MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **82** (2019) 515-528

ISSN 0340 - 6253

Short Note on Randić Energy

Luiz Emilio Allem†, Gonzalo Molina‡, Adrián Pastine‡

†*Instituto de Matemática, UFRGS, Porto Alegre, RS, 91509–900, Brazil*
‡*Universidad Nacional de San Luis, Departamento de Matemáticas, San Luis, Argentina*

adrian.pastine.tag@gmail.com, emilio.allem@ufrgs.br, lgmolina@unsl.edu.ar

(Received October 31, 2018)

Abstract

In this paper, we consider the Randić energy RE of simple connected graphs. We provide upper bounds for RE in terms of the number of vertices and the nullity of the graph. We present families of graphs that satisfy the Conjecture proposed by Gutman, Furtula and Bozkurt [9] about the maximal RE. For example, we show that starlikes of odd order satisfy the conjecture.

1 Introduction

The problem of finding the graphs with maximal and minimal energy has been extensively studied for several matrices. For the Adjacency matrix, Gutman [8] proved the following.

Theorem 1.1. *Let T be a tree on n vertices. Then*

$$E(S_n) \leq E(T) \leq E(P_n).$$

Where P_n and S_n stand for the n-vertex path and the n-vertex star. Radenković and Gutman [13] conjecturated the following about the Laplacian energy.

Conjecture 1. *Let T be a tree on n vertices. Then*

$$LE(P_n) \leq LE(T) \leq LE(S_n).$$

Fritscher et al. [7] proved that among the trees the star has maximal Laplacian energy. The problem of minimal Laplacian energy is still open.

In the paper of Gutman, Furtula and Bozkurt [9] on the energy of the Randić matrix, the authors conjecture that the graphs called sun, denoted by S^p, and double sun, denoted by $DS^{p,q}$, (see the definitions in the next section) have the largest Randić energy depending on the parity of n. More precisely they stated the following conjecture.

Conjecture 2. *Let G be a connected graph on n vertices. Then*

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

In this article we present bounds for the Randić energy. And some families of graphs that satisfy the conjecture above.

Let $G = (V, E)$ be an undirected graph with vertex set V and edge set E. The Randić matrix $R = [r_{ij}]$ of a graph G is defined [1,6,9] as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_u d_v}} & \text{if } uv \in E \\ 0 & \text{otherwise} \end{cases}$$

Denote the eigenvalues of R by $\lambda_1, \ldots, \lambda_n$. The multiset $\sigma_R = \{\lambda_1, \ldots, \lambda_n\}$ will be called the R-spectrum of the graph G.

The Randić energy $RE(G)$ of a graph G is

$$\sum_{i=1}^{n} |\lambda_i|.$$

Historically, the RE is related to a descriptor for molecular graphs used by Milan Randić in 1975 [14]. The normalized Laplacian matrix, defined by Chung [4], can be written using the Randić matrix as

$$\mathcal{L} = I_n - R.$$

And the eigenvalues of $\mathcal{L}$ are given by

$$\mu_i = 1 - \lambda_i$$

for $i = 1 \ldots n$. For graphs without isolated vertices Cavers [3] defined the normalized Laplacian energy as

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\mu_i - 1|.$$

An interesting fact about $E_{\mathcal{L}}(G)$, see [9], is that if G does not have isolated vertices then

$$RE(G) = E_{\mathcal{L}}(G).$$

Thus, results in this paper on Randić energy apply also to normalized Laplacian energy.

This paper is organized as follows. In Section 2, we present closed formulas for the Randić energy of the sun and the double sun. In Section 3, we use some known eigenvalues to provide upper bounds for RE in terms of the number of vertices and the nullity of the graph. In Section 4, we use bounds for the Randić index $R_{-1}(G)$ to improve bounds for RE. In Section 5, we show that some families of graphs, for example starlikes of odd order, satisfy the conjecture proposed in [9].

2 Randić energy of sun and double sun

In the work of Gutman, Furtula and Bozkurt [9] on the energy of the Randić matrix, two families of trees were defined, sun and double sun. For each $p \geq 0$, the *p-sun*, which we denote with S^p, is the tree of order $n = 2p+1$ formed by taking the star on $p+1$ vertices and subdividing each edge.

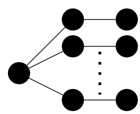

Figure 1. Sun S^p.

For $p, q \geq 0$ the *(p, q)-double sun*, denoted $D^{p,q}$, is the tree of order $n = 2(p + q + 1)$ obtained by connecting the centers of S^p and S^q with an edge. Without loss of generality we assume $p \geq q$. When $p - q \leq 1$ the double sun is called *balanced*.

