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Research Paper

Extremal Kragujevac Trees with Respect to Randić Energy

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Abstract

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The Randić matrix of G, represented as $R(G)$, is defined as the $n \times n$ matrix whose (i,j)-entry is $(d_i d_j)^{\frac{-1}{2}}$ if v_i and v_j are adjacent and 0 otherwise. The Randić energy of graph G is the sum of absolute values of the eigenvalues of $R(G)$. In this study, we determine the Kragujevac trees with a fixed degree and fixed order that have maximal and minimal Randić energy. Additionally, we obtain upper and lower bounds for the Randić energy of these trees.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$. The Randić matrix [1, 2] $R(G) = (r_{ij})$ of G whose vertex v_i has degree d_i is defined by $r_{ij} = \frac{1}{\sqrt{d_i d_j}}$ if the vertices v_i and v_j are adjacent, and $r_{ij} = 0$ otherwise. Denote the eigenvalues of the Randić matrix of G by $x_1, x_2, \ldots, x_n$. The multi set $SP_R(G) = \{x_1, x_2, \ldots, x_n\}$ is called the R-spectrum of the graph G. The Randić energy of G is defined as:

$$RE(G) = \sum_{i=1}^{n} |x_i|.$$

The Randić polynomial associated with the graph G, represented as $\phi_G(x)$, is defined as the characteristic polynomial of the Randić matrix $R(G)$, that is,

$$\phi_G(x) = det(xI_n - R(G)),$$

where I_n is the identity matrix of order n. If G is a tree of order n, then

$$\phi_G(x) = \sum_{k \geq 0} (-1)^k a_{2k} x^{n-2k}.$$

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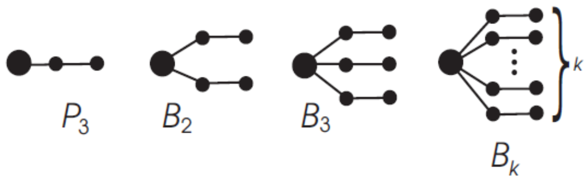

Figure 1: The branches of Kragujevac trees.

The Coulson-type integral of Randić energy of a tree is [3]

$$RE(G) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}Ln[\sum_{k\geq 0}(-1)^k a_{2k}x^{2k}]dx, \quad (1)$$

where $(-1)^k a_{2k} \geq 0$.

Let P_3 be the 3-vertex tree, rooted at one of its terminal vertices. For $k \geq 2$, B_k a branch of a Kragujevac tree is constructed by identifying the roots of k copies of P_3 (see Figure 1). We denote by $T(B_{k_1}, B_{k_2}, \ldots, B_{k_d})$ a Kragujevac tree of degree d where constructed by connecting the central vertex of $B_{k_1}, B_{k_2}, \ldots B_{k_d}$ to an isolated vertex (see Figure 2).

Recently, a number of studies have investigated and compared the numeric descriptors of Kragujevac trees [4–6]. In this paper, the Kragujevac trees with a fixed degree and a fixed order, having maximal and minimal Randić energy are determined by similar methods where are used in [6]. As an application, we obtain an upper bound and a lower bound for the Randić energy of these trees.

Let E_{n_i,n_j} be an $n_i \times n_j$ matrix whose $(1,1)$-entry is 1, and all other entries are zero. If A is a square matrix, then we will denote by $\bar{A}$, the obtained matrix from A by deleting its first row and first column. In the following theorem the main method of computation of characteristic polynomial of $R(G)$ is introduced.

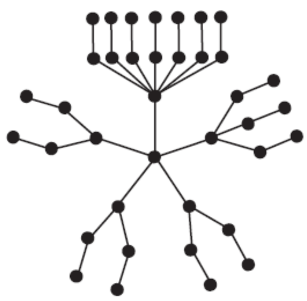

Figure 2: A Kragujevac tree of order 38 and degree 5.

