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Spectra and Randić Spectra of Caterpillar Graphs and Applications to the Energy

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Abstract

Let H be an undirected simple graph with vertices $v_1, \ldots, v_k$ and $G_1, \ldots, G_k$ be a sequence formed with k disjoint graphs G_i, $i = 1, \ldots, k$. The H-generalized composition (or H-join) of this sequence is denoted by $H[G_1, \ldots, G_k]$. In this work, we characterize the caterpillar graphs as a H-generalized composition and we study their spectra and Randić spectra, respectively. As an application, we obtain an improved and tight upper bound for the Energy and the Randić energy of these interesting trees.

1 Motivation and Preliminaries

We begin this section introducing the caterpillar tree and establishing some remarks where these interesting trees can be used in Mathematical Chemistry. In this work, we deal with undirected simple graphs hereafter simply called graphs. For each graph G, the vertex set is denoted by $\mathcal{V}(G)$ and its edge set by $\mathcal{E}(G)$. A path with r vertices, P_r, of a graph G is a sequence of r distinct vertices $v_1, \ldots, v_r$, such that $v_i v_{i+1} \in \mathcal{E}(G)$ for $i = 1, \ldots, r-1$. A tree is a connected graph without cycles. For $r \geq 0$, a star with

$r+1$ vertices, S_{r+1}, is a tree with a central vertex with degree r and all remaining r vertices are pendant. A caterpillar is a tree of order $n \geq 5$ (notice that a tree of order less than 5 is a path or a star) such that removing all the pendant vertices produces a path with at least two vertices. In particular, the caterpillar $T(q_1, \ldots, q_r)$ is obtained from a path P_r, with $r \geq 2$, attaching the central vertex of the star S_{q_i+1} $(1 \leq i \leq r)$ to the i-th vertex of the path P_r. Then, the order of the caterpillar is $n = r + q_1 + \cdots + q_r$. These trees are studied in detail in the theory of graph spectra (see for instance, [12–14]) and there are some connections with it in Mathematical Chemistry. *Molecular graphs* represent the structure of molecules. They are generated, in general, using the following rule: vertices stand for atoms and edges for bonds. There are two basic types of molecular graphs: those representing *saturated hydrocarbons* and those representing *conjugated π-electron systems*. In the second class, the molecular graph should have perfect matchings (called "Kekulé structure"). Below, a type of data reduction graph is exhibited. In the 1930s, the German scholar Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called *conjugated hydrocarbons* (conjugated π-electron systems) which have a system of connected p-orbitals with *delocalized* π-electrons (electrons in a molecule that are not associated with a single atom or a covalent bond). Thus, the HMO (Hückel molecular orbital model) enables to describe approximately the behavior of the so-called π-electrons in a conjugated molecule, especially in conjugated hydrocarbons. For more details see [11] and the references therein.

On the other hand, in Chemistry, *resonance* is a way of describing delocalized electrons within certain molecules. The individual hexagons of a given benzenoid system may or may not be resonant. Information on such resonance relations (among the individual hexagons) are best described using caterpillar trees (see [8]). To illustrate this fundamental relation we consider the two graphs in [8] presented below.

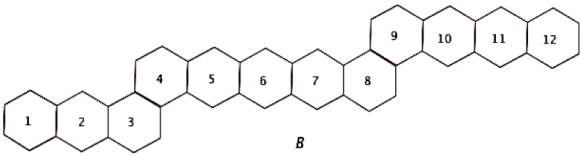

Figure 1: Benzenoid

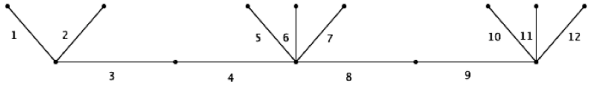

Figure 2: Associated caterpillar T

The hexagons of B may be grouped into subsets, namely $\{1,2,3\}$; $\{4,5,6,7,8\}$; $\{9,10,11,12\}$. Two hexagons are resonant provided that they don't belong to the same subset. Similarly the edges of T can be subdivided into analogous three subsets observing that in some cases only two edges of the two distinct subsets are adjacent. Thus, the number of selections of k mutually resonant (non-adjacent) hexagons in a benzenoid system (or polyhex graph) equals to the number of *k-matchings* of T (number of sets of k non-adjacent edges). For more details see in [8] and the references therein.

Returning to HMO theory, the total π-electron energy, E_π, is a quantum-chemical characteristic of conjugated molecules that agrees with their thermodynamic properties. For conjugated hydrocarbons in their ground electronic states, E_π is calculated from the eigenvalues of the adjacency matrix of the molecular graph:

$$E_\pi = n\alpha + E\beta,$$

where n is the number of carbon atoms, α and β are the HMO carbon-atom coulomb and carbon-carbon resonance integrals, respectively. For the majority conjugated π-electron systems

$$E = \sum_{i=1}^{n} |\lambda_i|, \tag{1}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix A of the underlying molecular graph. For molecular structure researches, E is the only interesting quantity. In fact, it is traditional to consider E as the total π-electron energy expressed in β-units. The spectral invariant defined by (1) is called the *energy* of G. For more details see [11] and the references therein.

