertex and u_{s-1} is a new small quasi-pendent vertex;

(2) There is just one pendent vertex in $N_{T'}(u_{s-1})$;

(3) $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.

Let T be the tree as shown in Figure 2(c), where T_1 is a subtree of T with $u_1 \in V(T_1)$ and $d_T(u_1) \geq 2$, $t \geq 7$. Let $T' = T - v_4v_5 \dots v_t + v_1v_4v_5 \dots v_t$ (as depicted in Figure 3). We say that T' is obtained from T by Operation II for v_1.

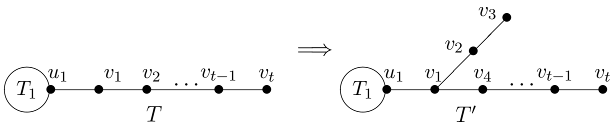

Figure 3. Operation II.

Lemma 3.4 *Let T' be obtained from T by Operation II. Then $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.*

Proof. Let the Randić characteristic polynomials of T and T' be

$$\phi_R(T,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T),k) x^{n-2k}, \quad \phi_R(T',x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'),k) x^{n-2k},$$

respectively, where $b(R(T),0) = b(R(T'),0) = 1$.

Note that $d_T(v_1) = 2$, $d_{T'}(v_1) = 3$, $d_T(v_3) = 2$, $d_{T'}(v_3) = 1$ and $d_T(u_1) = d_{T'}(u_1) \geq 2$. Then

$$\begin{aligned} & b(R(T'),1) - b(R(T),1) \\ = \; & R_{T'}(u_1v_1) + R_{T'}(v_1v_2) + R_{T'}(v_2v_3) + R_{T'}(v_1v_4) \\ & -(R_T(u_1v_1) + R_T(v_1v_2) + R_T(v_2v_3) + R_T(v_3v_4)) \\ = \; & \frac{1}{12} - \frac{1}{6d_T(u_1)} \geq 0. \end{aligned}$$

For $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$, denote $P = v_5v_6\ldots v_t$. Then

$$\begin{aligned} & b(M(T),k) \\ = \; & \sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) + \frac{1}{2d_T(u_1)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1-u_1)\cup P)} R_T(\alpha_{k-1}) \\ & + \frac{3}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) + \frac{1}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P-v_5))} R_T(\alpha_{k-1}) \\ & + \frac{1}{4d_T(u_1)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-u_1)\cup P)} R_T(\alpha_{k-2}) \\ & + \frac{1}{8d_T(u_1)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-u_1)\cup (P-v_5))} R_T(\alpha_{k-2}) \\ & + \frac{1}{16} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup P)} R_T(\alpha_{k-2}) + \frac{1}{8} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup (P-v_5))} R_T(\alpha_{k-2}) \\ & + \frac{1}{32d_T(u_1)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-u_1)\cup (P-v_5))} R_T(\alpha_{k-3}), \end{aligned}$$

$$\begin{aligned} & b(M(T'),k) \\ = \; & \sum_{\alpha_k \in \mathcal{M}_k(T_1 \cup P)} R_T(\alpha_k) + \frac{1}{3d_T(u_1)} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}((T_1-u_1)\cup P)} R_T(\alpha_{k-1}) \\ & + \frac{5}{6} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup P)} R_T(\alpha_{k-1}) + \frac{1}{4} \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1 \cup (P-v_5))} R_T(\alpha_{k-1}) \\ & + \frac{1}{6d_T(u_1)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-u_1)\cup P)} R_T(\alpha_{k-2}) \\ & + \frac{1}{12d_T(u_1)} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}((T_1-u_1)\cup (P-v_5))} R_T(\alpha_{k-2}) \end{aligned}$$

$$\begin{aligned} & + \frac{1}{12} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup P)} R_T(\alpha_{k-2}) + \frac{1}{6} \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1 \cup (P-v_5))} R_T(\alpha_{k-2}) \\ & + \frac{1}{24d_T(u_1)} \sum_{\alpha_{k-3} \in \mathcal{M}_{k-3}((T_1-u_1)\cup (P-v_5))} R_T(\alpha_{k-3}). \end{aligned}$$

Note that

$$\frac{1}{12}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup P)} R_T(\alpha_{k-1}) \geq \frac{1}{6d_T(u_1)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-u_1)\cup P)} R_T(\alpha_{k-1}),$$

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

$$\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup P)} R_T(\alpha_{k-2})$$
$$= \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))} R_T(\alpha_{k-2}) + \frac{1}{4}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))} R_T(\alpha_{k-3}).$$

