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Research Paper

ON THE MAXIMAL RANDIĆ ENERGY OF TREES WITH GIVEN DIAMETER

SHIVA SEPIDBON, NADER JAFARI RAD* AND AKBAR JAHANBANI

Abstract. For given integers n, d with $n \geq 5$ and $4 \leq d \leq n-1$, let T_d^n be the family of all trees of order n and diameter d. In this paper, we study trees $T \in T_d^n$ with maximal Randić energy. We prove that if $T \in T_d^n$ is a tree with maximal Randić energy then T is obtained from a path $P = v_0v_1 \dots v_d$ by adding n_i path(s) P_3 to each vertex v_i, for $i = 2, 3, 4, \dots, d-2$, where $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$. In particular, we present families of trees satisfying the Gutman-Furtula-Bozkurt Conjecture proposed in [Linear Algebra Appl., 442 (2014), 50–57].

1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$, and let $|V(G)| = n$ and $|E(G)| = m$. If the vertices v_i and v_j are adjacent, we write $v_iv_j \in E(G)$. For $i = 1, 2, \dots n$, let $d_{v_i} = d_G(v_i)$ be the degree of the vertex v_i. If $d_{v_i} = 1$, then v_i is a *pendant* vertex. A set of edges M of a graph G is a *matching* if no pair of edges of M share a

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*Corresponding author

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vertex. A matching of size k is referred as a *k-matching*. The *eccentricity* of a vertex v is the greatest distance from v to any other vertex of G. The *diameter* of a graph is the maximum over eccentricities of all vertices of the graph and is denoted by d. A diametrical path of a graph is the shortest path whose length is equal to the diameter of the graph.

For an integer $p \geq 0$, the tree S^p of order $n = 2p+1$, containing p pendant vertices, each attached to a vertex of degree 2, and a vertex of degree p, is called the *p-sun*.
For integers $p, q \geq 0$, the tree $DS^{p,q}$ 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*.

The *adjacency matrix* $A = A(G)$ of a graph G is defined by its entries as $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be *eigenvalues* of the adjacency matrix of G. According to the eigenvalues of the adjacency matrix, the *energy* of a graph is defined as

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} \mid \lambda_i \mid .$$

The concept of energy of a graph was first used by Gutman in chemistry to approximate *π-electron* energy, see([7], [8], [9]).

The *Randić matrix* is defined as $r_{ij} = \frac{1}{\sqrt{d_{v_i} d_{v_j}}}$ if $v_iv_j \in E(G)$ and 0 otherwise. The Randić matrix is real symmetric, so we can order its eigenvalues so that $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. The *Randić energy* (see [3]) is defined as

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

Gutman, Furtula and Bozkurt presented the following conjecture in [6] about the connected graphs with maximal Randić energy.

Conjecture 1.1 ([6]). *Let G be a connected graph on n vertices. Then*

$$\mathcal{E}_R(G) \leq \begin{cases} \mathcal{E}_R(S^p), & \text{if } n = 2p+1 \text{ is odd,} \\ \mathcal{E}_R(DS^{p,q}), & \text{if } n = 2(p+q+1) \text{ is even.} \end{cases}$$

Gao et al. in [5] presented the minimal Randić energy of trees with a given diameter. Gao in [4], showed that the generalized double suns of odd order satisfy Conjecture 1.1. The validity of Conjecture 1.1 over some other families of graphs is shown by Allem, Braga, Pastine and Molina, [1, 2].

Let T_d^n be the class of trees of order n with diameter $4 \leq d \leq n-1$. Let $T \in T_d^n$ and $M_k(T)$ be the set of all k-matchings of T, for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. For $e = uv \in E(T)$ and $\alpha_k = \{e_1, e_2, \ldots, e_k\} \in M_k(T)$, we denote $R_T(e) = R_T(uv) = \dfrac{1}{d_T(u)d_T(v)}$, and $R_T(\alpha_k) =$

$\prod_{i=1}^{k} R_T(e_i)$. The *R-polynomial* of T can be written as

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

where $b(R(T),0) = 1$ and $b(R(T),k) = \sum_{\alpha_k \in M_k(T)} R_T(\alpha_k)$ for $1 \le k \le \lfloor \frac{n}{2} \rfloor$ (see [10]).

Theorem 1.2 ([10]). *Let $T_1, T_2 \in T_d^n$, and their R-polynomials be*

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

respectively. If $b(R(T1),k) \ge b(R(T2),k)$ for all $k \ge 1$, and there is an integer number k such that $b(R(T_1),k) > b(R(T_2),k)$, then $\mathcal{E}_R(T_1) > \mathcal{E}_R(T_2)$.