If G is a bipartite graph, then its characteristic polynomial is

$$\phi(G,x) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^k b_{2k} x^{n-2k},$$

where $b_0 := 1$ and $b_{2k} \geq 0$. If $G = T$ is a tree then $b_{2k} := m(T,k)$, for all $k = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor$, where $m(T,k)$ equals to the number of k -matchings of T, (see [11]).

For two bipartite graphs G_1 and G_2, we define $G_1 \preceq G_2$ if and only if $b_{2k}(G_1) \leq b_{2k}(G_2)$ for all $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. Moreover, if there exists a k such that $b_{2k}(G_1) < b_{2k}(G_2)$ we write $G_1 \prec G_2$. The following result was proven. See [11].

$$\begin{aligned} G_1 &\preceq G_2 \Rightarrow E(G_1) \leq E(G_2) \\ G_1 &\prec G_2 \Rightarrow E(G_1) < E(G_2). \end{aligned}$$

By using these results the following other ones were obtained (see [11]). These results are consequence of previous observations, namely the order relation established above.

Here, a tree is called *double star* $S_{p,q}$ if it is obtained by joining the center of two stars S_p and S_q by an edge and a *comet* is a tree composed by a star and an appended path. For any number n and $2 \leq k \leq n-1$ the comet of order n with k pendant vertices is denoted by $P_{n,k}$. Note that it is formed by a path P_{n-k} of which one end vertex coincides with a pendant vertex of a star S_{k+1} of order $k+1$.

1. Let S_n and P_n denote the n vertices star and path, respectively. For any tree T with n vertices
$$E(S_n) \leq E(T) \leq E(P_n).$$

2. Let $S(n-2,2)$ and $S(n-3,3)$ denote two double stars of order n and $P_{n,n-3}$ denotes a comet of order n. If $T \ncong S_n$ then
$$E(S_n) < E(S(n-2,2)) < E(S(n-3,3)) < E(P_{n,n-3}) < E(T).$$

From the above it is clear that there exists a correlation among the resonance relations of a given benzenoid system and the energy of its associated caterpillar. This was a motivation for the study of the energy of the caterpillars.

Now, we introduce some more specific notation used throughout the text. We deal with graphs G of order n, and we set $\mathcal{V}(G) = \{v_1, \ldots, v_n\}$. An edge with end vertices v_i and v_j is denoted by v_iv_j and then we say that the vertices v_i and v_j are *adjacent* or *neighbors*. Sometimes, by convenience, the edge v_iv_j is represented by ij. The set of neighbors of v_i, $N_G(v_i)$, is called the *neighborhood* of v_i and its cardinality, d_i is the degree of v_i. The *maximum* and *minimum* degree of the vertices of G are denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively. A graph G is called *p-regular* whenever $\Delta = \delta = p$.

We denote the *adjacency matrix* of G by $\mathbf{A}_G$. The Laplacian matrix of G is $\mathbf{L} = \mathbf{L}_G = \mathbf{D}_G - \mathbf{A}_G$, where $\mathbf{D}_G$ is the diagonal matrix of vertex degrees of G. For spectral properties of these matrices see e.g. [6].

For a matrix $\mathbf{M}$ we denote its *spectrum* (the multiset of the eigenvalues of $\mathbf{M}$) by $\sigma_{\mathbf{M}}$. The multiplicities of the eigenvalues are represented in the multiset $\sigma_{\mathbf{M}}$ as powers in square brackets. For instance, $\sigma_{\mathbf{M}} = \{\alpha_1^{[m_1]}, \alpha_2^{[m_2]}, \ldots, \alpha_q^{[m_q]}\}$ denotes that α_1 has multiplicity m_1, α_2 has multiplicity m_2, and so on. If α is an eigenvalue of $\mathbf{M}$ and $\mathbf{x}$ one of its eigenvectors, the pair $(\alpha, \mathbf{x})$ is an eigenpair of $\mathbf{M}$. The spectrum of the adjacency matrix of a graph G, is just denoted by σ_G and the eigenvalues of $\mathbf{A}_G$, $\lambda_1(G) \geq \cdots \geq \lambda_n(G)$ are also called the eigenvalues of G.

Here, K_p is the complete graph of order p and the complement of a graph G is denoted by $\bar{G}$. We denote the square zero matrix, the all ones vector and the identity matrix of order n by $\mathbf{O}$, $\mathbf{e}_n$ and I_n , respectively. For the remaining basic terminology and notation used throughout the paper we refer the book [6].

2 Randić and Normalized Laplacian matrices

We start this section introducing a nonnegative graph matrix $\mathbf{R} = \mathbf{R}_G = (r_{ij})$, where $r_{ij} = 1/\sqrt{d_i\, d_j}$ if $v_i v_j \in \mathcal{E}(G)$, and zero otherwise. The proposed name for $\mathbf{R}$ was *Randić matrix* of the graph (see e.g. [2]). If $d_i = 0$, for some i, then the corresponding vertex is said isolated. By simplicity, we consider only graphs without isolated vertices, then the diagonal matrix $\mathbf{D}^{-1/2}$ exists (recall that $\mathbf{D}^{-1/2}$ is the diagonal matrix whose i-th diagonal entry is $1/\sqrt{d_i}$) and the matrix $\mathcal{L} = \mathcal{L}_G = \mathbf{D}^{-1/2}\, \mathbf{L}_G\, \mathbf{D}^{-1/2}$ is the *Normalized Laplacian matrix*. For spectral properties of this matrix, see e.g. [5]. It is easy to see that