So

$$\begin{aligned}
& b(M(T'),k) - b(M(T),k) \\
= & -\frac{1}{6d_T(u_1)}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}((T_1-u_1)\cup P)} R_T(\alpha_{k-1}) + \frac{1}{12}\sum_{\alpha_{k-1}\in\mathcal{M}_{k-1}(T_1\cup P)} R_T(\alpha_{k-1}) \\
& -\frac{1}{12d_T(u_1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup P)} R_T(\alpha_{k-2}) \\
& -\frac{1}{24d_T(u_1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))} R_T(\alpha_{k-2}) \\
& +\frac{1}{48}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup P)} R_T(\alpha_{k-2}) + \frac{1}{24}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_T(\alpha_{k-2}) \\
& +\frac{1}{96d_T(u_1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5))} R_T(\alpha_{k-3}) \\
\geq & -\frac{1}{12d_T(u_1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))} R_T(\alpha_{k-2}) \\
& -\frac{1}{12d_T(u_1)}\times\frac{1}{4}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))} R_T(\alpha_{k-3}) \\
& -\frac{1}{24d_T(u_1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))} R_T(\alpha_{k-2}) \\
& +\frac{1}{48}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))} R_T(\alpha_{k-2}) + \frac{1}{48}\times\frac{1}{4}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1\cup(P-v_5-v_6))} R_T(\alpha_{k-3})
\end{aligned}$$

$$+\frac{1}{24}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))}R_T(\alpha_{k-2})+\frac{1}{96d_T(u_1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5))}R_T(\alpha_{k-3})$$

$$= \frac{1}{16}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))}R_T(\alpha_{k-2})-\frac{1}{8d_T(u_1)}\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))}R_T(\alpha_{k-2})$$

$$+\frac{1}{192}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1\cup(P-v_5-v_6))}R_T(\alpha_{k-3})$$

$$-\frac{1}{96d_T(u_1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})$$

$$-\frac{1}{96d_T(u_1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3})$$

$$+\frac{1}{96d_T(u_1)}\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5))}R_T(\alpha_{k-3}).$$

Since $d_T(u_1)\geq 2$, and

$$\sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}(T_1\cup(P-v_5))}R_T(\alpha_{k-2}) \geq \sum_{\alpha_{k-2}\in\mathcal{M}_{k-2}((T_1-u_1)\cup(P-v_5))}R_T(\alpha_{k-2}),$$

$$\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}(T_1\cup(P-v_5-v_6))}R_T(\alpha_{k-3}) \geq \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3}),$$

$$\sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5))}R_T(\alpha_{k-3}) \geq \sum_{\alpha_{k-3}\in\mathcal{M}_{k-3}((T_1-u_1)\cup(P-v_5-v_6))}R_T(\alpha_{k-3}),$$

we get $b(M(T'),k)-b(M(T),k)\geq 0$.

By Lemma 2.1, $\mathcal{E}_R(T)\leq\mathcal{E}_R(T')$. ■

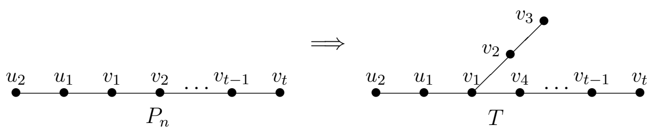

Figure 4.

Corollary 3.5 *Let T be the tree of order $n\geq 9$ (as depicted in Figure 4). Then*

$$\mathcal{E}_R(P_n)\leq\mathcal{E}_R(T).$$

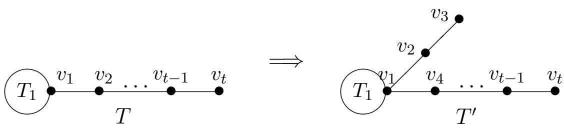

Figure 5. Operation III.

Lemma 3.6 ([8]) *Let T and T' be trees of order n as depicted in Figure 5, where $t \geq 5$, $d_T(v_1) \geq 3$, $N_T(v_1)$ has no pendent vertices, and T_1 is a subtree of T with $v_1 \in V(T_1)$. Then $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.*

4 Main result

In this section, we will show that for any coral tree $T \in \mathcal{T}(n)$, $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$. That is, P_n is the connected n-vertex graph with maximal Randić energy for $\mathcal{T}(n)$. Furthermore, we will prove that if for a graph G, $\mathcal{E}_R(G) \leq \mathcal{E}_R(P_n)$, then G satisfies Conjecture 1.1. That means that the coral trees set $T(n)$ is a family that satisfies Conjecture 1.1.