Theorem 1.1. *([7]). Let $A_{n_1}, A_{n_2}, \ldots, A_{n_k}$ be square matrices. If*

$$X = \begin{bmatrix} A_{n_1} & E_{n_1,n_2} & E_{n_1,n_3} & \cdots & E_{n_1,n_k} \\ E_{n_2,n_1} & A_{n_2} & E_{n_2,n_3} & \cdots & E_{n_2,n_k} \\ E_{n_3,n_1} & E_{n_3,n_2} & A_{n_3} & \cdots & E_{n_3,n_k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ E_{n_k,n_1} & E_{n_k,n_2} & E_{n_k,n_3} & \cdots & A_{n_k} \end{bmatrix},$$

then

$$det(X) = \begin{vmatrix} |A_{n_1}| & \alpha_{1,2} & \alpha_{1,3} & \cdots & \alpha_{1,k} \\ \alpha_{2,1} & |A_{n_2}| & \alpha_{2,3} & \cdots & \alpha_{2,k} \\ \alpha_{3,1} & \alpha_{3,2} & |A_{n_3}| & \cdots & \alpha_{3,k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{k,1} & \alpha_{k,2} & \alpha_{k,3} & \cdots & |A_{n_k}| \end{vmatrix},$$

where

$$\alpha_{ij} = \begin{cases} |\bar{A}_{n_i,nj}|, & if \;\; E_{n_i,n_j} \neq 0, \\ 0, & if \;\; E_{n_i,n_j} = 0. \end{cases}$$

2 Extremal Kragujevac trees

In this section, at first, the Randić polynomial of the branches of a Kragujevac tree is computed. To this purpose, we will use the following elementary lemma.

Lemma 2.1. *If x and y are arbitrary variables, then we have*

$$\begin{vmatrix} y & -1 & -1 & \ldots & -1 \\ -1 & x & 0 & \ldots & 0 \\ -1 & 0 & x & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \ldots & x \end{vmatrix}_{n+1,n+1} = x^{n-1}(xy-n).$$

Let v_i be a vertex of G for $1 \leq i \leq n$. In what follows, we need to delete a vertex of a graph without any change in the entries of $R(G - v_i)$. So we will denote by $\bar{R}(G - v_i)$ the square matrix where is obtained by deleting the i-th row and i-th column of $R(G)$ and denote by $\phi^{'}_G(x)$ the Randić polynomial of $\bar{R}(G - v_i)$.

Let G_1 and G_2 be two disjoint simple graph, $v_i \in V(G_i)$ for $i = 1, 2$ and G constructed by adjacent v_1 and v_2. In the following lemma the Randić polynomial of G will be computed.

Lemma 2.2. *Let $d(v_i)$ be the degree of v_i in G for $i = 1, 2$, then*

$$\phi_G(x) = \phi_{G_1}(x)\phi_{G_2}(x) - \frac{1}{d(v_1)d(v_2)}\phi^{'}_{G_1-v_1}(x)\phi^{'}_{G_2-v_2}(x).$$

Proof. Let $n_i = |V(G_i)|$ for $i = 1, 2$ where v_1 has the first label and label of v_2 is $n_1 + 1$ in $V(G)$. If the $(1, 1)$-entry of E_{n_1,n_2} is $\frac{1}{\sqrt{d(v_1)d(v_2)}}$ and all other enteries are 0, then the Randić matrix of G is

$$R(G) = \begin{bmatrix} R(G_1) & E_{n_1,n_2} \\ E^T_{n_1,n_2} & R(G_2) \end{bmatrix}.$$

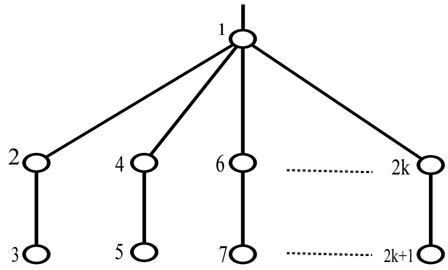

Figure 3: Labelling of the vertices of β_k in Lemma 2.3.

Using Theorem 1.1, Randić polynomial of G is given as

$$\begin{aligned}\phi_G(x) &= \frac{1}{d(v_1)d(v_2)}\begin{vmatrix} d(v_1)d(v_2)\phi_{G_1}(x) & \phi'_{G_1-v_1}(x) \\ \phi'_{G_2-v_2}(x) & \phi_{G_2}(x)\end{vmatrix} \\ &= \phi_{G_1}(x)\phi_{G_2}(x) - \frac{1}{d(v_1)d(v_2)}\phi'_{G_1-v_1}(x)\phi'_{G_2-v_2}(x).\end{aligned}$$

■

Let T be a Kragujevac tree and B_k be a branch of T. Note that the degree of the central vertex of B_k is $k+1$. Thus, in the calculation of the Randić polynomial of T we consider a tree such as β_k instate B_k where degree of its central vertex is $k+1$.

