

# On the Randić Energy of Caterpillar Graphs

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## Abstract

A caterpillar graph  $T(p_1, \dots, p_r)$  of order  $n = r + \sum_{i=1}^r p_i$ ,  $r \geq 2$ , is a tree such that removing all its pendent vertices gives rise to a path of order  $r$ . In this paper we establish a necessary and sufficient condition for a real number to be an eigenvalue of the Randić matrix of  $T(p_1, \dots, p_r)$ . This result is applied to determine the extremal caterpillars for the Randić energy of  $T(p_1, \dots, p_r)$  for cases  $r = 2$  (the double star) and  $r = 3$ . We characterize the extremal caterpillars for  $r = 2$ . Moreover, we study the family of caterpillars  $T(p, n - p - q - 3, q)$  of order  $n$ , where  $q$  is a function of  $p$ , and we characterize the extremal caterpillars for three cases:  $q = p$ ,  $q = n - p - b - 3$  and  $q = b$ , for  $b \in \{1, \dots, n - 6\}$  fixed. Some illustrative examples are included.

## 1 Introduction

It is worth to start this section defining the Randić matrix of a graph  $G$ , denoted by  $R_G = (r_{ij})$ , which is such that  $r_{ij} = \frac{1}{\sqrt{d_i d_j}}$  if  $ij \in E(G)$  and zero otherwise, where  $d_k$  is the degree of the vertex  $k$ . The spectrum of  $R_G$  is the multiset of its eigenvalues,  $\sigma_R(G) = \{\rho_1^{[m_1]}, \rho_2^{[m_2]}, \dots, \rho_s^{[m_s]}\}$ , where  $m_i$  stands for the multiplicity of  $\rho_i$ , for  $1 \leq i \leq s$ , and  $\rho_1 > \rho_2 > \dots > \rho_s$  are the distinct eigenvalues of  $R_G$ .

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It is well known that  $\rho_1(G) = 1$  whenever  $G$  is a graph with at least one edge (see [7, Th. 2.3]).

The *Randić energy* of a graph  $G$  is defined in [7] (see also [2,3]) as follows:

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

It is immediate that  $RE(G) = 0$  if and only if all the vertices of  $G$  are isolated vertices. Considering  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  as the eigenvalues of the adjacency matrix of a graph  $G$  of order  $n$ , the ordinary energy of  $G$  [8, 11], herein denoted by  $\mathcal{E}(G)$ , is defined as

$$\mathcal{E}(G) = \sum_{j=1}^n |\lambda_j|.$$

In [7], the Randić energy and the ordinary energy of the paths  $P_n$  and  $P_{n-2}$ , respectively, are related as follows.

$$RE(P_n) = 2 + \frac{1}{2}\mathcal{E}(P_{n-2}).$$

According to [5], if a graph  $G$  of order  $n$  has at least one edge, then

$$2 \leq RE(G) \leq n. \tag{1}$$

Furthermore, the lower bound in (1) is attained if and only if one component of  $G$  is a complete multipartite graph and all other components (if any) are isolated vertices. In particular,  $RE(G) = 2$  for complete graphs. The upper bound in (1) is attained only if  $n$  is even and  $G$  is isomorphic to  $\frac{n}{2}K_2$ , or  $n$  is odd and  $G$  is the disjoint union of  $\frac{n-3}{2}K_2$  plus a component which is a path  $P_2$  or a triangle  $K_3$ .

The characterization of connected graphs with maximal Randić energy remains an open problem as well as the following conjecture posed in [7] and computationally verified for graphs of order  $n$  up to  $n = 10$ .

**Conjecture 1** [7] *The connected graph with maximal Randić energy is a tree.*

The following more thinner conjecture, also posed in [7], remains open too.

**Conjecture 2** [7] *The connected graph of odd order  $n \geq 1$ , having maximal Randić energy is the sun [7, Fig. 2]. The connected graph of even order  $n \geq 2$ , having maximal Randić energy is the balanced double sun [7, Fig. 2].*

The aim of this paper is to determine the extremal graphs for the Randić energy of a family of caterpillars  $T(p_1, \dots, p_r)$  of order  $n = r + \sum_{i=1}^r p_i$  for cases  $r = 2$  and  $r = 3$ . The

paper is organized as follows. In Section 2 the notation and basic definitions of the main concepts used through the text are introduced. In Section 3 a caterpillar is considered as the H-join of graphs and some spectral results of graphs obtained by this operation are recalled. Moreover, we get a necessary and sufficient condition for a real number to be an eigenvalue of the Randić matrix. This result plays an important role throughout the paper. In Section 4 we characterize the extremal caterpillar graphs for  $r = 2$  (that are the double star) as well as we study the family of caterpillars  $T(p, n - p - q - 3, q)$  of order  $n$ , and we characterize extremal caterpillar graphs for three cases:  $q = p$ ,  $q = n - p - b - 3$  and  $q = b$ , for any  $b \in \{1, \dots, n - 6\}$  fixed.