$$\mathcal{L}_G = I_n - \mathbf{R}_G \tag{2}$$

implying there is an obvious relation between the eigenvalues of $\mathbf{R}_G$ and $\mathcal{L}_G$. Notice that the Normalized Laplacian matrix has the same inertia than $\mathbf{L}_G$, (see e.g. [9]), and then it is a positive semidefinite matrix. This fact and equality in (2) imply that 1 is the greatest Randić eigenvalue of any graph. Moreover, a standard verification shows that $\mathbf{D}^{1/2}\, \mathbf{e}$ is an eigenvector of the Randić matrix for the eigenvalue 1.

In [2], the concept of Randić energy of the graph G, $E_{\mathbf{R}}(G)$, was defined as the sum of the absolute values of the eigenvalues of the Randić matrix and some properties, namely

lower and upper bounds for it were established. See more literature related with this concept for instance in [2, 3, 7, 10] and in the references therein. Recently, lower and upper bounds for the Randić energy in terms of the number of the vertices, maximum degree, minimum degree and the determinant of the adjacency matrix of graphs were also presented, [7].

A generalization of the join operation was introduced in [4] as follows:

Consider a family of k graphs, $\mathcal{F} = \{G_1, \ldots, G_k\}$, where each graph G_i has order n_i, for $i = 1 \ldots k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Each vertex $v_i \in \mathcal{V}(H)$ is assigned to the graph $G_i \in \mathcal{F}$. The H-join of $G_1, \ldots, G_k$ is the graph $G = H[G_1, \ldots, G_k]$ such that $\mathcal{V}(G) = \bigcup_{i=1}^{k} \mathcal{V}(G_i)$ and edge set:

$$\mathcal{E}(G) = \left(\bigcup_{i=1}^{k} \mathcal{E}(G_i) \right) \cup \left(\bigcup_{uw \in \mathcal{E}(H)} \{ij : i \in \mathcal{V}(G_u), j \in \mathcal{V}(G_w)\} \right).$$

This operation, where H is an arbitrary graph of order k, is the same as the so called generalized composition, considered in [16] with the notation $H[G_1, \ldots, G_k]$. For better understanding we present here an example from [4].

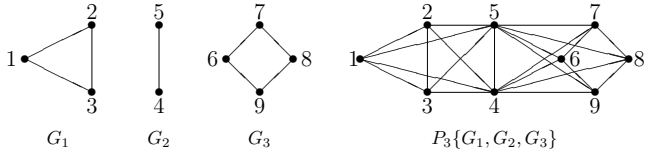

Figure 3: The H-join of $\mathcal{F} = \{K_3, K_2, C_4\}$, with $H = P_3$.

This paper is organized as follows: in Section 1 and 2 we present the motivation, notation and some concepts used throughout the text. In Section 3, we give the Adjacency and Randić spectra of H-join of graphs and, using these results, in Section 4, we characterize the non-zeros Randić eigenvalues of some caterpillars. Finally in Section 5, we obtain an explicit formula for an improved and tight upper bound for the energy and the Randić energy of a caterpillar.

3 Spectra and Randić spectra of H-join of graphs

The spectrum of the H-join of regular graphs was characterized in [4, Theorem 3]. Let H be a graph with k vertices without isolated vertices. Let $G_1, \ldots, G_k$ be a sequence of k

disjoint arbitrary p_j-regular graphs of orders n_j, $j = 1, \ldots, k$. Let $G = H[G_1, \ldots, G_k]$. For $j = 1, \ldots, k$ we use $\mathbf{A}_j$ to denote the adjacency matrices of G_j, respectively. Let $\mathbf{A}_H = (\delta_{ij})$ be the $k \times k$ adjacency matrix of H. Define

$$\widehat{C} = \begin{pmatrix} p_1 & \delta_{12}\sqrt{n_1 n_2} & \cdots & \delta_{1k}\sqrt{n_1 n_k} \\ \delta_{12}\sqrt{n_1 n_2} & p_2 & & \delta_{2k}\sqrt{n_2 n_k} \\ \vdots & & \ddots & \delta_{k-1,k}\sqrt{n_{k-1} n_k} \\ \delta_{1k}\sqrt{n_1 n_k} & & \delta_{k-1,k}\sqrt{n_{k-1} n_k} & p_k \end{pmatrix}. \tag{3}$$

Theorem 1. *[4] For $j = 1, \ldots, k$, let G_j be a p_j-regular graph of order n_j, with spectrum σ_{G_j}. If $G = H[G_1, \ldots, G_k]$, and $\widehat{C}$ as in (3), then*

$$\sigma(G) = \sigma_{\widehat{C}} \cup \left(\bigcup_{j=1}^{k} (\sigma_{G_j} \setminus \{p_j\}) \right).$$

Remark 1. *From (3) note that if $p_j = 0$, for all $j = 1, \ldots, k$, then $\mathbf{\Gamma}_k = \Lambda A_H \Lambda$, where $\Lambda^2 = diag(n_1, \ldots, n_k)$.*

Next, we present similar results concerning the Randić spectra of the H-join of a family of regular graphs.