In this paper, we study trees with a given diameter and maximal Randić energy, therefore, we find families of graphs satisfying Conjecture 1.1. We prove for $n \ge 5$ and $4 \le d \le n-1$, if $T \in T_d^n$ be a tree with maximal Randić energy then T is obtained from a path $P = v_0 v_1 \dots v_d$ by adding n_i path(s) P_3 to each vertex v_i, for $i = 2,3,4,\dots,d-2$, where $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$.

2. Operations

In this section, we introduce some operations which are useful to obtain the maximum Randić energy trees of order n and diameter d. The following operations 1 and 5 were introduced in [5] and [11], respectively.

Operation 1 ([5]). *Suppose that T is a tree, in addition, we assume that T_1 is a subtree of T, such that $v_1 \in V(T_1)$, $t \ge 3$ and $d_T(v_1) \ge 3$. Define $T' = T - \{v_1v_3, v_1v_4 \dots, v_1v_t\} + \{v_2v_3, v_3v_4 \dots, v_{t-1}v_t\}$. The above-referred graphs are illustrated in Figure 1.*

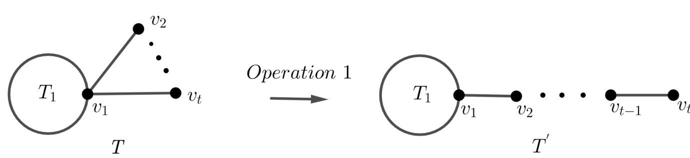

Figure 1. Trees T and T' for Operation 1.

We now present Operations 2, 3 and 4 as follows:

Operation 2. *Suppose that T is a tree, in addition, we assume that T_1 is a subtree of T. Define $T' = T - \{u_{s-1}u_s\} + \{v_tu_s\}$. The above-referred trees are illustrated in Figure 2.*

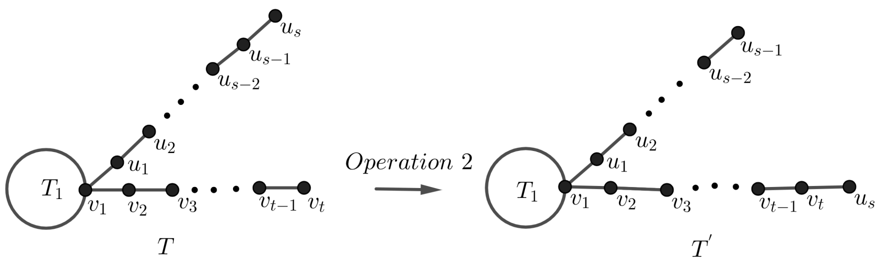

FIGURE 2. Trees T and T' for Operation 2.

Operation 3. *Suppose that* T *is a tree, in addition, we assume that* T_1 *is a subtree of* T*, such that* $v_1 \in V(T_1)$ *and* $d_T(v_1) \geq 3$. *Define* $T' = T - \{v_1u\} + \{v_tu\}$, $d_{T'}(v_1) \geq 2$, $d_T(v_1) = d_{T'}(v_1) + 1$. *The above-referred trees are illustrated in Figure 3.*

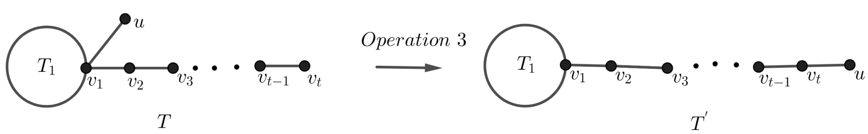

FIGURE 3. Trees T and T' for Operation 3.

Operation 4. *Suppose that* T *is a tree and* T_1 *is a subtree of* T*, such that* $v_1 \in V(T_1)$. *Define* $T' = T - \{u_{t-1}u_t\} + \{w_su_t\}$. *The above-referred trees are illustrated in Figure 4.*

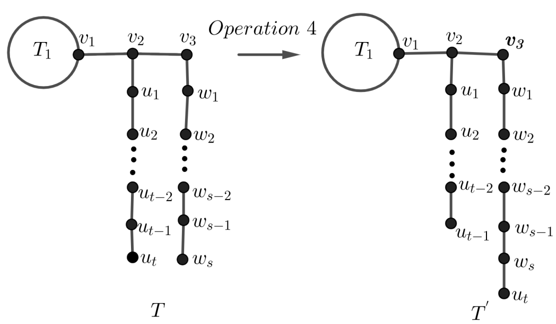

FIGURE 4. Trees T and T' for Operation 4.