## 2 Preliminaries

In this paper we deal with undirected simple graphs. For a graph  $G$  the vertex set is denoted by  $V(G)$  and the edge set by  $E(G)$  and  $|V(G)|$  is the order of  $G$ . The edges of  $G$  denoted by  $ij$ , where  $i$  and  $j$  are the end-vertices of the edge. When  $ij \in E(G)$  we say that the vertices  $i$  and  $j$  are adjacent and also that  $i$  is a neighbor of  $j$  (and conversely). The neighborhood of a vertex  $v \in V(G)$  is the set of its neighbors and is denoted by  $N_G(v) = \{w : vw \in E(G)\}$ . The degree of  $v$ , denoted by  $d_v$ , is the cardinality of  $N_G(v)$ . The vertices  $i$  with 0 degree are called isolated vertices. Two graphs  $G$  and  $H$  are isomorphic if there is a bijection  $\psi : V(G) \rightarrow V(H)$  such that  $ij \in E(G)$  if and only if  $\psi(i)\psi(j) \in E(H)$ . This binary relation between graphs is denoted by  $G \cong H$ . The complement graph of a graph  $G$ , denoted by  $\overline{G}$ , is such that  $V(\overline{G}) = V(G)$  and  $E(\overline{G}) = \{ij : ij \notin E(G)\}$ . The complete graph of order  $n$ , denote by  $K_n$ , is a graph where every pair of vertices are adjacent. The vertices of the complement of  $K_n$  are all isolated. The adjacency matrix of a graph  $G$  of order  $n = |V(G)|$  is  $n \times n$  symmetric matrix  $A_G = (a_{ij})$  such that  $a_{ij} = 1$  if  $ij \in E(G)$  and zero otherwise. The spectrum of a matrix  $M$  is the multiset of its eigenvalues denoted by  $\sigma_M$ . In particular, the spectrum of the adjacency matrix of a graph  $G$ , also called the spectrum of  $G$ , is  $\sigma(G) = \{\lambda_1^{[m_1]}, \lambda_2^{[m_2]}, \dots, \lambda_s^{[m_s]}\}$ , where  $m_i$  stands for the multiplicity of  $\lambda_i$ , for  $1 \leq i \leq s$ .

A path with  $r$  vertices, denoted by  $P_r$ , is a sequence of vertices  $v_1, v_2, \dots, v_r$  such that each vertex is adjacent to the next, that is  $v_i v_{i+1} \in E(G)$  for  $i = 1, \dots, r - 1$ . A cycle  $C_r$  is a closed path with  $r$  edges, that is, such that  $v_{r+1} = v_1$ . A tree is a connected acyclic graph; a star of order  $r$ , denoted by  $S_{r+1}$ , is a tree with a central vertex with degree  $r$  and all the other  $r$  vertices are pendent. A caterpillar is a tree such that removing all pendent

vertices give rise to a path with at least two vertices. In particular,  $T(p_1, \dots, p_r)$  denotes a caterpillar obtained by attaching the central vertex of a star  $S_{p_i+1}$  to the  $i$ -th vertex of  $P_r$ ,  $i = 1, \dots, r$ . The order of a caterpillar is  $n = r + \sum_{i=1}^r p_i$ .

A caterpillar  $T(p_1, \dots, p_r)$  can also be seen as the H-join  $H[G_1, \dots, G_r, G_{r+1}, \dots, G_{2r}]$ , where, for  $1 \leq i \leq r$ ,  $\begin{cases} G_i \cong K_1 \\ G_{i+r} \cong K_{p_i} \end{cases}$  and  $H$  is the caterpillar of order  $2r$ ,  $T(1, \dots, 1)$ , that is, a path  $P_r$  with one pendant vertex attached to each vertex of the path.

The null square and the identity matrices of order  $n$  are denoted by  $O_n$  and  $I_n$ , respectively.

### 3 The Randić spectrum of a caterpillar viewed as H-join

In this section, we consider a caterpillar as the H-join of a family of graphs (see [4]),  $T(p_1, \dots, p_r) = H[K_1, \dots, K_1, \overline{K_{p_1}}, \dots, \overline{K_{p_r}}]$ , where  $H$  is the caterpillar of order  $2r$ ,  $T(1, 1, \dots, 1)$ , that is, a path  $P_r$  with a pendant edge attached to each vertex of the path. The following result, given in [1], characterizes Randić spectra of H-join graphs.

**Theorem 3.1** [1] *Let  $H$  be a graph of order  $k$ . Let  $G_j$  be a  $d_j$ -regular graph of order  $n_j$ , with  $d_j \geq 0$ ,  $n_j \geq 1$ , for  $j = 1, \dots, k$  and  $G = H[G_1, \dots, G_k]$ . Let  $R_G$  be the Randić matrix of  $G$ . Then,*

$$\sigma_{R_G} = \sigma_{\Gamma_k} \cup \bigcup_{j=1}^k \left\{ \frac{\lambda}{N_j + d_j} : \lambda \in \sigma(A_{G_j}) \setminus \{d_j\} \right\},$$

where  $N_j = \sum_{i \in N_H(j)} n_i$ , for  $j = 1, 2, \dots, k$ ,

$$\Gamma_k = \begin{pmatrix} \frac{d_1}{N_1+d_1} & \rho_{12} & \dots & \rho_{1(k-1)} & \rho_{1k} \\ \rho_{12} & \frac{d_2}{N_2+d_2} & \dots & \rho_{2(k-1)} & \rho_{2k} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{1(k-1)} & \rho_{2(k-1)} & \dots & \frac{d_{k-1}}{N_{k-1}+d_{k-1}} & \rho_{(k-1)k} \\ \rho_{1k} & \rho_{2k} & \dots & \rho_{(k-1)k} & \frac{d_k}{N_k+d_k} \end{pmatrix}$$

and

$$\rho_{ij} = \delta_{ij} \frac{\sqrt{n_i n_j}}{\sqrt{(N_i + d_i)(N_j + d_j)}},$$

with  $\delta_{ij} = 1$  if  $ij \in E(H)$ , and zero otherwise, for  $i = 1, \dots, k-1$  and  $j = i+1, \dots, k$ .