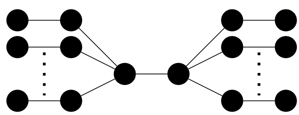

Figure 2. Double Sun $D^{p,q}$.

In [9] was conjectured that the connected graph with maximal Randić energy is a tree. More specifically, if $n \geq 1$ is odd, the sun is conjectured to have greatest Randić energy among graphs with n vertices. And, if $n \geq 2$ is even, then the balanced double sun is conjectured to have greatest Randić energy among graphs with n vertices.

Using the algorithm developed in [2], for locating eigenvalues in trees for the normalized Laplacian matrix, we can compute the characteristic polynomials of the sun and the balanced double sun.

The characteristic polynomial of the sun with $p \geq 1$ is:

$$\det(\lambda I - \mathcal{L}) = (-1)(\lambda - (\frac{2+\sqrt{2}}{2}))^{p-1}(\lambda - (\frac{2-\sqrt{2}}{2}))^{p-1}(\lambda)(\lambda-2)(\lambda-1).$$

It follows that

$$E_{\mathcal{L}}(S^p) = \sum_{i=1}^{n} |\lambda_i(l) - 1| = 2(p-1)\frac{\sqrt{2}}{2} + 2 = (n-3)\frac{\sqrt{2}}{2} + 2.$$

Suppose that $p \geq q$ and $p+q \geq 2$. Then, the characteristic polynomial of $D^{p,q}$ is:

$$\det(\lambda I - \mathcal{L}) = \lambda(\lambda-2)(\lambda - (\frac{2+\sqrt{2}}{2}))^{p+q-2}(x - (\frac{2-\sqrt{2}}{2}))^{p+q-2}(q(\lambda))$$

with

$$q(\lambda) = \lambda^4 - 4\lambda^3 + \frac{1}{4}\frac{(22p+20qp+22q+20)}{(q+1)(p+1)}\lambda^2 + \frac{1}{4}\frac{(-12p-8qp-12q-8)}{(q+1)(p+1)} + \frac{1}{4}\frac{(1+2p+2q)}{(q+1)(p+1)}.$$

It is known that the graph G is bipartite if and only if for each normalized laplacian eigenvalue λ, the value $2-\lambda$ is also an eigenvalue of G. Using this fact, we can write $q(\lambda)$ as

$$q(\lambda) = (\lambda - \lambda_a)(\lambda - \lambda_b)(\lambda - (2-\lambda_a))(\lambda - (2-\lambda_b))$$

with $\lambda_a \leq \lambda_b$. Now, we can compute the energy of the balanced double sun in both cases as follows:

If $p = q$ then

$$E_{\mathcal{L}}(D^{p,p}) = \frac{\sqrt{2}(n^2-4n-12) + 4\sqrt{n^2+4n+20}}{2(n+2)}.$$

If $q = p-1$ then

$$E_{\mathcal{L}}(D^{p,p-1}) = \frac{\sqrt{2}}{2n(n+4)}(n^3 - 2n^2 - 24 + 2\sqrt{n(n+4)(n^2+8+\sqrt{-64n+n^4+64})} + 2\sqrt{n(n+4)(n^2+8-\sqrt{-64n+n^4+64})}).$$

Now, we can rewrite the Conjecture 2 for the Randić energy using closed formulas.

Conjecture 3. *Let G be a connected graph on n vertices. Then for $k \geq 3$ odd we have that*

$$RE(G) \leq \begin{cases} RE(S^p) = E_{\mathcal{L}}(S^p) & \text{if } n = k \\ RE(DS^{p,p}) = E_{\mathcal{L}}(D^{p,p-1}) & \text{if } n = 2k \\ RE(DS^{p,p-1}) = E_{\mathcal{L}}(D^{p,p-1}) & \text{if } n = 2k+2 \end{cases}$$

3 Upper bounds for *RE*

In this section, we present upper bounds for RE in terms of the number of vertices and the nullity of G. The main tool we use to study the Randić energy of graphs is the trace of R^2, taking advantage of the eigenvalues we know for G.

The next Theorem is the generalized mean inequality that will be used in the results following it.

Theorem 3.1. *If $x_1, \ldots, x_n$ are nonnegative real numbers, p and q are positive integers, and $p < q$, then*

$$\left(\frac{1}{n}\sum_{i=1}^{n} x_i^p\right)^{1/p} \leq \left(\frac{1}{n}\sum_{i=1}^{n} x_i^q\right)^{1/q}$$

The next Lemma can also be found in [3]. But for completeness we present a proof here.