Operation 5 ([11]). *Suppose that* T *is a tree and* T_1 *is a subtree of* T*, with* $v_1 \in V(T_1)$ *such that* $d_T(v_1) \geq 2$, $t \geq 7$. *Define* $T' = T - \{v_4v_5 \ldots v_t\} + \{v_1v_4v_5 \ldots v_t\}$. *The above-referred trees are illustrated in Figure 5.*

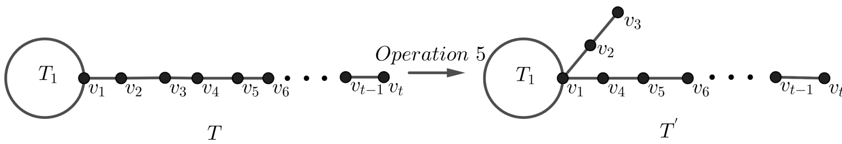

FIGURE 5. Trees T and T' for Operation 5.

3. Useful lemmas

In this section, we show that if a tree T' is obtained from a tree T by Operations 1, 2, 3, 4 and 5 then $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$. The following two lemmas corresponding to Operations 3.1 and 3.5 were presented in [5] and [11], respectively.

Lemma 3.1 ([5])**.** *Let T and T' be two trees satisfying the conditions of Operation 1. Then $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.*

We next present our lemmas for Operations 2, 3 and 4.

Lemma 3.2. *Let T and T' be two trees satisfying the conditions of Operation 2. Then $\mathcal{E}_R(T) = \mathcal{E}_R(T')$.*

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

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

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

$$\begin{aligned} b(R(T'),1) - b(R(T),1) &= R_{T'}(u_{s-2}u_{s-1}) + R_{T'}(v_{t-1}v_t) + R_{T'}(v_t u_s) \\ &\quad -R_T(u_{s-2}u_{s-1}) - R_T(u_{s-1}u_s) - R_T(v_{t-1}v_t) \\ &= \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} + \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \\ &\quad -\frac{1}{d_T(u_{s-2})d_T(u_{s-1})} - \frac{1}{d_T(u_{s-1})d_T(u_s)} - \frac{1}{d_T(v_{t-1})d_T(v_t)} \\ &= \frac{1}{2} + \frac{1}{4} + \frac{1}{2} - \frac{1}{4} - \frac{1}{2} - \frac{1}{2} \\ &= 0. \end{aligned}$$

That is, $b(R(T'),1)=b(R(T),1)$.

For $k=2,\dots,\lfloor\frac{n}{2}\rfloor$, we denote $P_1=v_1u_1u_2\dots u_{s-2}$ and $P_2=v_1v_2\dots v_{t-1}$, then we have

$$\begin{aligned}
b(R(T'),k)=&\sum_{\alpha_k\in M_k(T_1\cup(p_1\cup p_2))}R_{T'}(\alpha_k)\\
&+\Big(\frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})}+\frac{1}{d_{T'}(v_t)d_{T'}(u_s)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-1})\\
&+\Big(\frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})}\times\frac{1}{d_{T'}(v_t)d_{T'}(u_s)}\Big)\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-2})\\
&+\Big(\frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)}+\frac{1}{d_{T'}(v_t)d_{T'}(u_s)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1})\\
&+\Big(\frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})}+\frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)}\\
&+\frac{1}{d_{T'}(v_t)d_{T'}(u_s)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1})\\
&+\Big(\frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})}\times\frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)}\\
&+\frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})}\times\frac{1}{d_{T'}(v_t)d_{T'}(u_s)}\Big)\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-2})\\
=&\sum_{\alpha_k\in M_k(T_1\cup(p_1\cup p_2))}R_{T'}(\alpha_k)+\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-1})\\
&+\frac{1}{4}\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-2})+\frac{3}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1})\\
&+\frac{5}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1})\\
&+\frac{3}{8}\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-2}).
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
b(R(T),k)=&\sum_{\alpha_k\in M_k(T_1\cup(p_1\cup p_2))}R_T(\alpha_k)\\
&+\Big(\frac{1}{d_T(u_{s-2})d_T(u_{s-1})}+\frac{1}{d_T(u_{s-1})d_T(u_s)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_T(\alpha_{k-1})\\
&+\Big(\frac{1}{d_T(u_{s-1})d_T(u_s)}+\frac{1}{d_T(v_{t-1})d_T(v_t)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_T(\alpha_{k-1})\\
&+\Big(\frac{1}{d_T(u_{s-1})d_T(u_s)}\times\frac{1}{d_T(v_{t-1})d_T(v_t)}\Big)\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2})
\end{aligned}$$