It is clear that

$$\mathbf{R}_j = \begin{cases} \frac{1}{p_j}\mathbf{A}_j, & \text{if } p_j > 0 \\ \mathbf{O}, & \text{if } p_j = 0 \end{cases}$$

is the Randić matrix of the regular graph G_j. Define

$$N_j = \sum_{v_i \in N_H(v_j)} n_i, \qquad j = 1, \ldots, k. \tag{4}$$

and the $\frac{k(k-1)}{2}$-tuple of scalars

$$\rho = (\rho_{12}, \rho_{13}, \ldots, \rho_{1k}, \rho_{23}, \ldots, \rho_{2k}, \ldots, \rho_{(k-1)k}),$$

such that

$$\rho_{ij} = \frac{\delta_{ij}\sqrt{n_i n_j}}{\sqrt{(N_i + p_i)(N_j + p_j)}}, \tag{5}$$

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

$$\mathbf{R}_G = \begin{pmatrix} \frac{1}{N_1+p_1}\mathbf{A}_1 & \frac{\rho_{12}\mathbf{e}_{n_1}\mathbf{e}_{n_2}^T}{\sqrt{n_1 n_2}} & \cdots & \cdots & \frac{\rho_{1k}\mathbf{e}_{n_1}\mathbf{e}_{n_k}^T}{\sqrt{n_1 n_k}} \\ \frac{\rho_{12}\mathbf{e}_{n_2}\mathbf{e}_{n_1}^T}{\sqrt{n_1 n_2}} & \frac{1}{N_2+p_2}\mathbf{A}_2 & \frac{\rho_{23}\mathbf{e}_{n_2}\mathbf{e}_{n_3}^T}{\sqrt{n_2 n_3}} & \cdots & \frac{\rho_{2k}\mathbf{e}_{n_2}\mathbf{e}_{n_k}^T}{\sqrt{n_2 n_k}} \\ \vdots & \frac{\rho_{23}\mathbf{e}_{n_3}\mathbf{e}_{n_2}^T}{\sqrt{n_2 n_3}} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{\rho_{(k-1)k}\mathbf{e}_{n_{k-1}}\mathbf{e}_{n_k}^T}{\sqrt{n_{k-1} n_k}} \\ \frac{\rho_{1k}\mathbf{e}_{n_k}\mathbf{e}_{n_1}^T}{\sqrt{n_1 n_k}} & \frac{\rho_{2k}\mathbf{e}_{n_k}\mathbf{e}_{n_2}^T}{\sqrt{n_2 n_k}} & \cdots & \frac{\rho_{(k-1)k}\mathbf{e}_{n_k}\mathbf{e}_{n_{k-1}}^T}{\sqrt{n_{k-1} n_k}} & \frac{1}{N_k+p_k}\mathbf{A}_k \end{pmatrix} \tag{6}$$

is the Randić matrix of the H-join $G = H[G_1, \ldots, G_k]$. Let $\mathbf{\Gamma}_k$ be the $k \times k$ symmetric matrix

$$\mathbf{\Gamma}_k = \begin{pmatrix} \frac{p_1}{N_1+p_1} & \rho_{12} & \cdots & \rho_{1(k-1)} & \rho_{1k} \\ \rho_{12} & \frac{p_2}{N_2+p_2} & \cdots & \rho_{2(k-1)} & \rho_{2k} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{1k} & \rho_{2k} & \cdots & \rho_{(k-1)k} & \frac{p_k}{N_k+p_k} \end{pmatrix}. \tag{7}$$

The following result characterizes the Randić spectra of the H -joins.

Theorem 2. *Let H be a graph on k vertices. Let G_i be a p_j -regular graph on n_j vertices with $p_j \geq 0$, $n_j \geq 1$, for $j = 1, \ldots, k$ and $G = H[G_1, \ldots, G_k]$. Let $\mathbf{R}_G$ be the Randić matrix of G. Then*

$$\sigma_{\mathbf{R}_G} = \sigma_{\mathbf{\Gamma}_k} \cup \bigcup_{j=1}^{k} \left\{ \tfrac{\lambda}{N_j+p_j} : \lambda \in \sigma_{G_j} \setminus \{p_j\} \right\}.$$

Proof. This follows directly from Theorem 3 in [4] due to the construction of the matrix in (6). □

Remark 2. *From the formula of the entries (5) note that if $p_j = 0$, for all $j = 1, \ldots, k$, then $\mathbf{\Gamma}_k = \Sigma A_H \Sigma$ where $\Sigma^2 = diag\left(\frac{n_1}{N_1}, \ldots, \frac{n_k}{N_k}\right)$.*

4 An application to some spectra of special caterpillars

For the caterpillar $T(q_1, \ldots, q_r)$, where $r \geq 3$ and $q_i \geq 1$, with $i = 1, \ldots, r$, we label its vertices as follows:

1. We start labeling, from left to right, the vertices of P_r,

2. then, (and again from left to right) we use the labels $r + i$ for the pendant vertices at i, for all $1 \leq i \leq n - r$.