Lemma 3.2. *Let G be a graph of order n with no isolated vertices. Then*

$$RE(G) \leq \sqrt{n\, tr(R^2)}.$$

Proof: Applying Theorem 3.1 with $p = 1$, $q = 2$, $x_i = |\lambda_i|$ yields

$$\begin{aligned}
\frac{1}{n}\sum_{i=1}^{n} |\lambda_i| &\leq \left(\frac{1}{n}\sum_{i=1}^{n} |\lambda_i|^2\right)^{1/2} \\
\sum_{i=1}^{n} |\lambda_i| &\leq n\frac{1}{\sqrt{n}}\left(\sum_{i=1}^{n} |\lambda_i|^2\right)^{1/2} \\
\sum_{i=1}^{n} |\lambda_i| &\leq \sqrt{n}\left(\sum_{i=1}^{n} |\lambda_i|^2\right)^{1/2}.
\end{aligned}$$

And the last inequality is exactly $RE(G) \leq \sqrt{n\, tr(R^2)}$. ■

Notice that Lemma 3.2 can be improved when some of the eigenvalues for R are known. Consider Ψ a sub-multiset of σ_R and denote the multiset difference by $\sigma_R \setminus \Psi$.

Theorem 3.3. *Let G be a graph, and let Ψ be a sub-multiset of σ_R. Then*

$$RE(G) \leq \sqrt{(n - |\Psi|)\left(tr(R^2) - \sum_{\lambda\in\Psi}\lambda^2\right)} + \sum_{\lambda\in\Psi}|\lambda|.$$

Proof: Notice that

$$RE(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{\lambda\in\sigma_R\setminus\Psi} |\lambda| + \sum_{\lambda\in\Psi}|\lambda|.$$

Applying Theorem 3.1 to the elements of $\sigma_R \setminus \Psi$ yields

$$\frac{1}{|\sigma_R \setminus \Psi|} \sum_{\lambda \in \sigma_R \setminus \Psi} |\lambda| \leq \left(\frac{1}{|\sigma_R \setminus \Psi|} \sum_{\lambda \in \sigma_R \setminus \Psi} (|\lambda|)^2 \right)^{1/2}$$

$$\sum_{\lambda \in \sigma_R \setminus \Psi} |\lambda| \leq \left(|\sigma_R \setminus \Psi| \sum_{\lambda \in \sigma_R \setminus \Psi} (\lambda)^2 \right)^{1/2}.$$

But $|\sigma_R \setminus \Psi| = n - |\Psi|$, and $\sum_{\lambda \in \sigma_R \setminus \Psi} (\lambda)^2 = tr(R^2) - \sum_{\lambda \in \Psi} \lambda^2$. Thus

$$\sum_{\lambda \in \sigma_R \setminus \Psi} |\lambda| \leq \left((n - |\Psi|) \left(tr(R^2) - \sum_{\lambda \in \Psi} \lambda^2 \right) \right)^{1/2}.$$

Hence

$$RE(G) \leq \sqrt{(n - |\Psi|) \left(tr(R^2) - \sum_{\lambda \in \Psi} \lambda^2 \right)} + \sum_{\lambda \in \Psi} |\lambda|.$$

We can apply Theorem 3.3 to graphs in general, using that 1 is an eigenvalues of R for every graph G, and using that -1 is an eigenvalue whenever the graph is bipartite. Furthermore, we can use the dimension of the null space, denoted by $null(R)$, as that counts the multiplicity of 0 as an eigenvalue. Notice that $\sum_{\lambda \in \Psi} \lambda^2 = \sum_{\lambda \in \Psi} |\lambda| = 1$ in the general case, and $\sum_{\lambda \in \Psi} \lambda^2 = \sum_{\lambda \in \Psi} |\lambda| = 2$ in the bipartite case. Hence, we obtain the following.

Corollary 3.4. *If G is a graph, then*

$$RE(G) \leq \sqrt{(n - 1 - null(R))(tr(R^2) - 1)} + 1.$$

Furthermore, if G is bipartite, then

$$RE(G) \leq \sqrt{(n - 2 - null(R))(tr(R^2) - 2)} + 2.$$

Corollary 3.4 will be our main tool to obtain an upper bound on $RE(G)$ in the following sections.

4 Upper bounds using $R_{-1}(G)$

The randić index of G, denoted by $R_{-1}(G)$, satisfies the equality

$$R_{-1}(G) = \frac{1}{2}\, tr(R^2).$$

Hence, any upper bound of $R_{-1}(G)$ may yield an upper bound for $RE(G)$.