$$
\begin{aligned}
&+\Big(\frac{1}{d_T(u_{s-2})d_T(u_{s-1})}+\frac{1}{d_T(u_{s-1})d_T(u_s)}\\
&+\frac{1}{d_T(v_{t-1})d_T(v_t)}\Big)\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-1})\\
&+\Big(\frac{1}{d_T(u_{s-2})d_T(u_{s-1})}\times\frac{1}{d_T(v_{t-1})d_T(v_t)}\\
&+\frac{1}{d_T(u_{s-1})d_T(u_s)}\times\frac{1}{d_T(v_{t-1})d_T(v_t)}\Big)\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2})\\
=&\sum_{\alpha_k\in M_k(T_1\cup(p_1\cup p_2))}R_T(\alpha_k)+\frac{3}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_T(\alpha_{k-1})\\
&+\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_1-v_{t-1}))}R_T(\alpha_{k-1})+\frac{1}{4}\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2})\\
&+\frac{5}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-1})+\frac{3}{8}\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2}).
\end{aligned}
$$

since

$$
\begin{aligned}
\sum_{\alpha_k\in M_k(T_1\cup p_1\cup p_2)}R_T(\alpha_k)&=\sum_{\alpha_k\in M_k(T_1\cup p_1\cup p_2)}R_{T'}(\alpha_k),\\
\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_T(\alpha_{k-1})&=\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-1}),\\
\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2})&=\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_{T'}(\alpha_{k-2}),\\
\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup p_2)}R_T(\alpha_{k-1})&=\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p_1\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1}),\\
\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-1})&=\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-1}),\\
\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_T(\alpha_{k-2})&=\sum_{\alpha_{k-2}\in M_{k-2}(T_1\cup(p_1-u_{s-2})\cup(p_2-v_{t-1}))}R_{T'}(\alpha_{k-2}),
\end{aligned}
$$

it is easy to see that $b(R(T'),k)-b(R(T),k)$ =0. This implies $b(R(T'),1)=b(R(T),1)$. By Theorem 1.2, the lemma holds. □

Lemma 3.3. *Let T and T' be two trees satisfying the conditions of Operation 3. Then $\mathcal{E}_R(T)\le\mathcal{E}_R(T')$.*

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

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

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

$$\begin{aligned} b(R(T'),1) - b(R(T),1) &= R_{T'}(v_1v_2) + R_{T'}(v_{t-1}v_t) + R_{T'}(v_tu) \\ &\quad -R_T(v_1u) - R_T(v_1v_2) - R_T(v_{t-1}v_t) \\ &= \frac{1}{d_{T'}(v_1)d_{T'}(v_2)} + \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u)} \\ &\quad -\frac{1}{d_T(v_1)d_T(u)} - \frac{1}{d_T(v_1)d_T(v_2)} - \frac{1}{d_T(v_{t-1})d_T(v_t)} \\ &= \frac{1}{2d_{T'}(v_1)} + \frac{1}{4} + \frac{1}{2} - \frac{1}{d_T(v_1)} - \frac{1}{2d_T(v_1)} - \frac{1}{2} \\ &= \frac{1}{4} + \frac{1}{2d_{T'}(v_1)} - \frac{3}{2d_T(v_1)} > 0. \end{aligned}$$

This implies $b(R(T'),1) > b(R(T),1)$.

For $k = 2, \dots, \lfloor \frac{n}{2} \rfloor$, we denote $p = v_2v_3 \dots v_{t-1}$. Then

$$\begin{aligned} b(R(T'),k) &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_{T'}(\alpha_k) + \frac{1}{d_{T'}(v_t)d_{T'}(u)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) \\ &\quad + \frac{1}{d_{T'}(v_t)d_{T'}(u)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - v_2))} R_{T'}(\alpha_{k-1}) \\ &\quad + \left(\frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u)}\right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - v_{t-1})} R_{T'}(\alpha_{k-1}) \\ &\quad + \left(\frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u)}\right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - \{v_2, v_{t-1}\})} R_{T'}(\alpha_{k-1}) \\ &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_{T'}(\alpha_k) + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) \\ &\quad + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - v_2))} R_{T'}(\alpha_{k-1}) + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - v_{t-1})} R_{T'}(\alpha_{k-1}) \\ &\quad + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - \{v_2, v_{t-1}\})} R_{T'}(\alpha_{k-1}). \end{aligned}$$