Lemma 4.1 *Let $T \in \mathcal{T}(n)$ be a coral tree with two small quasi-pendent vertices. If there is just one pendent vertex in the neighborhood of a small quasi-pendent vertex, then $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.*

Proof. Without loss of generality, we assume that v_2, v_{n-1} are two small quasi-pendent vertices. Then T is a tree as depicted in Figure 6, where T_1 is a subtree of order $n-2$. Consider the tree T' which is obtained from T by replacing T_1 with the path of order $n-2$. Clearly, T' is a path of order n as depicted in Figure 6. For $1 \leq i < j \leq n$, use P_{v_i,v_j} to denote the path of T' from v_i to v_j.

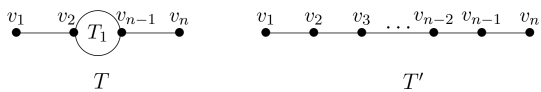

Figure 6.

Let the Randić characteristic polynomials of T and T' be

$$\phi_R(T,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T),k) x^{n-2k}, \quad \phi_R(T',x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'),k) x^{n-2k},$$

respectively, where $b(R(T),0) = b(R(T'),0) = 1$.

Note that the following facts.

- $R_{T'}(v_1v_2) = \frac{1}{2} \geq R_T(v_1v_2)$, $R_{T'}(v_{n-1}v_n) = \frac{1}{2} \geq R_T(v_{n-1}v_n)$.
- For each edge $v_iv_j \in E(T'), 2 \leq i < j \leq n-1$, $R_{T'}(v_iv_j) = \frac{1}{4}$. For each edge $uv \in E(T) \setminus \{v_1v_2, v_{n-1}v_n\}$, $R_T(uv) \leq \frac{1}{4}$.

- For any positive integer l, by Lemma 2.2,

$$\sum_{\alpha'_l \in \mathcal{M}_l(P_{v_2,v_{n-1}})} R_{T'}(\alpha'_l) = (\frac{1}{4})^l |\mathcal{M}_l(P_{v_2,v_{n-1}})| \geq \sum_{\alpha_l \in \mathcal{M}_l(T_1)} R_T(\alpha_l),$$

$$\sum_{\alpha'_l \in \mathcal{M}_l(P_{v_3,v_{n-1}})} R_{T'}(\alpha'_l) = (\frac{1}{4})^l |\mathcal{M}_l(P_{v_3,v_{n-1}})| \geq \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_2)} R_T(\alpha_l),$$

$$\sum_{\alpha'_l \in \mathcal{M}_l(P_{v_2,v_{n-2}})} R_{T'}(\alpha'_l) = (\frac{1}{4})^l |\mathcal{M}_l(P_{v_2,v_{n-2}})| \geq \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_{n-1})} R_T(\alpha_l),$$

$$\sum_{\alpha'_l \in \mathcal{M}_l(P_{v_3,v_{n-2}})} R_{T'}(\alpha'_l) = (\frac{1}{4})^l |\mathcal{M}_l(P_{v_3,v_{n-2}})| \geq \sum_{\alpha_l \in \mathcal{M}_l(T_1 - v_2 - v_{n-1})} R_T(\alpha_l).$$

It is clear that $b(R(T'), k) \geq b(R(T), k)$ for $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

By Lemma 2.1, $\mathcal{E}_R(T) \leq \mathcal{E}_R(T') = \mathcal{E}_R(P_n)$. ■

Theorem 4.2 *Let $T \in \mathcal{T}(n)$ be a coral tree. Then $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.*

Proof. If $T \in \mathcal{T}(n)$ is a coral tree with two small quasi-pendent vertices and there is just one pendent vertex in the neighborhood of a small quasi-pendent vertex, then by Lemma 4.1, $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.

Otherwise, by Lemma 3.3, there is $T' \in \mathcal{T}(n)$ satisfies the following conditions.

(1) $T' \in \mathcal{T}(n)$ is a coral tree with two small quasi-pendent vertices;

(2) There is just one pendent vertex in the neighborhood of a small quasi-pendent vertex;

(3) $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.

Therefore $\mathcal{E}_R(T) \leq \mathcal{E}_R(T') \leq \mathcal{E}_R(P_n)$. ■

Theorem 4.3 *Let n be odd. Then $\mathcal{E}_R(P_n) \leq \mathcal{E}_R(Su_{\frac{n-1}{2}})$.*

Proof. **Case 1.** $3 \leq n \leq 7$.