Let $H_0 = T(1, \ldots, 1)$ be the caterpillar with $2r$ vertices obtained from a path P_r, with $r \geq 2$, attaching the central vertex of the star S_2 to the i-th vertex of the path P_r, $1 \leq i \leq r$. Using the described labeling of the vertices, the adjacency matrix of H_0, takes the form

$$\mathbf{A}_{H_0} = \begin{pmatrix} \mathbf{A}_{P_r} & \mathbf{I}_r \\ \mathbf{I}_r & \mathbf{O} \end{pmatrix}, \tag{8}$$

recall that $\mathbf{A}_{P_r}$ is the adjacency matrix of the path P_r.

Using the notation in the above section

$$T(q_1,\ldots,q_r) = H_0\left[K_1,\ldots,K_1,\overline{K}_{q_1},\ldots,\overline{K}_{q_r}\right]. \tag{9}$$

By the identification in (9), the cardinality n_i is

$$n_i = \begin{cases} 1, & \text{if } i = 1,\ldots,r \\ q_{i-r}, & \text{if } i = r+1,\ldots,2r, \end{cases}$$

the regularity p_i is equal to zero, for $1 \leq i \leq 2r$. Hence by applying Theorem 1 to $T(q_1,\ldots,q_r)$ we obtain.

Theorem 3. *Let $H_0 = T(1,\ldots,1)$ be the caterpillar with $2r$ vertices. Let $G = T(q_1,\ldots,q_r)$ the caterpillar with $n = r + \sum_{i=1}^{r} q_i$ vertices as described above. Let $\mathbf{A}_G$ be the adjacency G. Then*

$$\sigma_{\mathbf{A}_G} = \left\{0^{\left[\sum_{i=1}^{r}(q_i-1)\right]}\right\} \cup \sigma_{\mathbf{C}_{2r}},$$

where $\mathbf{C}_{2r}$ is the $2r \times 2r$ matrix

$$\mathbf{C}_{2r} = \begin{pmatrix} \mathbf{A}_{P_r} & \Lambda_r \\ \Lambda_r & \mathbf{O} \end{pmatrix}, \tag{10}$$

with $\Lambda_r^2 = diag\,(q_1,\ldots,q_r)$.

Next, using Theorem 2 we characterize the Randić spectrum of $T(q_1,\ldots,q_r)$. Let $\mathbf{A}_{H_0} = (\delta_{ij})$ the $2r \times 2r$ adjacency matrix of H_0 as in (8). The value of N_i in (4) becomes

$$N_i = \begin{cases} q_i + 1, & \text{if } i \in \{1, r\} \\ q_i + 2, & \text{if } i \in \{2,\ldots,r-1\} \\ 1, & \text{if } i \in \{r+1,\ldots,2r\}. \end{cases}$$

Here we consider Remark 2. For convenience, let us consider the following diagonal matrix,

$$\begin{aligned} \Sigma^2 &= diag\left(\tfrac{n_1}{N_1},\ldots,\tfrac{n_{2r}}{N_{2r}}\right) \\ &= diag\left(\tfrac{1}{q_1+1},\ldots,\tfrac{1}{q_j+2},\ldots,\tfrac{1}{q_r+1},q_1,\ldots,q_r\right) \end{aligned}$$

and define

$$\mathbf{\Gamma}_{2r} = \Sigma \mathbf{A}_{H_0} \Sigma = (\nu_{ij})_{1 \leq i,j \leq 2r} \tag{11}$$

where

$$\nu_{ij}=\begin{cases}\frac{1}{\sqrt{(q_i+1)(q_j+2)}}, & (i,j)\in\{(1,2)\}\cup\{(r,r-1)\},\\ \frac{1}{\sqrt{(q_i+2)(q_j+1)}}, & (i,j)\in\{(2,1)\}\cup\{(r-1,r)\},\\ \frac{1}{\sqrt{(q_i+2)(q_j+2)}}, & (i,j)\in\{(t,t+1)\}_{t=2}^{r-2}\cup\{(t,t-1)\}_{t=3}^{r-1},\\ \sqrt{\frac{q_i}{q_{j-r}+1}}, & (i,j)\in\{(1,r+1),(r,2r)\},\\ \sqrt{\frac{q_{i-r}}{q_j+1}}, & (i,j)\in\{(r+1,1),(2r,r)\},\\ \sqrt{\frac{q_i}{q_{j-r}+2}}, & (i,j)\in\{(t,t+r)\}_{t=2}^{r-1},\\ \sqrt{\frac{q_{i-r}}{q_j+2}}, & (i,j)\in\{(t+r,t)\}_{t=2}^{r-1},\\ 0, & \text{otherwise.}\end{cases}\tag{12}$$

As a consequence of Theorem 2 we obtain the next result.

$$\sigma_{\mathbf{R}_{T(q_1,\ldots,q_r)}}=\left\{0^{\left[\sum_{i=1}^{r}(q_i-1)\right]}\right\}\cup\sigma_{\mathbf{\Gamma}_{2r}}.$$

Example 1. *For the caterpillar* $T(3,2,4)=H_0\left[K_1,K_1,K_1,\overline{K}_3,\overline{K}_2,\overline{K}_4\right]$*, the matrix in (11) becomes*

$$\mathbf{\Gamma}_6=\begin{pmatrix}0&\frac{1}{4}&0&\sqrt{\frac{3}{4}}&0&0\\ \frac{1}{4}&0&\frac{1}{\sqrt{20}}&0&\sqrt{\frac{2}{4}}&0\\ 0&\frac{1}{\sqrt{20}}&0&0&0&\sqrt{\frac{4}{5}}\\ \sqrt{\frac{3}{4}}&0&0&0&0&0\\ 0&\sqrt{\frac{2}{4}}&0&0&0&0\\ 0&0&\sqrt{\frac{4}{5}}&0&0&0\end{pmatrix}$$

Then $\sigma_{\mathbf{R}_{T(3,2,4)}}=\left\{0^{[6]}\right\}\cup\sigma_{\mathbf{\Gamma}_6}=\left\{0^{[6]}\right\}\cup\{\pm1.0000,\pm0.8808,\pm0.6218\}$.