Similarly, we have

$$\begin{aligned} b(R(T),k) &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_T(\alpha_k) + \frac{1}{d_T(v_{t-1})d_T(v_t)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p - v_{t-1})} R_T(\alpha_{k-1}) \\ &\quad + \frac{1}{d_T(v_{t-1})d_T(v_t)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - \{v_2, v_{t-1}\})} R_T(\alpha_{k-1}) \\ &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_T(\alpha_k) + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p - v_{t-1})} R_T(\alpha_{k-1}) \\ &\quad + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p - \{v_2, v_{t-1}\})} R_T(\alpha_{k-1}). \end{aligned}$$

Note that

$$\begin{aligned}\sum_{\alpha_k\in M_k(T_1\cup p)} R_{T'}(\alpha_k) &= \sum_{\alpha_k\in M_k(T_1\cup p)} R_T(\alpha_k),\\ \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_{t-1})} R_{T'}(\alpha_{k-1}) &= \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_{t-1})} R_T(\alpha_{k-1}),\\ \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1}) &= \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_T(\alpha_{k-1}),\end{aligned}$$

So, we get

$$\begin{aligned}b(R(T'),k)-b(R(T),k) &= \frac{1}{2}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p)} R_{T'}(\alpha_{k-1})+\frac{1}{2}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_2)} R_{T'}(\alpha_{k-1})\\ &+\frac{1}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_{t-1}))} R_{T'}(\alpha_{k-1})\\ &+\frac{1}{4}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1}).\end{aligned}$$

On the other hand, since

$$\begin{aligned}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup p)} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1}),\\ \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_2))} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1}),\\ \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-v_{t-1})} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1}),\end{aligned}$$

we get

$$b(R(T'),k)-b(R(T),k)\geq \frac{3}{2}\sum_{\alpha_{k-1}\in M_{k-1}(T_1\cup(p-\{v_2,v_{t-1}\})} R_{T'}(\alpha_{k-1})>0.$$

that is, $b(R(T'),k)>b(R(T),k)$. By Theorem 1.2, the lemma holds. □

Lemma 3.4. *Let T and T' be two trees satisfying the conditions of Operation 4. Then $\mathcal{E}_R(T)=\mathcal{E}_R(T')$.*

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

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

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

$$\begin{aligned} b(R(T'),1) - b(R(T),1) &= R_{T'}(u_{t-2}u_{t-1}) + R_{T'}(w_{s-1}w_s) + R_{T'}(w_s u_t) \\ &\quad - R_T(u_{t-2}u_{t-1}) - R_T(u_{t-1}u_t) - R_T(w_{s-1}w_s) \\ &= \frac{1}{d_{T'}(u_{t-2})d_{T'}(u_{t-1})} + \frac{1}{d_{T'}(w_{s-1})d_{T'}(w_s)} + \frac{1}{d_{T'}(w_s)d_{T'}(u_t)} \\ &\quad - \frac{1}{d_T(u_{t-2})d_T(u_{t-1})} - \frac{1}{d_T(u_{t-1})d_T(u_t)} - \frac{1}{d_T(w_{s-1})d_T(w_s)} \\ &= \frac{1}{2} + \frac{1}{4} + \frac{1}{2} - \frac{1}{4} - \frac{1}{2} - \frac{1}{2} = 0. \end{aligned}$$

Thus the above eequality is equivalent to $b(R(T'),1) = b(R(T),1)$.
For $k = 2, \ldots, \lfloor \frac{n}{2} \rfloor$, we use $p_1 = v_1v_2v_3$ and $p_2 = v_2u_1u_2 \ldots u_{t-2}$, $p_3 = v_3w_1w_2 \ldots w_{s-1}$. By the same argument as lemma 3.2, we can prove that $b(R(T'),k) = b(R(T),k)$. □

In [11], the following lemma is proved.

Lemma 3.5 ([11]). *Let T and T' be two trees satisfying the conditions of Operation 5. Then $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$.*

4. Main result

Let $T(n_2, n_3, \ldots, n_{d-2})$ be the class of trees T such that T is obtained from a path $P = v_0v_1 \ldots v_d$ by adding n_i path(s) P_3 to each vertex v_i, for $i = 2, 3, 4, \ldots, d-2$, where $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$. Also, let $T'(n_2, n_3, \ldots, n_{d-2})$ be the class of trees T' such that T' is obtained from a tree $T \in T(n_2, n_3, \ldots, n_{d-2})$ by adding a leaf to one of the path(s) p_3.