**Remark 1** It is clear that the Randić matrix of a  $d_j$ -regular graph  $G_j$  is  $R_{G_j} = \frac{1}{d_j} A_{G_j}$  if  $d_j > 0$  and zero otherwise. On the other hand, if  $d_j = 0$ , for  $j = 1, \dots, k$ , then  $\Gamma_k = \Omega A_H \Omega$ , with  $\Omega = \text{diag} \left\{ \sqrt{\frac{n_1}{N_1}}, \dots, \sqrt{\frac{n_k}{N_k}} \right\}$ .

Since  $K_1$  and  $\overline{K_{p_i}}$ , for  $i = 1, \dots, r$ , are 0-regular graphs, we have the following result, which plays an important role in this paper:

**Corollary 3.1** *Let  $H = T(1, 1, \dots, 1)$  be the caterpillar of order  $2r$ ,  $r \geq 2$ , obtained from a path  $P_r$  and a pendent vertex attached to each vertex of the path. Let  $T = T(p_1, \dots, p_r) = H[K_1, \dots, K_1, \overline{K_{p_1}}, \dots, \overline{K_{p_r}}]$  be a caterpillar of order  $n = r + \sum_{i=1}^r p_i$ . Then,*

$$\sigma_{R_T} = \sigma_{\Gamma_{2r}} \cup \left\{ 0^{[\sum_{i=1}^r (p_i - 1)]} \right\}.$$

As a consequence, in order to obtain the spectrum of the Randić matrix of  $T(p_1, \dots, p_r)$  we focus our attention on the spectrum of  $\Gamma_{2r}$ . Firstly, note that

$$\Omega = \text{diag} \left\{ \sqrt{\frac{1}{N_1}}, \dots, \sqrt{\frac{1}{N_r}}, \sqrt{\frac{p_1}{N_{r+1}}}, \dots, \sqrt{\frac{p_r}{N_{2r}}} \right\} = \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix}$$

with

$$\Omega_1 = \text{diag} \left\{ \sqrt{\frac{1}{N_1}}, \dots, \sqrt{\frac{1}{N_r}} \right\}, \quad \Omega_2 = \text{diag} \left\{ \sqrt{\frac{p_1}{N_{r+1}}}, \dots, \sqrt{\frac{p_r}{N_{2r}}} \right\}, \quad (2)$$

Therefore, we can write

$$\Gamma_{2r} = \Omega A_H \Omega = \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix} \begin{bmatrix} A_{P_r} & I_r \\ I_r & O_r \end{bmatrix} \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix} = \begin{bmatrix} A & B \\ B & O_r \end{bmatrix}, \quad (3)$$

where

$$A = \Omega_1 A_{P_r} \Omega_1 \quad \text{and} \quad B = \Omega_1 \Omega_2. \quad (4)$$

It is worth to recall a famous determinantal identity presented by Issa Schur in 1917 [12] referred as the formula of Schur by Gantmacher [6, p. 46]. In the sixties, the term Schur complement was introduced by Emilie Haynsworth [9] jointly with the following notation. Considering a square matrix  $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ , where  $A$  and  $D$  are square block matrices and  $A$  is nonsingular, the Schur complement of  $A$  in  $M$  is defined as

$$M/A = D - CA^{-1}B.$$

For more details see [10]. Using the above notation, the next theorem states the Schur determinantal identity. For the readers convenience, the very short proof presented in [10] is reproduced.

**Theorem 3.2** [12] *Let  $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ , where  $A$  and  $D$  are square submatrices of order  $m$  and  $n$ , respectively. If  $A$  is nonsingular then*

$$\det(M) = \det(A) \cdot \det(M/A).$$

**Proof** It is immediate that

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I_m & 0 \\ CA^{-1} & I_n \end{bmatrix} \begin{bmatrix} A & B \\ 0 & D - CA^{-1}B \end{bmatrix}.$$

The identity follows by taking the determinant of both sides. ■

Similarly, if  $D$  is nonsingular then

$$\det(M) = \det(A - BD^{-1}C) \cdot \det(D). \quad (5)$$

Note that  $\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I_m & BD^{-1} \\ 0 & I_n \end{bmatrix} \begin{bmatrix} A - BD^{-1}C & 0 \\ C & D \end{bmatrix}$ .

From (5), we may establish the following spectral characterization for the matrix  $\Gamma_{2r}$ , which will play an important role in getting our main results:

**Theorem 3.3** *Let  $H = T(1, 1, \dots, 1)$  be the caterpillar of order  $2r$ ,  $r \geq 2$  and let  $\Gamma_{2r}$  be partitioned as in (3). Then,  $\lambda \in \sigma_{\Gamma_{2r}}$  if and only if*

$$\det(\lambda^2 I_r - \lambda A - B^2) = 0,$$

where  $A$  and  $B$  are defined as in (4).

**Proof** The characteristic polynomial of  $\Gamma_{2r}$  is

$$p_{\Gamma_{2r}}(\lambda) = \det(\lambda I_{2r} - \Gamma_{2r}) = \det \left( \begin{bmatrix} \lambda I_r - A & -B \\ -B & \lambda I_r \end{bmatrix} \right).$$

Thus, applying (5), we obtain

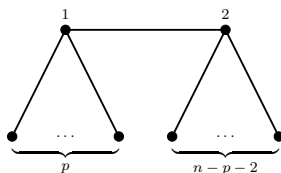
$$\begin{aligned} p_{\Gamma_{2r}}(\lambda) &= \det(\lambda I_r) \cdot \det \left( \lambda I_r - A - B \left( \frac{1}{\lambda} I_r \right) B \right) \\ &= \lambda^r \cdot \det \left( \left( \frac{1}{\lambda} \right) (\lambda^2 I_r - \lambda A - B^2) \right) \\ &= \lambda^r \cdot \left( \frac{1}{\lambda} \right)^r \cdot \det(\lambda^2 I_r - \lambda A - B^2) = \det(\lambda^2 I_r - \lambda A - B^2). \end{aligned}$$

■

## 4 Extremal caterpillar graphs for Randić energy

In this section, we obtain the extremal graphs in the family of caterpillars, for  $r = 2, 3$ .