Lemma 2.3. *Let k be a positive integer. The characteristic polynomial of β_k is given as:*

$$\phi_{\beta_k}(x) = x\left(x^2 - \frac{1}{2}\right)^{k-1}\left(x^2 - \frac{2k+1}{2k+2}\right).$$

Proof. Let the vertices of β_k be labelled as shown in Figure 3 and
$A = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$, $Z = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ and $C = \begin{bmatrix} \frac{1}{\sqrt{2(k+1)}} & 0 \end{bmatrix}$, then

$$R_{\beta_k}(x) = \begin{bmatrix} 0 & C & C & C & \ldots & C \\ C^T & A & Z & Z & \ldots & Z \\ C^T & Z & A & Z & \ldots & Z \\ C^T & Z & Z & A & \ldots & Z \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ C^T & Z & Z & Z & \ldots & A \end{bmatrix}.$$

Since $\phi_A(x) = x^2 - \frac{1}{2}$ and $\phi_{\bar{A}}(x) = x$, thus by use of Theorem 1.1, the characteristic polynomial of β_k is computed as follows:

$$\phi_{\beta_k}(x) = \left|\begin{array}{cccccc} x & \frac{-1}{\sqrt{2(k+1)}} & \frac{-1}{\sqrt{2(k+1)}} & \frac{-1}{\sqrt{2(k+1)}} & \cdots & \frac{-1}{\sqrt{2(k+1)}} \\ \frac{-x}{\sqrt{2(k+1)}} & x^2-\frac{1}{2} & 0 & 0 & \cdots & 0 \\ \frac{-x}{\sqrt{2(k+1)}} & 0 & x^2-\frac{1}{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{-x}{\sqrt{2(k+1)}} & 0 & 0 & 0 & \cdots & x^2-\frac{1}{2} \end{array}\right]$$

$$= \frac{x^k}{2(k+1)}\left|\begin{array}{ccccccc} 2(k+1)x & 1 & 1 & \cdots & 1 & & \\ 1 & \frac{x^2-\frac{1}{2}}{x} & 0 & 0 & \cdots & 0 \\ 1 & 0 & \frac{x^2-\frac{1}{2}}{x} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & \frac{x^2-\frac{1}{2}}{x} \end{array}\right].$$

Therefore, by using Lemma 2.1, we get

$$\begin{aligned} \phi_{\beta_k}(x) &= \frac{x^k}{2(k+1)}\left(\frac{x^2-\frac{1}{2}}{x}\right)^{k-1}\left(2(k+1)x(\frac{x^2-\frac{1}{2}}{x})-k\right) \\ &= x\left(x^2-\frac{1}{2}\right)^{k-1}\left(x^2-\frac{2k+1}{2k+2}\right). \end{aligned}$$

■

Let $R^{'}(G)$ denote the square matrix obtained from $R(G)$ by replacing any positive integer instead of the degree of a vertex of G. In what follows, we need to verify the sign of the coefficients of the characteristic polynomial of $R^{'}(G)$ where we will call it the modified Randić polynomial of G and denote by $\bar{\phi}_G(x)$.

Lemma 2.4. *The sigsn of the coefficients of $\phi_G(x)$ and $\bar{\phi}_G(x)$ are the same.*

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$ and $d_i = deg(v_i)$. Without losing the generality, suppose that in the construction of $R(G)$, we consider the positive integer $d_1^{'}$ instead of d_1. Let $\delta_{1,i} = 1$ if $v = v_1$ adjacent to $v_i \in V(G)$, otherwise $\delta_{1,i} = 0$. For

$$C = \left[\frac{\delta_{1,2}}{\sqrt{d_1^{'}d_2}}, \frac{\delta_{1,3}}{\sqrt{d_1^{'}d_3}}, \dots, \frac{\delta_{1,n}}{\sqrt{d_1^{'}d_n}}\right],$$

we have

$$\bar{\phi}_G(x) = \left|\begin{array}{cc} x & C \\ C^T & R(G-v_1) \end{array}\right|.$$