5 Bounds for the energy and Randić energy of some caterpillars

In what follows we use a result in [1] to give bounds for the energy and the Randić energy of some caterpillars.

A symmetric imprimitive matrix $\mathbf{M}$ (see [15, Chap. 3]) must have index 2. By the Frobenius Form of an Irreducible Matrix [15, Theorem 3.1], in this case there exists a permutation matrix $\mathbf{P}$ such that

$$\mathbf{M}=\mathbf{P}^t\begin{pmatrix}\mathbf{0}&\mathbf{M}_{12}\\ \mathbf{M}_{21}&\mathbf{0}\end{pmatrix}P.\tag{13}$$

Let $|\mathbf{P}|$ be the Frobenius matrix norm of a square matrix $\mathbf{P}$. Considering a consequence of the Cauchy-Schwarz inequality in [1], among others results, a sharp upper bound of

the energy of a symmetric imprimitive matrix $\mathbf{M}$ was obtained. As a consequence, an improved upper bound for the energy of a bipartite graph was obtained.

Theorem 4. *[1] Let* $\mathbf{M}$ *be an imprimitive symmetric matrix whose Frobenius form is given in Eq. (13). If* $\mathbf{M}_{12}$ *has order* $m_1 \times m_2$*, and* $\mathbf{M}_{21}$ *has order* $m_2 \times m_1$ *and* $\widetilde{m} = \min\{m_1, m_2\}$*, then*

$$E(\mathbf{M}) \leq 2\lambda_1(\mathbf{M}) + 2\sqrt{(\widetilde{m}-1)\left(|\mathbf{M}|^2/2 - \lambda_1^2(\mathbf{M})\right)}.$$

Equality holds if and only if $\widetilde{m} = 1$ *or if* $\mathbf{M}$ *has* $2(\widetilde{m}-1)$ *eigenvalues distinct of* $\pm\lambda_1(\mathbf{M})$ *with the same modulus, namely* $\sqrt{\frac{|\mathbf{M}|^2/2 - \lambda_1^2(\mathbf{M})}{\widetilde{m}-1}}$ *and* $|m_2 - m_1|$ *eigenvalues equal to* 0*.*

Let now $H_0 = T(1, \ldots, 1)$ defined as before. Using the described above labeling of the vertices for H_0, one can see that the set of vertices of H_0 can be split into two set X and Y such that X is formed with vertices of the path whose label is odd and the pendent vertices which are neighbors of the vertices of the path whose label is even. In consequence, both sets X and Y have the same cardinality, $\widetilde{m} = r$. The following theorems will be proved by replacing the matrix $\mathbf{M}$ in Theorem 4 by the matrix in (10) (at Theorem 5) and by the matrix in (11) (at Theorem 6). In consequence, these theorems have essentially the same proof and therefore only the proof of Theorem 6 will be given.

Theorem 5. *Let* $T(q_1, \ldots, q_r)$ *be the caterpillar obtained from a path* P_r*, with* $r \geq 3$*, identifying the central vertex of the star* S_{q_i+1} $(i = 1 \ldots, r)$ *to the* i*-th vertex of the path* P_r*. Then*

$$E(T(q_1, \ldots, q_r)) \leq 2\lambda_1(\mathbf{C}_{2r}) + 2\sqrt{(r-1)\left(\tfrac{|\mathbf{C}_{2r}|^2}{2} - \lambda_1^2(\mathbf{C}_{2r})\right)}. \tag{14}$$

Equality holds if and only if $\mathbf{C}_{2r}$ *has* $2(r-1)$ *eigenvalues distinct from* $\pm\lambda_1(\mathbf{C}_{2r})$ *with the same modulus, namely* $\sqrt{\frac{\frac{|\mathbf{C}_{2r}|^2}{2} - 1}{r-1}}$*.*

The next theorem gives an upper bound for the Randić energy of $T(q_1, \ldots, q_r)$.