If $n = 3$, then $P_3 \cong Su_1$.

If $n = 5$, then $P_5 \cong Su_2$.

If $n = 7$, we denote $T = Su_3$ and

$$\phi_R(T, x) = \sum_{k=0}^{\lfloor \frac{7}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k}, \quad \phi_R(P_7, x) = \sum_{k=0}^{\lfloor \frac{7}{2} \rfloor} (-1)^k b(R(P_7), k) x^{n-2k},$$

where $b(R(T),0) = b(R(P_7),0) = 1$. Note that

$$b(M(T),1) - b(M(P_7),1) = 2 - 2 = 0,$$
$$b(M(T),2) - b(M(P_7),2) = \frac{5}{4} - \frac{19}{16} > 0,$$
$$b(M(T),3) - b(M(P_7),3) = \frac{1}{4} - \frac{3}{16} > 0.$$

By Lemma 2.1, $\mathcal{E}_R(P_7) < \mathcal{E}_R(T)$.

Case 2. $n \geq 9$.

Let T be the tree as depicted in Figure 4. By Corollary 3.5, $\mathcal{E}_R(P_n) \leq \mathcal{E}_R(T)$. Applying Operation III to T successively, by Lemma 3.6, we find that the Randić energy is increasing as $d_T(v_1)$ is increasing. So, $\mathcal{E}_R(P_n) \leq \mathcal{E}_R(Su_{\frac{n-1}{2}})$.

The theorem now follows. ■

Theorem 4.4 *Let n be even. Then* $\mathcal{E}_R(P_n) \leq \mathcal{E}_R(DSu_{\lfloor \frac{n-2}{4} \rfloor, \lceil \frac{n-2}{4} \rceil})$.

Proof. **Case 1.** $2 \leq n \leq 12$.

If $n = 2$, then $P_2 \cong DSu_{0,0}$.

If $n = 4$, then $P_4 \cong DSu_{0,1}$.

If $n = 6$, then $P_6 \cong DSu_{1,1}$.

If $n = 8$, we denote $T = DSu_{1,2}$ and

$$\phi_R(T,x) = \sum_{k=0}^{4} (-1)^k b(R(T),k) x^{n-2k}, \quad \phi_R(P_8,x) = \sum_{k=0}^{4} (-1)^k b(R(P_8),k) x^{n-2k},$$

where $b(R(T),0) = b(R(P_8),0) = 1$. Note that

$$b(M((T),1) - b(M(P_8),1) = \frac{9}{4} - \frac{9}{4} = 0,$$
$$b(M(T),2) - b(M(P_8),2) = \frac{5}{3} - \frac{13}{8} > 0,$$
$$b(M(T),3) - b(M(P_8),3) = \frac{7}{16} - \frac{25}{64} > 0,$$
$$b(M(T),4) - b(M(P_8),4) = \frac{1}{48} - \frac{1}{64} > 0.$$

By Lemma 2.1, $\mathcal{E}_R(P_8) < \mathcal{E}_R(DSu_{1,2})$.

If $n = 10$, we denote $T = DSu_{2,2}$ and

$$\phi_R(T,x) = \sum_{k=0}^{5} (-1)^k b(R(T),k) x^{n-2k}, \quad \phi_R(P_{10},x) = \sum_{k=0}^{5} (-1)^k b(R(P_{10}),k) x^{n-2k},$$

where $b(R(T),0) = b(R(P_{10}),0) = 1$. Note that

$$\begin{aligned}
b(M(T),1) - b(M(P_{10}),1) &= \frac{25}{9} - \frac{11}{4} > 0,\\
b(M(T),2) - b(M(P_{10}),2) &= \frac{17}{6} - \frac{43}{16} > 0,\\
b(M(T),3) - b(M(P_{10}),3) &= \frac{23}{18} - \frac{35}{32} > 0,\\
b(M(T),4) - b(M(P_{10}),4) &= \frac{25}{144} - \frac{41}{256} > 0,\\
b(M(T),5) - b(M(P_{10}),5) &= \frac{1}{144} - \frac{1}{256} > 0.
\end{aligned}$$

By Lemma 2.1, $\mathcal{E}_R(P_{10}) < \mathcal{E}_R(DSu_{2,2})$.