#### 4.1 Extremal caterpillar graphs $\mathbf{T}(p, n - p - 2)$ , $p = 1, \dots, \lfloor \frac{n-2}{2} \rfloor$ .



**Theorem 4.1** Let  $T_p = T(p, n - p - 2)$ ,  $p = 1, \dots, \lfloor \frac{n-2}{2} \rfloor$  be a caterpillar of order  $n \geq 4$ . Then

$$2 + \sqrt{\frac{2(n-3)}{n-2}} \leq RE(T_p) \leq 4 - \frac{4}{n}.$$

The lower bound is attained if and only if  $p = 1$  (the graph obtained by attaching a pendent vertex to a pendent vertex of  $S_{n-1}$ ) and the upper bound is attained if and only if  $T_p$  has even order and  $p = \frac{n-2}{2}$ .

**Proof** By Theorem 3.3, the eigenvalues of  $\sigma_{\Gamma_4}$  are the zeros of the polynomial  $\det(\lambda^2 I_2 - \lambda A - B^2) = 0$  where (see (4)),

$$A = \begin{bmatrix} 0 & \frac{1}{\sqrt{(p+1)(n-p-1)}} \\ \frac{1}{\sqrt{(p+1)(n-p-1)}} & 0 \end{bmatrix} \text{ and } B = \begin{bmatrix} \frac{\sqrt{p}}{\sqrt{p+1}} & 0 \\ 0 & \frac{\sqrt{n-p-2}}{\sqrt{n-p-1}} \end{bmatrix}.$$

So,

$$\begin{aligned} \det(\lambda^2 I_2 - \lambda A - B^2) &= \det \begin{bmatrix} \lambda^2 - \frac{p}{p+1} & -\frac{\lambda}{\sqrt{(p+1)(n-p-1)}} \\ -\frac{\lambda}{\sqrt{(p+1)(n-p-1)}} & \lambda^2 - \frac{n-p-2}{n-p-1} \end{bmatrix} \\ &= \left( \lambda^2 - \frac{p}{p+1} \right) \left( \lambda^2 - \frac{n-p-2}{n-p-1} \right) - \frac{\lambda^2}{(p+1)(n-p-1)} \\ &= \frac{\lambda^2 - 1}{(p+1)(n-p-1)} \left( (p+1)(n-p-1)\lambda^2 - p(n-p-2) \right). \end{aligned}$$

Consequently,

$$\sigma_{\Gamma_4} = \left\{ \pm \sqrt{\frac{p(n-p-2)}{(p+1)(n-p-1)}}, \pm 1 \right\}.$$

and

$$RE(T_p) = \sum_{i=1}^n |\lambda_i(T_p)| = 2 + 2\sqrt{\frac{p(n-p-2)}{(p+1)(n-p-1)}},$$

for all  $p = 1, \dots, \lfloor \frac{n-2}{2} \rfloor$ . For  $1 \leq x \leq \lfloor \frac{n-2}{2} \rfloor$ , let  $f(x) = \frac{x(n-x-2)}{(x+1)(n-x-1)}$ . Then,

$$f'(x) = \frac{(n-1)(n-2(x+1))}{(x+1)^2(n-x-1)^2} \geq 0.$$

if and only if  $1 \leq x \leq \frac{n-2}{2}$ . Therefore,  $f$  is an increasing function in this interval, and consequently,

$$2 + \sqrt{\frac{2(n-3)}{n-2}} \leq RE(T_p) \leq RE(T_{\lfloor \frac{n-2}{2} \rfloor}),$$

for all  $p = 1, \dots, \lfloor \frac{n-2}{2} \rfloor$ . Finally, if  $n$  is even,

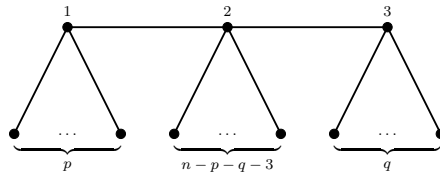
$$RE(T_{\lfloor \frac{n-2}{2} \rfloor}) = RE(T_{\frac{n-2}{2}}) = 2 + 2 \left( \frac{n-2}{n} \right) = 4 - \frac{4}{n},$$

and if  $n$  is odd,

$$RE(T_{\lfloor \frac{n-2}{2} \rfloor}) = RE(T_{\lfloor \frac{n-3}{2} + \frac{1}{2} \rfloor}) = RE(T_{\frac{n-3}{2}}) = 2 + 2 \left( \sqrt{\frac{n-3}{n+2}} \right) < 4 - \frac{4}{n}$$

for all  $n \geq 3$ . ■

### 4.2 Extremal caterpillar graphs $\Gamma(p, n - p - q - 3, q)$ , $p, q \in \{1, \dots, n - 5\}$



For this class of caterpillars,

$$\Omega_1 = \text{diag} \left\{ \frac{1}{\sqrt{p+1}}, \frac{1}{\sqrt{n-p-q-1}}, \frac{1}{\sqrt{q+1}} \right\}$$

and

$$\Omega_2 = \text{diag} \left\{ \sqrt{p}, \sqrt{n-p-q-3}, \sqrt{q} \right\}.$$

Therefore (see (2), (3) and (4))