If

$$D = \left[\frac{\delta_{1,2}}{\sqrt{d_1d_2}}, \frac{\delta_{1,3}}{\sqrt{d_1d_3}}, \dots, \frac{\delta_{1,n}}{\sqrt{d_1d_n}}\right],$$

then

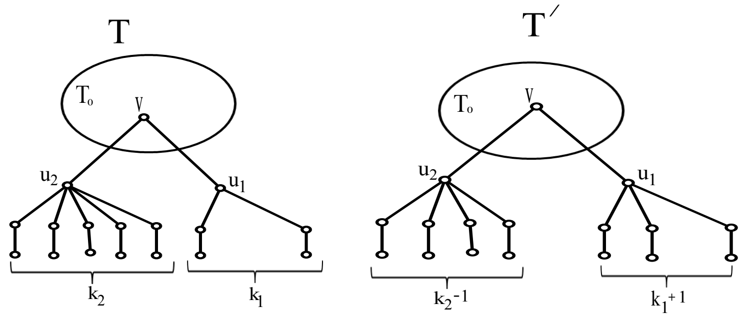

Figure 4: The Kragujevac trees considered in Lemma 2.5.

$$\bar{\phi}_G(x) = \begin{vmatrix} \frac{d_1' x}{d_1} & D \\ D^T & R(G - v_1) \end{vmatrix}.$$

Thus in the computation of $\bar{\phi}_G(x)$ only the $(1,1)$- entry of $det(xI - R(G))$ changes from x to $\frac{d_1' x}{d_1}$ and the coefficients of $\bar{\phi}_G(x)$ and $\phi_G(x)$ are the same. ■

Let k_1 and k_2 be integers such that $2 \leq k_1 \leq k_2 - 2$. Suppose that T_0 is a subtree of a Kragujevac tree T obtained by deleting the branches B_{k_1} and B_{k_2} from T with v as its central vertex. So, T is constructed by attaching v to the root vertices of B_{k_1} and B_{k_2}. Construct the tree $T^{'}$ by attaching v in T_0 to the root vertices of new branches, B_{k_1+1} and B_{k_2-1} (see Figure 4).

Lemma 2.5. *If* $\phi_T(x) = \sum_{i\geq 0}(-1)^i a_{2i} x^{n-2i}$ *and* $\phi_{T'}(x) = \sum_{i\geq 0}(-1)^i a_{2i}^{'} x^{n-2i}$*, then* $a_{2i}^{'} \geq a_{2i}$ *for* $i \geq 0$*.*

Proof. Let u_i denote the central vertex of B_{k_i} for $i = 1, 2$ and let $d = d(v)$ in T. By using Lemma 2.2 for edges vu_1 and vu_2, we have

$$\begin{aligned} \phi_T(x) &= \phi_{T_0}(x)\phi_{\beta_{k_1}}(x)\phi_{\beta_{k_2}}(x) - \frac{\phi_{T_0-v}^{'}(x)\phi_{\beta_{k_1}}(x)\phi_{\beta_{k_2}-u_2}^{'}(x)}{d(k_1+1)} - \\ &\quad \frac{\phi_{T_0-v}^{'}(x)\phi_{\beta_{k_1}-u_1}^{'}(x)\phi_{\beta_{k_2}}(x)}{d(k_2+1)}. \end{aligned}$$

And

$$\begin{aligned} \phi_{T'}(x) &= \phi_{T_0}(x)\phi_{\beta_{k_1+1}}(x)\phi_{\beta_{k_2-1}}(x) - \frac{\phi_{T_0-v}^{'}(x)\phi_{\beta_{k_1+1}}(x)\phi_{\beta_{k_2-1}-u_2}^{'}(x)}{dk_2} - \\ &\quad \frac{\phi_{T_0-v}^{'}(x)\phi_{\beta_{k_1+1}-u_1}^{'}(x)\phi_{\beta_{k_2-1}}(x)}{d(k_1+2)}. \end{aligned}$$

