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On the Randić Energy of Caterpillar Graphs

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Abstract

A caterpillar graph $T(p_1,\ldots,p_r)$ 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 $T(p_1,\ldots,p_r)$. This result is applied to determine the extremal caterpillars for the Randić energy of $T(p_1,\ldots,p_r)$ 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 $T\big(p, n-p-q-3, q\big)$ 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 $b \in \{1,\ldots,n-6\}$ 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, $\sigma_R(G) = \{\rho_1^{[m_1]}, \rho_2^{[m_2]}, \ldots, \rho_s^{[m_s]}\}$, where m_i stands for the multiplicity of ρ_i, for $1 \leq i \leq s$, and $\rho_1 > \rho_2 > \cdots > \rho_s$ 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 $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ 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

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

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 disjoin 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 $T(p_1, \cdots p_r)$ 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 a 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 $T\big(p, n-p-q-3, q\big)$ of order n, and we characterize extremal caterpillar graphs for three cases: $q = p$, $q = n-p-b-3$ and $q = b$, for any $b \in \{1, \ldots, n-6\}$ 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 $\psi : V(G) \to V(H)$ 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 σ_M. In particular, the spectrum of the adjacency matrix of a graph G, also called the spectrum of G, is $\sigma(G) = \{\lambda_1^{[m_1]}, \lambda_2^{[m_2]}, \ldots, \lambda_s^{[m_s]}\}$, where m_i stands for the multiplicity of λ_i, for $1 \le i \le s$.

A path with r vertices, denoted by P_r, is a sequence of vertices $v_1, v_2, \ldots, v_r$ such that each vertex is adjacent to the next, that is $v_1 v_{i+1} \in E(G)$ for $i = 1, \ldots, r-1$. 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, $T(p_1, \ldots, p_r)$ denotes a caterpillar obtained by attaching the central vertex of a star S_{p_i+1} to the i-th vertex of P_r, $i = 1, \ldots r$. The order of a caterpillar is $n = r + \sum_{i=1}^{r} p_i$.

A caterpillar $T(p_1, \ldots, p_r)$ can also be seen as the H-join $H[G_1, \ldots, G_r, G_{r+1}, \ldots, G_{2r}]$, where, for $1 \leq i \leq r$, $\begin{cases} G_i & \cong & K_1 \\ G_{i+r} & \cong & \overline{K_{p_i}} \end{cases}$ and H is the caterpillar of order $2r$, $T(1, \ldots, 1)$, 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]), $T(p_1, \ldots, p_r) = H[K_1, \ldots, K_1, \overline{K_{p_1}}, \ldots, \overline{K_{p_r}}]$, where H is the caterpillar of order $2r$, $T(1, 1, \ldots, 1)$, 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 $j = 1, \ldots, k$ and $G = H[G_1, \ldots, G_k]$. Let R_G be the Randić matrix of G. Then,*

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

where $N_j = \sum\limits_{i \in N_H(j)} n_i$, for $j = 1, 2, \ldots, k$,

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

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 $i = 1 \ldots, k-1$ and $j = i+1, \ldots, k$.

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 $j = 1, \ldots, k$, then $\Gamma_k = \Omega A_H \Omega$, with $\Omega = \text{diag}\left\{ \sqrt{\frac{n_1}{N_1}}, \ldots, \sqrt{\frac{n_k}{N_k}} \right\}$.

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

Corollary 3.1 *Let $H = T(1, 1, \ldots, 1)$ 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 $T = T(p_1, \ldots, p_r) = H[K_1, \ldots, K_1, \overline{K_{p_1}}, \ldots, \overline{K_{p_r}}]$ 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 $T(p_1, \ldots, p_r)$ we focus our attention on the spectrum of Γ_{2r}. Firstly, note that

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

with

$$\Omega_1 = \text{diag}\left\{ \sqrt{\frac{1}{N_1}}, \ldots, \sqrt{\frac{1}{N_r}} \right\}, \qquad \Omega_2 = \text{diag}\left\{ \sqrt{\frac{p_1}{N_{r+1}}}, \ldots, \sqrt{\frac{p_r}{N_{2r}}} \right\}, \tag{2}$$

Therefore, we can write

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

where

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

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

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

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 Γ_{2r}, which will play an important role in getting our main results:

Theorem 3.3 *Let $H = T(1, 1, \ldots, 1)$ be the caterpillar of order $2r$, $r \geq 2$ and let Γ_{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 Γ_{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

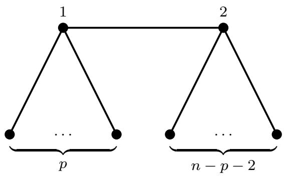
$$\begin{aligned} p_{\Gamma_{2r}}(\lambda) &= det(\lambda I_r) \cdot det\left(\lambda I_r - A - B\left(\frac{1}{\lambda} I_r\right) B\right) \\ &= \lambda^r \cdot det\left(\left(\frac{1}{\lambda}\right)(\lambda^2 I_r - \lambda A - B^2)\right) \\ &= \lambda^r \cdot \left(\frac{1}{\lambda}\right)^r \cdot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

■

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 $\mathbf{T(p, n-p-2)}$, $\mathbf{p = 1, \ldots, \lfloor \frac{n-2}{2} \rfloor}$.



Theorem 4.1 *Let $T_p = T(p, n-p-2)$, $p = 1, \ldots, \lfloor \frac{n-2}{2} \rfloor$ 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 σ_{Γ_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 $p = 1, \ldots, \lfloor \frac{n-2}{2} \rfloor$. 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,

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

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 $p = 1, \ldots, \left\lfloor \frac{n-2}{2} \right\rfloor$. Finally, if n is even,

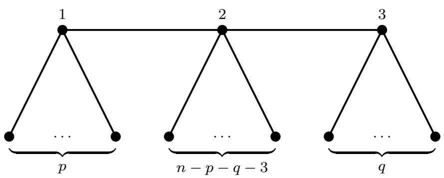
$$RE(T_{\lfloor \frac{n-2}{2} \rfloor}) = RE(T_{\frac{n-2}{2}}) = 2 + 2\left(\frac{n-2}{n}\right) = 4 - \frac{4}{n},$$

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 $\mathbf{T(p, n-p-q-3, q)}$, $\mathbf{p, q \in \{1, \ldots, n-5\}}$



For this class of caterpillars,

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

and

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

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

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

$$\det(\lambda^2 I_3 - \lambda A - B^2) =$$

$$= \left(\lambda^2 - \frac{p}{p+1}\right) \det\left(\begin{bmatrix} \lambda^2 - \frac{n-p-q-3}{n-p-q-1} & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} & \lambda^2 - \frac{q}{q+1} \end{bmatrix}\right)$$

$$+ \left(\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}}\right) \det\left(\begin{bmatrix} -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ 0 & \lambda^2 - \frac{q}{q+1} \end{bmatrix}\right)$$

$$= \left(\lambda^2 - \frac{p}{p+1}\right) \left[\left(\lambda^2 - \frac{n-p-q-3}{n-p-q-1}\right)\left(\lambda^2 - \frac{q}{q+1}\right) - \frac{\lambda^2}{(q+1)(n-p-q-1)}\right]$$

$$- \left(\frac{\lambda^2}{(p+1)(n-p-q-1)}\right)\left(\lambda^2 - \frac{q}{q+1}\right)$$

$$= \frac{\left(\lambda^2(p+1) - p\right)\left[\left(\lambda^2(n-p-q-1) - (n-p-q-3)\right)\left(\lambda^2(q+1) - q\right) - \lambda^2\right] - \lambda^2\left(\lambda^2(q+1) - q\right)}{(p+1)(q+1)(n-p-q-1)}.$$

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

$$\det(\lambda^2 I_3 - \lambda A - B^2) = \frac{1}{(p+1)(q+1)(n-p-q-1)}\Big[(p+1)(q+1)(n-p-q-1)\lambda^6$$

$$- \left[(n-p-q-2)\left(q(2p+1)+p\right) + (p+1)(q+1)(n-p-q-1)\right]\lambda^4$$

$$+ \left[pq(n-p-q-3) + (n-p-q-2)\left(q(2p+1)+p\right)\right]\lambda^2 - pq(n-p-q-3)\Big]$$

$$= \frac{(\lambda^2-1)\Big[(p+1)(q+1)(n-p-q-1)\lambda^4 - (n-p-q-2)\left(q(2p+1)+p\right)\lambda^2 + pq(n-p-q-3)\Big]}{(p+1)(q+1)(n-p-q-1)}$$