$$\Gamma_6 = \Omega A_H \Omega = \begin{bmatrix} A & B \\ B & O_3 \end{bmatrix},$$

with

$$A = \Omega_1 A_{P_3} \Omega_1 = \begin{bmatrix} 0 & \frac{1}{\sqrt{p+1}\sqrt{n-p-q-1}} & 0 \\ \frac{1}{\sqrt{p+1}\sqrt{n-p-q-1}} & 0 & \frac{1}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ 0 & \frac{1}{\sqrt{q+1}\sqrt{n-p-q-1}} & 0 \end{bmatrix}$$

and

$$B = \Omega_1 \Omega_2 = \begin{bmatrix} \frac{\sqrt{p}}{\sqrt{p+1}} & 0 & 0 \\ 0 & \frac{\sqrt{n-p-q-3}}{\sqrt{n-p-q-1}} & 0 \\ 0 & 0 & \frac{\sqrt{q}}{\sqrt{q+1}} \end{bmatrix}.$$



By Theorem 3.3, as

$$\lambda^2 I_3 - \lambda A - B^2 = \begin{bmatrix} \lambda^2 - \frac{p}{p+1} & -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} & 0 \\ -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} & \lambda^2 - \frac{n-p-q-3}{n-p-q-1} & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ 0 & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} & \lambda^2 - \frac{q}{q+1} \end{bmatrix},$$

$$\begin{aligned} \det(\lambda^2 I_3 - \lambda A - B^2) &= \\ &= \left( \lambda^2 - \frac{p}{p+1} \right) \det \left( \begin{bmatrix} \lambda^2 - \frac{n-p-q-3}{n-p-q-1} & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} & \lambda^2 - \frac{q}{q+1} \end{bmatrix} \right) \\ &+ \left( \frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} \right) \det \left( \begin{bmatrix} -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ 0 & \lambda^2 - \frac{q}{q+1} \end{bmatrix} \right) \\ &= \left( \lambda^2 - \frac{p}{p+1} \right) \left[ \left( \lambda^2 - \frac{n-p-q-3}{n-p-q-1} \right) \left( \lambda^2 - \frac{q}{q+1} \right) - \frac{\lambda^2}{(q+1)(n-p-q-1)} \right] \\ &- \left( \frac{\lambda^2}{(p+1)(n-p-q-1)} \right) \left( \lambda^2 - \frac{q}{q+1} \right) \\ &= \frac{(\lambda^2(p+1) - p) [(\lambda^2(n-p-q-1) - (n-p-q-3)) (\lambda^2(q+1) - q) - \lambda^2] - \lambda^2 (\lambda^2(q+1) - q)}{(p+1)(q+1)(n-p-q-1)}. \end{aligned}$$

After some algebraic manipulation on the above expression, we get that

$$\begin{aligned} \det(\lambda^2 I_3 - \lambda A - B^2) &= \frac{1}{(p+1)(q+1)(n-p-q-1)} \left[ (p+1)(q+1)(n-p-q-1)\lambda^6 \right. \\ &- [(n-p-q-2)(q(2p+1)+p) + (p+1)(q+1)(n-p-q-1)]\lambda^4 \\ &+ [pq(n-p-q-3) + (n-p-q-2)(q(2p+1)+p)]\lambda^2 - pq(n-p-q-3) \left. \right] \\ &= \frac{(\lambda^2 - 1) \left[ (p+1)(q+1)(n-p-q-1)\lambda^4 - (n-p-q-2)(q(2p+1)+p)\lambda^2 + pq(n-p-q-3) \right]}{(p+1)(q+1)(n-p-q-1)} \\ &= \frac{1}{\eta(n,p,q)} (\lambda^2 - 1) \left[ \eta(n,p,q)\lambda^4 - \zeta(n,p,q)\lambda^2 + \chi(n,p,q) \right], \end{aligned}$$

being

$$\begin{cases} \eta(n,p,q) &= (p+1)(q+1)(n-p-q-1), \\ \zeta(n,p,q) &= (n-p-q-2)(q(2p+1)+p) \\ \chi(n,p,q) &= pq(n-p-q-3). \end{cases} \quad (6)$$

When obtaining the roots of the biquadratic equation

$$\eta(n, p, q)\lambda^4 - \zeta(n, p, q)\lambda^2 + \chi(n, p, q) = 0,$$

we determinate the roots of the equation  $\det(\lambda^2 I_3 - \lambda A - B^2) = 0$ , given by:

$$\lambda_{1,2} = \pm 1$$

$$\lambda_{3,4} = \pm \sqrt{\frac{\zeta(n, p, q) + \sqrt{\zeta^2(n, p, q) - 4\eta(n, p, q)\chi(n, p, q)}}{2\eta(n, p, q)}}$$

$$\lambda_{5,6} = \pm \sqrt{\frac{\zeta(n, p, q) - \sqrt{\zeta^2(n, p, q) - 4\eta(n, p, q)\chi(n, p, q)}}{2\eta(n, p, q)}}.$$

Using the notation

$$\begin{cases} \alpha(n, p, q) &= \frac{\zeta(n, p, q)}{2\eta(n, p, q)}, \\ \gamma(n, p, q) &= \frac{\chi(n, p, q)}{\eta(n, p, q)}, \\ \beta(n, p, q) &= \sqrt{\alpha^2(n, p, q) - \gamma(n, p, q)}, \end{cases} \quad (7)$$

we get, for a general caterpillar  $T_{p,q} = T(p, n - 3 - p - q, q)$ ,

$$RE(T_{p,q}) = 2 \left( 1 + \sqrt{\alpha(n, p, q) + \beta(n, p, q)} + \sqrt{\alpha(n, p, q) - \beta(n, p, q)} \right). \quad (8)$$