Theorem 4.1. *Let $T \in T_d^n$ be a tree with maximal Randić energy, where $4 \leq d \leq n-1$ and $n \geq 5$. If n is odd and d is even or n is even and d is odd, then $T \in T(n_2, n_3, \ldots, n_{d-2})$. If both n and d are odd or both n and d are even, then $T \in T'(n_2, n_3, \ldots, n_{d-2})$.*

Proof. Let $T \in T_d^n$ be a tree with maximal Randić energy, where $4 \leq d \leq n-1$ and $n \geq 5$. We prove that if n is odd and d is even or n is even and d is odd, then there is a tree $T' \in T(n_2, n_3, \ldots, n_{d-2})$ such that $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$, and if both n and d are odd or both n and d are even, then there is a tree $T' \in T'(n_2, n_3, \ldots, n_{d-2})$ such that $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$. Let $P = v_0v_1v_2 \ldots v_d$ be a diametrical path in T. By Lemma 3.1, there is a tree $T_1 \in T_d^n$ such that $\mathcal{E}_R(T) \leq \mathcal{E}_R(T_1)$. By Lemmas 3.2 and 3.3, there is a tree $T_2 \in T_d^n$ such that $\mathcal{E}_R(T_1) \leq \mathcal{E}_R(T_2)$. Now, if there is a pendant vertex on the tree T_2, applying Operation 3, then there is a tree $T_3 \in T_d^n$ as show in Figure 6 such that $\mathcal{E}_R(T_2) \leq \mathcal{E}_R(T_3)$.

Note that by Lemma 3.4 we have even number of vertices in each path connected to the diametrical path in Figure 6. Finally by Lemma 3.5 there is a tree $T_4 \in T(n_2, n_3, \ldots, n_{d-2})$ as shown in Figure 7 such that $\mathcal{E}_R(T_3) \leq \mathcal{E}_R(T_4)$. □

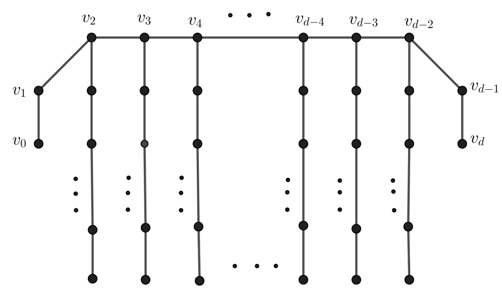

FIGURE 6. The tree T_3.

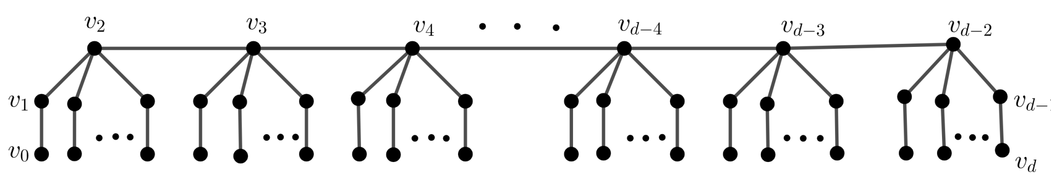

FIGURE 7. The tree T_4.

As a consequence of Theorem 4.1, we obtain the following which proves the validity of Conjecture 1.1 for particular classes of trees.

Corollary 4.2. *Let $T \in T_d^n$. Then*

$$\mathcal{E}_R(T) \leq \begin{cases} \mathcal{E}_R(S^p) & \text{if } d=4 \text{ and } n=2p+1 \\ \mathcal{E}_R(DS^{p,q}) & \text{if } d=5 \text{ and } n=2(p+q+1). \end{cases}$$

5. Conclusion

In this paper, using Operations 1, 2, 3, 4 and 5 we have determined trees $T \in T_d^n$ with maximal Randić energy. In particular, we presented families of trees satisfying Conjecture 1.1.

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Shiva Sepidbon
Department of Mathematics,
Shahed University,
Tehran, Iran.
shiva.sepidbon@shahed.ac.ir

Nader Jafari Rad
Department of Mathematics,
Shahed University,
Tehran, Iran.
n.jafarirad@shahed.ac.ir

Akbar Jahanbani
Department of Mathematics,
Azarbaijan Shahid Madani University,
Tabriz, Iran.
akbarjahanbani92@gmail.com