Theorem 6. *Let* $T(q_1, \ldots, q_r)$ *be the caterpillar obtained from a path* P_r*, with* $r \geq 3$*, identifying the central vertex of the star* S_{q_i+1} $(i = 1 \ldots, r)$ *to the* i*-th vertex of the path* P_r*. Then*

$$E_{\mathbf{R}}(T(q_1, \ldots, q_r)) \leq 2 + 2\sqrt{(r-1)\left(\tfrac{|\mathbf{\Gamma}_{2r}|^2}{2} - 1\right)}. \tag{15}$$

Equality holds if and only if $\mathbf{\Gamma}_{2r}$ *has* $2(r-1)$ *eigenvalues distinct from* ± 1 *with the same modulus, namely* $\sqrt{\frac{\frac{|\mathbf{\Gamma}_{2r}|^2}{2} - 1}{r-1}}$*.*

Proof. The adjacency matrix, $\mathbf{A}_{H_0}$ and so $\mathbf{\Gamma}_{2r}$, have the Frobenius form

$$\begin{pmatrix} 0 & \mathbf{V}_{12} \\ \mathbf{V}_{21} & 0 \end{pmatrix},$$

where both matrices $\mathbf{V}_{12}$ and $\mathbf{V}_{21}$ have order r. By the results in the above section, the nonzero eigenvalues of $T(q_1,\ldots,q_r)$ are the eigenvalues of $\mathbf{\Gamma}_{2r}$ in (11). By a direct application of Theorem 4, replacing $\mathbf{M}$ by $\mathbf{\Gamma}_{2r}$, where $\widetilde{m}=r$, the result follows. □

Remark 3. *With the next develoments we find a new upper bound for the energy of caterpillars. For* $0<x<\frac{|\mathbf{C}_{2r}|}{\sqrt{2}}$, *let* $f(x)=x+\sqrt{(r-1)\left(\frac{|\mathbf{C}_{2r}|^2}{2}-x^2\right)}$. *Then* $f'(x)=1-\frac{(r-1)x}{\sqrt{(r-1)\left(\frac{|\mathbf{C}_{2r}|^2}{2}-x^2\right)}}<0$ *if and only if*

$$(r-1)\left(\frac{|\mathbf{C}_{2r}|^2}{2}-x^2\right)<(r-1)^2x^2 \Leftrightarrow \frac{|\mathbf{C}_{2r}|}{\sqrt{2r}}<x.$$

Therefore, $f(x)$ *is a non-increasing function in the open interval* $I=\left(\frac{|\mathbf{C}_{2r}|}{\sqrt{2r}},\frac{|\mathbf{C}_{2r}|}{\sqrt{2}}\right)$. *Let* $\mathbf{e}$ *and* $\|\cdot\|$*denote the* $2r$*-dimensional all ones vector and the Euclidean vector norm of* $\mathbb{R}^{2r}$, *respectively. By the Rayleigh quotient*

$$\lambda_1^2(\mathbf{C}_{2r})\geq\frac{\mathbf{e}^*\mathbf{C}_{2r}^2\mathbf{e}}{\mathbf{e}^*\mathbf{e}}\geq\frac{trace\left(\mathbf{C}_{2r}^2\right)}{2r}=\frac{|\mathbf{C}_{2r}|^2}{2r}\Rightarrow\lambda_1(\mathbf{C}_{2r})\geq\frac{|\mathbf{C}_{2r}|}{\sqrt{2r}}$$

and

$$|\mathbf{C}_{2r}|^2\geq 2\lambda_1^2(\mathbf{C}_{2r})\Rightarrow\frac{|\mathbf{C}_{2r}|}{\sqrt{2}}\geq\lambda_1(\mathbf{C}_{2r}).$$

Hence, $\lambda_1(\mathbf{C}_{2r})\in I$. *On the other hand,*

$$trace\left(\mathbf{C}_{2r}^2\right)\leq\mathbf{e}^*\mathbf{C}_{2r}^2\mathbf{e}\leq 2r\lambda_1^2\Rightarrow|\mathbf{C}_{2r}|\leq\|\mathbf{C}_{2r}\mathbf{e}\|\leq\sqrt{2r}\lambda_1.$$

Hence, $\frac{\|\mathbf{C}_{2r}\mathbf{e}\|}{\sqrt{2r}}\in I$ *and*

$$f\left(\frac{\|\mathbf{C}_{2r}\mathbf{e}\|}{\sqrt{2r}}\right)\geq f(\lambda_1),$$

and by (14) we arrive at

$$E(T(q_1,\ldots,q_r))\leq 2f\left(\frac{\|\mathbf{C}_{2r}\mathbf{e}\|}{\sqrt{2r}}\right)=2\left(\frac{\|\mathbf{C}_{2r}\mathbf{e}\|}{\sqrt{2r}}+\sqrt{(r-1)\left(\frac{|\mathbf{C}_{2r}|^2}{2}-\frac{\|\mathbf{C}_{2r}\mathbf{e}\|^2}{2r}\right)}\right).$$

Now, by the computation of $\frac{|\mathbf{C}_{2r}|^2}{2}$, we obtain the following result.

Theorem 7. *Let* $T(q_1,\ldots,q_r)$ *be the caterpillar obtained from a path* P_r, *with* $r\geq 2$, *attaching the central vertex of the star* S_{q_i+1} $(i=1,\ldots,r)$ *to the* i*-th vertex of the path* P_r. *Then*

$$E(T(q_1,\ldots,q_r))\leq$$

$$2\lambda_1(\mathbf{C}_{2r})+2\sqrt{(r-1)\left(n-1-\lambda_1^2(\mathbf{C}_{2r})\right)}\leq\sqrt{\tfrac{2}{r}}\|\mathbf{C}_{2r}\mathbf{e}\|+\sqrt{\tfrac{2}{r}}\sqrt{(r-1)\left(2r(n-1)-\|\mathbf{C}_{2r}\mathbf{e}\|^2\right)}.$$

Equality holds if and only if $\mathbf{C}_{2r}$ *has* $2(r-1)$ *eigenvalues distinct from* $\pm\lambda_1(\mathbf{C}_{2r})$ *with the same modulus and* $(\lambda_1(\mathbf{C}_{2r}),\mathbf{e})$ *is an eigenpair of* $\mathbf{C}_{2r}$.