Since $\phi^{'}_{\beta_{k_i}-u_i}(x) = (x^2 - \frac{1}{2})^{k_i}$, for $i = 1, 2$, by using Lemma 2.3, we have

$$\begin{aligned} \phi_{T'}(x) - \phi_T(x) &= -\phi_{T_0}(x)x^2(x^2 - \frac{1}{2})^{k_1+k_2-2}(x^2-\alpha) \\ &\quad -\phi^{'}_{T_0-v}(x)x(x^2-\frac{1}{2})^{k_1+k_2-1}(x^2-\beta), \end{aligned} \quad (2)$$

where $\alpha = \frac{2(k_2^2-k_1^2)-5k_1+k_2-3}{2(k_2^2-k_1^2)+2k_2-6k_1-4}$ and $\beta = \frac{k_2^2-k_1^2-2k_1-1}{k_2^2-k_1^2+k_2-3k_1-2}$. Since $k_2 \geq k_1 + 2$, in follows that $\alpha, \beta > 0$. Thus, in (2), $\phi_{T_0}(x)x^2(x^2 - \frac{1}{2})^{k_1+k_2-2}(x^2-\alpha)$ can considered as Randić (or modified Randić) polynomial of a graph contains T_0, $k_1 + k_2$ copy of P_2 (the path of order 2) and two disjoint vertices. Also $\phi^{'}_{T_0-v}(x)x(x^2 - \frac{1}{2})^{k_1+k_2-1}(x^2-\beta)$ can considered as modified Randić polynomial of a graph contains $T_0 - v$, $k_1 + k_2$ copies of P_2 and a disjoint vertex.

Therefore by using Lemma 2.4, $\phi_{T'}(x) - \phi_T(x)$ is a polynomial of degree $n - 2$ where the sing of coefficient of x^{2i} is equal to the sign of the coefficient of x^{2i} in $\phi_T(x)$ for $0 \leq i \leq \lfloor \frac{n}{2} \rfloor - 1$. Thus, $a^{'}_{2i} \geq a_{2i}$ for $i \geq 0$. ■

The trees T and $T^{'}$ are Kragujevac trees with same order and degree. Because of the requirement $k_2 - 2 \geq k_1 \geq 2$, in the transformation $T \to T^{'}$, a larger branch is diminished and a smaller branch is increased. Since the Randić energy of trees is a monotonically increasing function of parameters $(-1)^i a_{2i}$ for $i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$, by Lemma 2.5 and (1) we get the our main results [3].

Lemma 2.6. *If T and $T^{'}$ be Kragujevac trees of order n and degree d with structure as indicated in Figure 4, then for $2 < k_1 \leq k_2 - 2$, the Randić energy of $T^{'}$ is greater than the Randić energy of T.*

Continuing the argument used in Lemma 2.6, and repeatedly applying the transformations $T \to T^{'}$ as far as possible for any Kragujevac tree, we can obtain the Kragujevac trees with maximum Randić energy or minimum Randić energy as follows:

Theorem 2.7. *Within the Kragujevac trees with order n and degree d, the trees such that either all branches isomorphic to B_k if*

$$k = \frac{1}{2}(\frac{n-1}{d} - 1),$$

is an integer, or branches isomorphic to B_k and B_{k-1} for

$$k = \lceil \frac{1}{2}(\frac{n-1}{d} - 1) \rceil.$$

have maximal Randić energy. Therefore in a Kragujevac tree with maximal Randić energy the branches are either equal or almost equal.

Finally, by using the transformations of the type $T^{'} \to T$ as far as it is possible, we can obtain the Kragujevac trees with minimum Randić energy.

Theorem 2.8. *Within the Kragujevac trees with order n and degree d, trees such that all branches are isomorphic to B_2 and a single branch is isomorphic to B_k where*

$$k = \frac{1}{2}\lfloor n - 2 - 5(d-1) \rfloor,$$

have minimal Randić energy.

3 Bounds of Randić energy of the Kragujevac trees

In this section, we obtain an upper bound and a lower bound for the Randić energy of a Kragujevac tree in terms of its order and degree.