$$= \frac{1}{\eta(n,p,q)}(\lambda^2-1)\Big[\eta(n,p,q)\lambda^4 - \zeta(n,p,q)\lambda^2 + \chi(n,p,q)\Big],$$

being

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

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:

$$\begin{aligned}
\lambda_{1,2} &= \pm 1 \\
\lambda_{3,4} &= \pm\sqrt{\frac{\zeta(n,p,q) + \sqrt{\zeta^2(n,p,q) - 4\eta(n,p,q)\chi(n,p,q)}}{2\eta(n,p,q)}} \\
\lambda_{5,6} &= \pm\sqrt{\frac{\zeta(n,p,q) - \sqrt{\zeta^2(n,p,q) - 4\eta(n,p,q)\chi(n,p,q)}}{2\eta(n,p,q)}}.
\end{aligned}$$

Using the notation

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

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

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

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

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

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,

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

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

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

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)

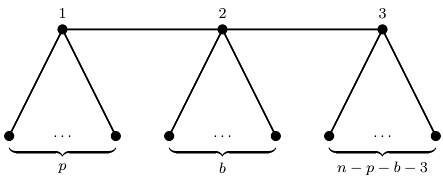
$$\gamma'(x) \leq \lambda(x) < 2\alpha'(x). \tag{11}$$

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

$$2\alpha'(x) < \lambda(x) \leq \gamma'(x). \tag{12}$$

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 $b \in \{1, \ldots, n-6\}$ fixed.

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



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

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

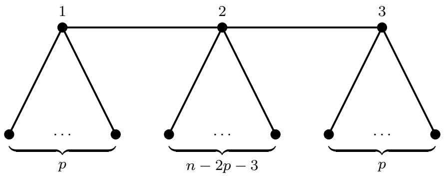
Proof Without loss of generality, we take $1 \leq p \leq \lfloor \frac{n-b-3}{2} \rfloor$, since for $p = 1, \ldots, n-b-4$, T_p and $T_{n-p-b-3}$ are isomorphic graphs. Replacing q by $n-p-b-3$ in (8), and considering the function $f(x)$, as in (9), for $1 \leq x \leq \frac{n-b-3}{2}$,

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

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

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 $\mathbf{T}(\mathbf{p}, \mathbf{n}-\mathbf{2p}-\mathbf{3}, \mathbf{p})$



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

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

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

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

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

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

and

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

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

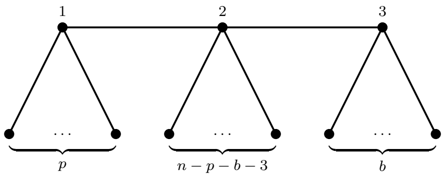
Similarly, $\gamma'(x) \geq 0$ if only if $x\big(2x^2-(4n-6)x+n^2-4n+3\big) \geq 0$, that is, for $0 \leq x \leq r_1$ or $x \geq r_2$ with $r_{1,2} = \frac{1}{2}\left(2n-3 \mp \sqrt{2n(n-2)+3}\right)$.

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 $z = round(\bar{z}) \in [round(r),\ round(s)]$, 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 $b \in \{1, \ldots, n-6\}$ fixed and $p = 1, \ldots, n-b-4$. Then,*

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

with

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

and

$$s = \frac{1}{b}\Bigg(-\big((b+1)(n-b)-1\big) + \sqrt{(b+1)(n-b-1)\big((2b+1)(n-1)-2b^2\big)}\Bigg). \tag{14}$$

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

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

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

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

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

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

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

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 $z = round(\bar{z}) \in I = [round(r), \ round(s)]$. Furthermore, $f(n-b-4) < f(1)$, which completes the proof. ■

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 a estimated interval

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

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 $b \in \{1, \ldots, n-6\}$ fixed, for each $p = 1, \ldots, n-b-4$. In this case, we want to point out that the interval I does not necessarily has range less than 1. In fact, that interval have 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:

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

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

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

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

$$\begin{aligned} \Delta_1 &= \sqrt{8}(n+b-1)(n-b-2) - 3(n-1)(n-2) + (3n-2)b > 0, \text{ and,} \\ \Delta_2 &= \sqrt{8}(n+b-1)(n-b-2) + 3(n-1)(n-2) - (3n-2)b > 0. \end{aligned}$$

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

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

Since

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

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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