In order to obtain the extreme graphs for certain subfamilies of caterpillar of the form  $T(p, n - p - q - 3, q)$ , for  $n \geq 7$ , we consider  $q$  as a function of  $x$  such that  $1 \leq q(x) \leq n - 5$  for  $1 \leq x \leq n - 5$  and define

$$f(x) = \sqrt{\alpha(x) + \beta(x)} + \sqrt{\alpha(x) - \beta(x)}, \quad (9)$$

where  $\alpha(x) := \alpha(n, x, q(x))$  and  $\beta(x) = \sqrt{\alpha^2(x) - \gamma(x)} := \beta(n, x, q(x))$  as in (7). Therefore,

$$\begin{aligned} f'(x) &= \frac{1}{2} \left( \frac{\alpha'(x) + \beta'(x)}{\sqrt{\alpha(x) + \beta(x)}} + \frac{\alpha'(x) - \beta'(x)}{\sqrt{\alpha(x) - \beta(x)}} \right) \\ &= \frac{1}{2} \left( \frac{f(x)\alpha'(x) + (\sqrt{\alpha(x) - \beta(x)} - \sqrt{\alpha(x) + \beta(x)})\beta'(x)}{\sqrt{\gamma(x)}} \right) \\ &= \frac{1}{2} \left( \frac{f^2(x)\alpha'(x) - 2\beta(x)\beta'(x)}{f(x)\sqrt{\gamma(x)}} \right) \\ &= \frac{\alpha'(x)(f^2(x) - 2\alpha(x)) + \gamma'(x)}{2f(x)\sqrt{\gamma(x)}} \\ &= \frac{2\alpha'(x)\sqrt{\gamma(x)} + \gamma'(x)}{2f(x)\sqrt{\gamma(x)}}, \end{aligned}$$

where,  $\gamma(x) := \gamma(n, x, q(x))$ . So,

$$f'(x) \geq 0 \quad \text{if and only if} \quad \lambda(x) := 2\alpha'(x)\sqrt{\gamma(x)} + \gamma'(x) \geq 0. \quad (10)$$

Taking into account (6) and (7), it is easy to see that  $0 \leq \gamma(x) < 1$ , for all  $1 \leq x \leq n-5$ . Thus,

i. If  $\alpha'(x) \geq 0$  and  $\gamma'(x) \leq 0$ , for  $x \in I \subset [1, n-5]$ , then by (10)

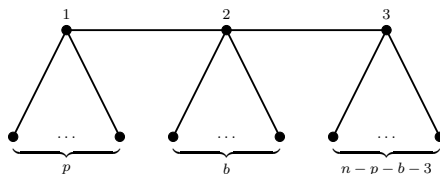
$$\gamma'(x) \leq \lambda(x) < 2\alpha'(x). \quad (11)$$

ii. If  $\alpha'(x) \leq 0$  and  $\gamma'(x) \geq 0$ , for  $x \in I \subset [1, n-5]$ , then by (10)

$$2\alpha'(x) < \lambda(x) \leq \gamma'(x). \quad (12)$$

Next we characterize the extremal caterpillars  $T(p, n-2p-3, q)$  for three specific cases:  $q = p$ ,  $q = n-p-b-3$  and  $q = b$ , for any  $b \in \{1, \dots, n-6\}$  fixed.

#### 4.2.1 Extremal graphs for the family of caterpillars $T(p, b, n-p-b-3)$



**Theorem 4.2** Let  $T_p = T(p, b, n-p-b-3)$  be a caterpillar of order  $n \geq 7$ , with  $b \in \{1, \dots, n-6\}$  fixed and  $p = 1, \dots, n-b-4$ . Then

$$RE(T_1) \leq RE(T_p) \leq RE\left(T_{\lfloor \frac{n-b-3}{2} \rfloor}\right).$$

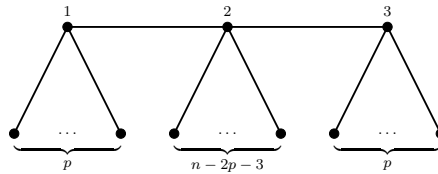
**Proof** Without loss of generality, we take  $1 \leq p \leq \lfloor \frac{n-b-3}{2} \rfloor$ , since for  $p = 1, \dots, n-b-4$ ,  $T_p$  and  $T_{n-p-b-3}$  are isomorphic graphs. Replacing  $q$  by  $n-p-b-3$  in (8), and considering the function  $f(x)$ , as in (9), for  $1 \leq x \leq \frac{n-b-3}{2}$ ,

$$\alpha'(x) = \frac{(b+1)(n-b-1)(n-2x-b-3)}{2(b+2)((x+1)(n-x-b-2))^2},$$

$$\gamma'(x) = \frac{b(n-b-2)(n-2x-b-3)}{(b+2)(x+1)^2(n-x-b-2)^2}.$$

we have both  $\alpha'(x) \geq 0$  and  $\gamma'(x) \geq 0$  if and only if  $1 \leq x \leq \frac{n-b-3}{2}$ . Thus, by (10),  $f$  increases in the interval  $[1, \frac{n-b-3}{2}]$  and the proof is complete. ■