Theorem 3.1. *Let $T = T(B_{k_1}, B_{k_2}, \ldots, B_{k_d})$ be a Kragujevac tree. The characteristic polynomial of T is computed as*

$$x^{d-1}(x^2-\frac{1}{2})^{\sum_{i=1}^{d}(k_i-1)}\Big(x^2\prod_{i=1}^{d}(x^2-\frac{2k_i+1}{2k_i+2})-\sum_{i=1}^{d}\frac{x^2-\frac{1}{2}}{d(k_i+1)}\prod_{j\neq i=1}^{d}(x^2-\frac{2k_j+1}{2k_j+2})\Big).$$

Proof. Let the central vertex of T be labeled 1 and let the vertices of B_{k_1}, B_{k_2}, ..., B_{k_d} have consecutive labels. If R_1, R_2, ..., R_d denote the Randić matrix of β_{k_1}, β_{k_2}, ..., β_{k_d} respectively, $O_{m,n}$ denotes the $m \times n$ zero matrix and

$$C=\left[\frac{1}{\sqrt{d(k_1+1)}},\underbrace{0,\ldots,0}_{2k_1},[\frac{1}{\sqrt{d(k_2+1)}},\underbrace{0,\ldots,0}_{2k_2},\ldots,\frac{1}{\sqrt{d(k_d+1)}},\underbrace{0,\ldots,0}_{2k_d}\right],$$

then the Randić matrix of T is given as:

$$R_T(x) = \begin{bmatrix} 0 & C & C & C & \cdots & C \\ C^T & R_1 & O_{2k_1+1,2k_2+1} & O_{2k_1+1,2k_3+1} & \cdots & O_{2k_1+1,2k_d+1} \\ C^T & O_{2k_2+1,2k_1+1} & R_2 & O_{2k_2+1,2k_3+1} & \cdots & O_{2k_2+1,2k_d+1} \\ C^T & O_{2k_3+1,2k_1+1} & O_{2k_3+1,2k_2+1} & R_3 & \cdots & O_{2k_3+1,2k_d+1} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ C^T & O_{2k_d+1,2k_1+1} & O_{2k_d+1,2k_2+1} & O_{2k_d+1,2k_3+1} & \cdots & R_d \end{bmatrix}.$$

If $\bar{R}_{k_i}$ denotes determinant of the square matrix obtained by deleting the first column and the first row of $det(xI - R(\beta_{k_i}))$ for $1 \le i \le d$, then using Theorem 1.1, we have

$$\phi_T(x) = \begin{vmatrix} x & \frac{1}{\sqrt{d(k_1+1)}} & \frac{1}{\sqrt{d(k_2+1)}} & \cdots & \frac{1}{\sqrt{d(k_d+1)}} & \\ \frac{\bar{R}_{k_1}}{\sqrt{d(k_1+1)}} & R_{\beta_{k_1}}(x) & 0 & 0 & \cdots & 0 \\ \frac{\bar{R}_{k_2}}{\sqrt{d(k_2+1)}} & 0 & R_{\beta_{k_2}}(x) & 0 & \cdots & 0 \\ \frac{\bar{R}_{k_3}}{\sqrt{d(k_3+1)}} & 0 & 0 & R_{\beta_{k_3}}(x) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\bar{R}_{k_d}}{\sqrt{d(k_d+1)}} & 0 & 0 & 0 & \cdots & R_{\beta_{k_d}}(x) \end{vmatrix}$$

$$= \prod_{i=1}^{d}\frac{\bar{R}_{B_{k_i}}(x)}{d(k_i+1)} \begin{vmatrix} x & 1 & 1 & \cdots & 1 \\ 1 & \frac{d(k_1+1)R_{\beta_{k_1}}(x)}{\bar{R}_{k_1}} & 0 & \cdots & 0 \\ 1 & 0 & \frac{d(k_2+1)R_{B\beta_{k_2}}(x)}{\bar{R}_{k_2}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & \frac{d(k_d+1)R_{\beta_{k_d}}(x)}{\bar{R}_{k_d}} \end{vmatrix}.$$