Next, from the calculation of $|\frac{\Gamma_{2k}}{2}|^2$, an explicit formula of the above upper bound for the Randić energy is obtained.

Theorem 8. *Let* $T(q_1,\ldots,q_r)$ *be the caterpillar obtained from a path* P_r, *with* $r\geq 2$, *attaching the central vertex of the star* S_{q_i+1} $(1\leq i\leq r)$ *to the* i*-th vertex of the path* P_r. *Then*

$$E_{\mathbf{R}}(T(q_1,\ldots,q_r))\leq\Upsilon,$$

where

$$\Upsilon=2+2\sqrt{(r-1)\left(\tfrac{1+q_1q_2+2q_1}{(q_1+1)(q_2+2)}+\tfrac{1+q_rq_{r-1}+2q_r}{(q_r+1)(q_{r-1}+2)}+\tfrac{q_{r-1}}{q_{r-1}+2}+\sum_{i=2}^{r-2}\tfrac{1+q_iq_{i+1}+2q_i}{(q_i+2)(q_{i+1}+2)}-1\right)}. \quad (16)$$

Equality holds if and only if $\mathbf{\Gamma}_{2r}$ *has* $2(r-1)$ *eigenvalues distinct of* ±1 *with the same modulus, namely*

$$\sqrt{\frac{\left(\tfrac{1+q_1q_2+2q_1}{(q_1+1)(q_2+2)}+\tfrac{1+q_rq_{r-1}+2q_r}{(q_r+1)(q_{r-1}+2)}+\tfrac{q_{r-1}}{q_{r-1}+2}+\sum_{i=2}^{r-2}\tfrac{1+q_iq_{i+1}+2q_i}{(q_i+2)(q_{i+1}+2)}\right)-1}{r-1}}.$$

Proof. Using the entries of $\mathbf{\Gamma}_{2r}$ in (12) and by a direct computation we see that

$$\frac{|\mathbf{\Gamma}_{2r}|^2}{2}=$$

$$\begin{aligned}
&\tfrac{1}{(q_1+1)(q_2+2)}+\tfrac{1}{(q_r+1)(q_{r-1}+2)}+\tfrac{q_1}{q_1+1}+\tfrac{q_r}{q_r+1}+\sum_{i=2}^{r-2}\tfrac{1}{(q_i+2)(q_{i+1}+2)}+\sum_{i=2}^{r-1}\tfrac{q_i}{q_i+2}\\
=\;&\tfrac{1}{(q_1+1)(q_2+2)}+\tfrac{1}{(q_r+1)(q_{r-1}+2)}+\tfrac{q_1}{q_1+1}+\tfrac{q_r}{q_r+1}+\sum_{i=2}^{r-2}\left(\tfrac{1}{(q_i+2)(q_{i+1}+2)}+\tfrac{q_i}{q_i+2}\right)+\tfrac{q_{r-1}}{q_{r-1}+2}\\
=\;&\tfrac{1+q_1q_2+2q_1}{(q_1+1)(q_2+2)}+\tfrac{1+q_rq_{r-1}+2q_r}{(q_r+1)(q_{r-1}+2)}+\tfrac{q_{r-1}}{q_{r-1}+2}+\sum_{i=2}^{r-2}\tfrac{1+q_iq_{i+1}+2q_i}{(q_i+2)(q_{i+1}+2)}.
\end{aligned}$$

By a direct replacement of the last formula in (15) the result is obtained. □

Below, a table with some values for the largest upper bound in Theorem 7 is presented.

r	$(q_1,\ldots,q_r)$	$E(T(q_1,\ldots,q_r))$	T. 7
4	$(5,5,5,5)$	18.5410	18.8769
6	$(9,9,8,9,10,9)$	36.8012	37.3700
7	$(11,9,12,12,12,10,13)$	47.8409	48.5471.

Again, a table with some values for the upper bound in (16) is presented.

r	$(q_1, \ldots, q_r)$	$E_{\mathbf{R}}(T(q_1, \ldots, q_r))$	(16)
4	$(5, 5, 5, 5)$	7.0711	7.0950
6	$(8, 9, 9, 7, 10, 7)$	10.9906	11.0106
7	$(10, 9, 7, 9, 10, 11, 9)$	12.8792	12.9027.

Remark 4. *We remark that if $q_j = 0$, for some j, the matrix Γ_k in (7) becomes of order $k = 2r - s$, where s is the number of vertices of the path without pendent vertices. Moreover, the set of vertices can, again, be split into two sets of vertices X and Y, where X is formed with the vertices of the path with odd label and the pendant vertices that are neighbors to the vertices of the path with even label. In this case, by Theorem 4, 0 is an eigenvalue of Γ_{2r-s} with multiplicity at least $||X| - |Y||$.*

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