4.2.2 Extremal graphs for the family of caterpillar  $T(p, n - 2p - 3, p)$



**Theorem 4.3** Let  $T_p = T(p, n - 2p - 3, p)$  be a caterpillar of order  $n \geq 7$ , with  $p = 1, \dots, \lfloor \frac{n-4}{2} \rfloor$ . Then

$$RE(T_1) \leq RE(T_p) \leq RE(T_z),$$

where  $z$  is an integer number in  $I = [\text{round}(r), \text{round}(s)]$ , with

$$r = \frac{1}{2} \left( 2n - 3 - \sqrt{2n(n-2) + 3} \right) \quad \text{and} \quad s = \frac{1}{2} \left( 2(n-1) - \sqrt{2n(n-1)} \right).$$

**Proof** From (8), replacing  $q$  by  $p$ , consider (see (9))  $f(x)$  for  $1 \leq x \leq \frac{n-4}{2}$ . The derivatives of  $\alpha$  and  $\gamma$  are

$$\alpha'(x) = \frac{2x^2 - (4n - 4)x + n^2 - 3n + 2}{(x + 1)^2(n - 2x - 1)^2}$$

and

$$\gamma'(x) = \frac{2x(2x^2 - (4n - 6)x + n^2 - 4n + 3)}{(x + 1)^3(n - 2x - 1)^2}$$

thus, we have  $\alpha'(x) \geq 0$  if only if  $2x^2 - (4n - 4)x + n^2 - 3n + 2 \geq 0$  which occurs for  $x \leq s_1$  or  $x \geq s_2$  with  $s_{1,2} = \frac{1}{2} \left( 2(n-1) \mp \sqrt{2n(n-1)} \right)$ .

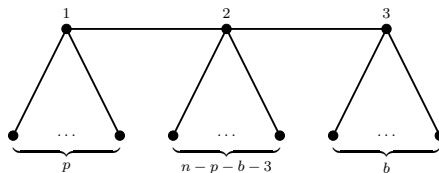
Similarly,  $\gamma'(x) \geq 0$  if only if  $x(2x^2 - (4n - 6)x + n^2 - 4n + 3) \geq 0$ , that is, for  $0 \leq x \leq r_1$  or  $x \geq r_2$  with  $r_{1,2} = \frac{1}{2} \left( 2n - 3 \mp \sqrt{2n(n-2) + 3} \right)$ .

We have  $1 < r_1 < s_1 < \frac{n-4}{2} < r_2, s_2$ . Therefore (see (10), (11) and (12)),  $f$  increases in the interval  $[1, r_1]$  and decreases in  $[s_1, \frac{n-4}{2}]$ . By Bolzano's Theorem, there exists  $\bar{z} \in (r_1, s_1)$  such that  $f'(\bar{z}) = 0$ . Since  $s_1 - r_1 < 0.5$ , we take  $z = \text{round}(\bar{z}) \in [\text{round}(r), \text{round}(s)]$ , where  $r = r_1$  and  $s = s_1$ . Finally,  $f(1) < f(\frac{n-4}{2})$ , so  $f(1)$  is the minimum of this function. ■

**Example 1** A table with some values for  $RE(T_{z-1})$ ,  $RE(T_z)$ ,  $RE(T_{z+1})$  and extremal caterpillars  $T(p, n - 3 - 2p, p)$  are presented below.

$n$	$r$	$s$	$z$	$RE(T_{z-1})$	$RE(T_z)$	$RE(T_{z+1})$	extremal graph
19	4.762261	4.923303	5	5.388854	5.406881	5.363498	$T(5, 6, 5)$
21	5.349028	5.508623	5	5.421848	5.458735	5.455208	$T(5, 8, 5)$
35	9.453171	9.607378	10	5.672191	5.672395	5.662869	$T(10, 12, 10)$
50	13.84816	14.000000	14	5.768798	5.770057	5.768229	$T(14, 19, 14)$

### 4.2.3 Extremal graphs of the family of caterpillars $\mathbf{T}(p, n - p - b - 3, b)$



**Theorem 4.4** Let  $T_p = T(p, n - p - b - 3, b)$  be a caterpillar of order  $n \geq 7$ , with  $b \in \{1, \dots, n - 6\}$  fixed and  $p = 1, \dots, n - b - 4$ . Then,

$$RE(T_{n-b-4}) \leq RE(T_p) \leq RE(T_z), \text{ where } z \in I = [\text{round}(r), \text{round}(s)],$$

with

$$r = -(n - b - 1) + \sqrt{2(n - b - 1)(n - b - 2)} \quad (13)$$

and

$$s = \frac{1}{b} \left( -((b + 1)(n - b) - 1) + \sqrt{(b + 1)(n - b - 1)((2b + 1)(n - 1) - 2b^2)} \right). \quad (14)$$

**Proof** Replacing  $q$  by  $b$  in (8), we define  $f(x)$  as in (9) for  $1 \leq x \leq n - b - 4$ . We compute

$$\alpha'(x) = \frac{-bx^2 - 2((b + 1)(n - b) - 1)x + (b + 1)n^2 - (b + 1)(2b + 3)n + b(b + 2)^2 + 2}{2(b + 1)((x + 1)(n - x - b - 1))^2},$$

$$\gamma'(x) = \frac{b(-x^2 - 2(n - b - 1)x + n^2 - 2(b + 2)n + (b + 3)(b + 1))}{(b + 1)((x + 1)(n - x - b - 1))^2}.$$