Therefore, by using Lemma 2.1, we get

$$\begin{aligned}\phi_T(x) &= \prod_{i=1}^{d}\frac{\bar{R}_{k_i}}{d(k_i+1)}\Bigg(x\prod_{i=1}^{d}\frac{d(k_i+1)R_{B_{k_i}}(x)}{\bar{R}_{k_i}} - \sum_{i=1}^{d}\prod_{j\neq i=1}^{d}\frac{d(k_j+1)R_{B_{k_j}}(x)}{\bar{R}_{k_j}}\Bigg)\\ &= x\prod_{i=1}^{d}R_{B_{k_i}}(x) - \sum_{i=1}^{d}\frac{\bar{R}_{k_i}}{d(k_i+1)}\prod_{j\neq i=1}^{d}R_{B_{k_j}}(x). \end{aligned} \quad (3)$$

Since $\bar{R}_{k_i} = (x^2-\frac{1}{2})^{k_i}$, for $1 \le i \le d$, by using Lemma 2.3, we have

$$x^{d-1}(x^2-\frac{1}{2})^{\sum_{i=1}^{d}(k_i-1)}\Bigg(x^2\prod_{i=1}^{d}(x^2-\frac{2k_i+1}{2k_i+2}) - \sum_{i=1}^{d}\frac{x^2-\frac{1}{2}}{d(k_i+1)}\prod_{j\neq i=1}^{d}(x^2-\frac{2k_j+1}{2k_j+2})\Bigg).$$

■

Corollary 3.2. *The characteristic polynomial of* $T = T(B_k, \underbrace{B_2, B_2, \ldots, B_2}_{d-1})$ *is computed as*

$$\begin{aligned}\phi_T(x) &= x^{d-1}(x^2-\frac{1}{2})^{k+d-2}(x^2-\frac{5}{6})^{d-2}(x^2-1)\\ &\quad (12d(k+1)x^4-(14kd+8d-4k+8)x^2+2kd+d-2k+4).\end{aligned}$$

Proof. Let $k_1 = k$ and $k_i = 2$ for $2 \le i \le d$. By using (3), we get

$$\begin{aligned}R_T(x) &= x(R_{\beta_2}(x))^{d-1}R_{\beta_k}(x) - \frac{d-1}{3d}\bar{R}_{k_2}(R_{\beta_k}(x))^{d-2}R_{\beta_k}(x) -\\ &\quad \frac{1}{d(k+1)}\bar{R}_{k_1}(R_{\beta_2}(x))^{d-1}\\ &= x^{d-1}(x^2-\frac{1}{2})^{k+d-2}(x^2-\frac{5}{6})^{d-2}\Bigg(x^2(x^2-\frac{2k+1}{2k+2})(x^2-\frac{5}{6})\\ &\quad -\frac{d-1}{3d}\left(x^2-\frac{1}{2}\right)\left(x^2-\frac{2k+1}{2k+2}\right)-\frac{1}{d(k+1)}(x^2-\frac{1}{2})(x^2-\frac{5}{6})\Bigg)\\ &= x^{d-1}(x^2-\frac{1}{2})^{k+d-2}(x^2-\frac{5}{6})^{d-2}(x^2-1)\\ &\quad (12d(k+1)x^4-(14kd+8d-4k+8)x^2+2kd+d-2k+4).\end{aligned}$$

■

Corollary 3.3. *The characteristic polynomial of* $T = T(\underbrace{B_{k-1}, B_{k-1}, \ldots, B_{k-1}}_{d_1}, \underbrace{B_k, B_k, \ldots, B_k}_{d-d_1})$ *is computed as:*

$$\begin{aligned}R_T(x) &= x^{d-1}(x^2-\frac{1}{2})^{(k-1)d-d_1}(x^2-\frac{2k-1}{2k})^{d_1-1}(x^2-\frac{2k+1}{2k+2})^{d-d_1-1}(x^2-1)\\ &\Bigg(4kd(k+1)x^4-(4kd(k+1)+2(2d_1-d))x^2+2kd+2d_1-d\Bigg)x^2+2d_1-d).\end{aligned}$$