If $n = 12$, we denote $T = DSu_{2,3}$ and

$$\phi_R(T,x) = \sum_{k=0}^{6}(-1)^k b(R(T),k)x^{n-2k}, \quad \phi_R(P_{12},x) = \sum_{k=0}^{6}(-1)^k b(R(P_{12}),k)x^{n-2k},$$

where $b(R(T),0) = b(R(P_{12}),0) = 1$. Note that

$$\begin{aligned}
b(M(T),1) - b(M(P_{12}),1) &= \frac{79}{24} - \frac{13}{4} = \frac{1}{24} > 0,\\
b(M(T),2) - b(M(P_{12}),2) &= \frac{101}{24} - 4 > 0,\\
b(M(T),3) - b(M(P_{12}),3) &= \frac{251}{72} - \frac{133}{64} > 0,\\
b(M(T),4) - b(M(P_{12}),4) &= \frac{83}{96} - \frac{139}{256} > 0,\\
b(M(T),5) - b(M(P_{12}),5) &= \frac{17}{192} - \frac{39}{1024} > 0,\\
b(M(T),6) - b(M(P_{12}),6) &= \frac{1}{384} - \frac{1}{1024} > 0.
\end{aligned}$$

By Lemma 2.1, $\mathcal{E}_R(P_{12}) < \mathcal{E}_R(DSu_{2,3})$.

Case 2. $n \geq 14$.

Denote by T' and T'' the trees depicted in Figures 7(a) and 7(b), where $x = \frac{n}{2}$ if $\frac{n}{2}$ is odd, and $x = \frac{n-2}{2}$ if $\frac{n}{2}$ is even.

Let T be the tree of order $n \geq 14$ as depicted in Figure 4. By Corollary 3.5, $\mathcal{E}_R(P_n) < \mathcal{E}_R(T)$. Applying Operation III to T successively, by Lemma 3.6, $\mathcal{E}_R(P_n) < \mathcal{E}_R(T')$.

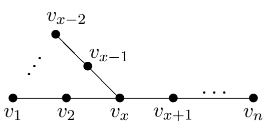

Figure 7(a). Tree T'

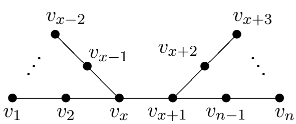

Figure 7(b). Tree T''

Applying Operation II to T' for v_{x+1} firstly, then applying Operation III to the resulting tree successively, by Lemmas 3.4 and 3.6, we find that the Randić energy is increasing as $d_T(v_{x+1})$ is increasing. So, $\mathcal{E}_R(P_n) < \mathcal{E}_R(T') < \mathcal{E}_R(T'')$, where T'' is $DSu_{\lfloor \frac{n-2}{4} \rfloor, \lceil \frac{n-2}{4} \rceil}$ as depicted in Figure 7(b). ■

By Theorems 4.2, 4.3 and 4.4, we get the following results.

(1) For $T \in \mathcal{T}(n)$, $\mathcal{E}_R(T) \leq \mathcal{E}_R(P_n)$.

(2) For a graph G, if $\mathcal{E}_R(G) \leq \mathcal{E}_R(P_n)$, then G satisfies Conjecture 1.1.

(3) $\mathcal{T}(n)$ is a family of trees that satisfies Conjecture 1.1.

References

[1] L. E. Allem, R. O. Braga, A. Pastine, Randić index and energy, *MATCH Commun. Math. Comput. Chem.* **83** (2020) 611–622.

[2] L. E. Allem, G. Molina, A. Pastine, Short note on Randić energy, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 515–528.

[3] S. B. Bozkurt, A. D. Güngör, I. Gutman, Randić spectral radius and Randić energy, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 321–334.

[4] S. B. Bozkurt, A. D. Güngör, I. Gutman, A. S. Cevik, Randić matrix and Randić energy, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 239–250.

[5] D. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Applications*, Barth Verlag, Heidelberg, 1995.

[6] K. C. Das, S. Sorgun, On Randić energy of graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 227–238.

[7] K. C. Das, S. Sorgun, I. Gutman, On Randić energy, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 81–92.

[8] W. Gao, The Randić energy of generalized double sun, *Czech. Math. J.* (2021) `https://doi.org/10.21136/CMJ.2021.0463-20`.

[9] Y. Gao, W. Gao, Y. Shao, The minimal Randić energy of trees with given diameter, *Appl. Math. Comput.* **411** (2021) #126489.

[10] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[11] I. Gutman, B. Furtula, S. B. Bozkurt, On Randić energy, *Lin. Algebra Appl.* **442** (2014) 50–57.

[12] J. He, Y. M. Liu, J. K. Tian, Note on the Randić energy of graphs, *Kragujevac J. Math.* **42** (2018) 209–215.

[13] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.