We have  $\alpha'(x) \geq 0$  if only if  $s_1 \leq x \leq s_2$  with

$$s_{1,2} = \frac{1}{b} \left( -((b + 1)(n - b) - 1) \mp \sqrt{(b + 1)(n - b - 1)((2b + 1)(n - 1) - 2b^2)} \right),$$

and  $\gamma'(x) \geq 0$  if only if  $r_1 \leq x \leq r_2$  with

$$r_{1,2} = -(n - b - 1) \mp \sqrt{2(n - b - 1)(n - b - 2)}.$$

We have  $1 < r_2 < s_2 < n - b - 4$ . So, for  $s = s_2$  and  $r = r_2$ , we get that (see (10), (11) and (12))  $f$  is increasing in  $[1, r]$  and decreasing in  $[s, n - b - 4]$ . Therefore, there exists  $\bar{z} \in (r, s)$  such that  $f'(\bar{z}) = 0$ . So, we take  $z = \text{round}(\bar{z}) \in I = [\text{round}(r), \text{round}(s)]$ . Furthermore,  $f(n - b - 4) < f(1)$ , which completes the proof.  $\blacksquare$

**Example 2** To obtain the maximal Randić energy caterpillar graphs  $T(p_1, p_2, p_3)$  of order  $n = 33$ , we apply Theorems 5, 6 and 7, for slight different values of  $b$ , shown in the following table.

Theorem	$b$	$r$	$s$	$z$	$RE(T_z)$	extremal graph
4.2	12			9	5.653986727	$T(9, 12, 9)$
4.2	9			10	5.639354482	$T(10, 9, 11)$
4.3	9	8.867059	9.021749	9	5.653986727	$T(9, 12, 9)$
4.4	9	8.811947	9.031236	9	5.653986727	$T(9, 12, 9)$
4.4	8	9.226495	9.469988	9	5.652375900	$T(9, 13, 8)$
4.4	10	8.397368	8.597041	9	5.651878107	$T(8, 12, 10)$

**Remark 2** In Theorem 4.4, we find an estimated interval

$$I = [\text{round}(r), \text{round}(s)],$$

where  $r$  and  $s$  are given in (13) and (14), respectively, which contains the value of  $z$  that maximizes Randić energy for the family of caterpillars  $T_p = T(p, n - p - b - 3, b)$ ,  $n \geq 7$ , with  $b \in \{1, \dots, n - 6\}$  fixed, for each  $p = 1, \dots, n - b - 4$ . In this case, we want to point out that the interval  $I$  does not necessarily have range less than 1. In fact, that interval has length less than 1 if and only if

$$g(n, b) = 8(n + b - 1)^2(n - b - 1)(n - b - 2) - (3n^2 - 3bn - 9n + 2b + 6)^2 > 0,$$

and this function  $g(n, b)$  can be written as:

$$g(n, b) = 8(n + b - 1)^2(n - b - 1)(n - b - 2) - \left(3(n - 1)(n - 2) - (3n - 2)b\right)^2.$$

Since  $n - b - 1 > n - b - 2 > 0$  then  $g(n, b) > h(n, b)$ , with

$$\begin{aligned} h(n, b) &= 8(n + b - 1)^2(n - b - 2)^2 - \left(3(n - 1)(n - 2) - (3n - 2)b\right)^2 \\ &= \left(\sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + (3n - 2)b\right) \\ &\quad \times \left(\sqrt{8}(n + b - 1)(n - b - 2) + 3(n - 1)(n - 2) - (3n - 2)b\right). \end{aligned}$$

For each  $n$ , we find the values of  $b$  such that

$$\Delta_1 = \sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + (3n - 2)b > 0, \text{ and,}$$

$$\Delta_2 = \sqrt{8}(n + b - 1)(n - b - 2) + 3(n - 1)(n - 2) - (3n - 2)b > 0.$$

Taking into account that  $3n - 2 > 3(n - 1) > 0$ , then

$$\begin{aligned} \Delta_1 &> \sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + 3(n - 1)b \\ &= \left(\sqrt{8}b - (3 - \sqrt{8})(n - 1)\right)(n - b - 2). \end{aligned}$$

Since

$$\sqrt{8}b - (3 - \sqrt{8})(n - 1) > 0 \Leftrightarrow b > \frac{(3 - \sqrt{8})(n - 1)}{\sqrt{8}} \simeq 0.06066(n - 1),$$

for such values of  $b$ ,  $\Delta_1 > 0$ . Now, let us show that

$$\Delta_2 = \sqrt{8}(n + b - 1)(n - b - 2) - (3n - 2)b + 3(n - 1)(n - 2) > 0.$$

From

$$-(3n - 2)b + 3(n - 1)(n - 2) > 0 \Leftrightarrow b < \frac{3(n - 1)(n - 2)}{3n - 2}$$

and

$$n - 6 < \frac{3(n - 1)(n - 2)}{3n - 2} \Leftrightarrow 3n^3 - 20n + 12 < 3(n^2 - 3n + 2) \Leftrightarrow 6 < 11n \quad (\text{which is true}),$$

it follows that  $\Delta_2 > 0$ , for  $1 \leq b \leq n - 6 < \frac{3(n-1)(n-2)}{3n-2}$ .

From the above, for  $n \geq 7$  and  $b \in \mathbb{N}$  such that  $0.06066(n - 1) \leq b \leq n - 6$ ,

$$g(n, b) > h(n, b) = \Delta_1 \Delta_2 > 0.$$

Given  $n \geq 7$ , consider  $b_{\min}$  the smallest integer  $b \geq 1$  such that  $g(n, b) > 0$  and let  $b^* = 0.06066(n - 1)$ . For different values of  $n$ ,  $b^*$  remains close to the exact value  $b_{\min}$ :

$n$	$b_{\min}$	$b^*$
20	1	1.1525
30	2	1.7591
50	3	2.9723
100	6	6.0053
500	30	30.269
1000	61	60.599
5000	303	303.24
10000	606	606.54
20000	1213	1213.1

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