Proof. Let $k_i = k-1$ for $1 \le i \le d_1$ and $k_i = k$ for $2d_1+1 \le i \le d$. By using Theorem 3.1, we get

$$\begin{aligned}
R_T(x) &= [R_{\beta_{k-1}}(x)]^{d_1-1}[R_{\beta_k}(x)]^{d-d_1-1}\Big(xR_{\beta_{k-1}}(x)R_{\beta_k}(x) - \frac{d_1}{dk}\bar{R}_{k_1}R_{\beta_k}(x) \\
&\quad -\frac{d-d_1}{d(k+1)}R_{\bar{\beta}_{k-1}}(x)\bar{R}_{k_d}\Big) \\
&= x^{d-1}(x^2-\frac{1}{2})^{(k-1)d-d_1}(x^2-\frac{2k-1}{2k})^{d_1-1}(x^2-\frac{2k+1}{2k+2})^{d-d_1-1} \\
&\quad \Big(x^2(x^2-\frac{2k1}{2k})(x^2-\frac{2k+1}{2k+2}) \\
&\quad -\frac{d_1}{d(k+1)}(x^2-\frac{1}{2})(x^2-\frac{2k+3}{2k+4}) - \frac{d-d_1}{d(k+2)}x(x^2-\frac{1}{2})(x^2-\frac{2k+1}{2k+2})\Big) \\
&= x^{d-1}(x^2-\frac{1}{2})^{(k-1)d-d_1}(x^2-\frac{2k-1}{2k})^{d_1-1}(x^2-\frac{2k+1}{2k+2})^{d-d_1-1}(x^2-1) \\
&\quad \Big(4kd(k+1)x^4-(4kd(k+1)+2(2d_1-d))x^2+2kd+2d_1-d\Big).
\end{aligned}$$

■

Theorem 3.4. *A lower bound for Randić energy of Kragujevac trees of order n and degree d is given as:*

$$2+\sqrt{2}(d+k-2)+\frac{2\sqrt{5}(d-2)}{\sqrt{6}}+\frac{\sqrt{7kd+4(d+1)-2k\pm\sqrt{(5k+2)^2d^2-4(k-2)^2(d-1)}}}{\sqrt{3d(k+1)}}.$$

Proof. Let $T = T(B_k, \underbrace{B_2, B_2, \ldots, B_2}_{d-1})$ be a Kragujevac tree of order n and degree d where $n = 5(d-1)+2k+2$. By using Corollary 3.2, the spectrum of $R(T)$ contains 0 with multiplicity $d-1$, $\frac{1}{\sqrt{2}}$ with multiplicity $k+d-2$, $\frac{5}{6}$ with multiplicity $d-2$, ± 1 and

$$\frac{\pm\sqrt{7kd+4(d+1)-2k\pm\sqrt{(5k+2)^2d^2-4(k-2)^2(d-1)}}}{\sqrt{12d(k+1)}}.$$

Thus the Randič energy of T is computed as

$$\begin{aligned}
RE(T) &= \sum_{i=1}^{n}|x_i| \\
&= 2+\frac{2(k+d-2)}{\sqrt{2}}+\frac{2\sqrt{5}(d-2)}{\sqrt{6}} \\
&\quad +\frac{2\sqrt{7kd+4(d+1)-2k\pm\sqrt{(5k+2)^2d^2-4(k-2)^2(d-1)}}}{\sqrt{12d(k+1)}}.
\end{aligned}$$

The result can be obtained by using Theorem 2.8. ■

Let T be a Kragujevac tree with maximum Randić energy of order n and degree d. By Theorem 2.7, if $k = \lceil \frac{1}{2}(\frac{n-1}{d}-1)\rceil$, then $T = T(\underbrace{B_{k-1}, B_{k-1}, \ldots, B_{k-1}}_{d_1}, \underbrace{B_k, B_k, \ldots, B_k}_{d-d_1})$ for

$d_1 = \frac{kd-n+1}{2}$. By Corollary 3.3, an upper bound for the Randić energy of the Kragujevac trees is given as follows:

Theorem 3.5. *Let T be a Kragujevac tree of order n and degree d, then*

$$RE(T) \leq 2 + \sqrt{2}((k-1)d - d_1) + 2(d_1 - 1)\sqrt{\frac{2k-1}{2k}} + 2(d - d_1 - 1)\sqrt{\frac{2k+1}{2k+2}}$$
$$+\sqrt{\frac{2dk(k+1) + 2d_1 - d \pm \sqrt{4k^2d^2(k^2-1) + (2d_1 - d)^2}}{dk(k+1)}}.$$

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