In the next Theorem we summarize some upper bounds for $R_{-1}(G)$.

Theorem 4.1. *In [3], Cavers et al. showed that if G is a connected graph on $n \geq 3$ vertices. Then*

$$R_{-1}(G) \leq \frac{15(n+1)}{56}.$$

In [5], Clark and Moon proved that if T is a tree, then

$$R_{-1}(T) \leq \frac{5n+8}{18}.$$

In [10, 12], they proved that if T is a tree of order $n \geq 103$, then

$$R_{-1}(T) \leq \frac{15n-1}{56}.$$

Applying Corollary 3.4 together with Theorem 4.1 yields

Corollary 4.2. *Let G be a graph, then*

$$RE(G) \leq \sqrt{(n-1-\mathit{null}(R))\frac{15n-13}{28}} + 1.$$

Let G be a bipartite graph, then

$$RE(G) \leq \sqrt{(n-2-\mathit{null}(R))\frac{15n-41}{28}} + 2.$$

Let T be a tree, then

$$RE(T) \leq \sqrt{(n-2-\mathit{null}(R))\frac{5n-10}{9}} + 2.$$

Let T be a tree of order $n \geq 103$, then

$$RE(T) \leq \sqrt{(n-2-\mathit{null}(R))\frac{15n-57}{28}} + 2.$$

It is known that trees of odd order have nullity at least one. If we consider $\mathit{null}(R) = 0$ for trees of even order and $\mathit{null}(R) = 1$ for trees of odd order in Corollary 4.2 we obtain the following result.

Corollary 4.3. *Let T be a tree of even order $n \geq 2$, then*

$$RE(T) \leq \sqrt{(n-2)\frac{5n-10}{9}} + 2. \tag{1}$$

Let T be a tree of odd order $n \geq 2$, then

$$RE(T) \leq \sqrt{(n-3)\frac{5n-10}{9}} + 2. \tag{2}$$

Let T be a tree of even order $n \geq 103$, then

$$RE(T) \leq \sqrt{(n-2)\frac{15n-57}{28}} + 2. \tag{3}$$

Let T be a tree of odd order $n \geq 103$, then

$$RE(T) \leq \sqrt{(n-3)\frac{15n-57}{28}} + 2. \tag{4}$$

In [6] the following bound for the energy of trees was found.

Theorem 4.4. *[6] Let T be a tree of order n, then*

$$RE(T) \leq 2\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \frac{5n+8}{18}}. \tag{5}$$

With a simple calculation we can compare the bounds in Corollary 4.3 and Theorem 4.4. If n is even we use $\lfloor n/2 \rfloor = n/2$. Then (1) $<$ (5) if $n \geq 3$ and (1) $=$ (5) if $n = 2$. If n is odd we use $\lfloor n/2 \rfloor = (n-1)/2$. Then (2) $<$ (5) if $n \geq 3$.

Corollary 4.2 also suggests that if $null(R)$ is sufficiently large, then $RE(G) \leq (n-3)\frac{\sqrt{2}}{2} + 2$. The following theorem gives a lower bound for the nullity that yields the inequality.

Theorem 4.5. *If $null(R) \geq \dfrac{n^2 + 56n - 141 - 28(n-3)\sqrt{2}}{15n-13}$, then $RE(G) \leq (n-3)\frac{\sqrt{2}}{2} + 2$.*

Proof: If G is a graph, then writing Corollary 3.4 in terms of $R_{-1}(G)$ yields

$$RE(G) \leq \sqrt{n-1-null(R)}\sqrt{2R_{-1}(G)-1} + 1.$$

Using Theorem 4.1,

$$\begin{aligned} RE(G) \leq& \sqrt{n-1-null(R)}\sqrt{\frac{15(n+1)}{28} - 1} + 1 \\ =& \sqrt{n-1-null(R)}\sqrt{\frac{15n-13}{28}} + 1. \end{aligned}$$

Thus, we want

$$\sqrt{n-1-null(R)}\sqrt{\frac{15n-13}{28}} + 1 \leq (n-3)\frac{\sqrt{2}}{2} + 2,$$

$$\begin{aligned}
(n-1-\mathit{null}(R))\frac{15n-13}{28} &\le ((n-3)\frac{\sqrt{2}}{2}+1)^2,\\
(n-1-\mathit{null}(R))\frac{15n-13}{28} &\le (n^2-6n+9)\frac{1}{2}+(n-3)\sqrt{2}+1,\\
(n-1-\mathit{null}(R))(15n-13) &\le 14n^2-84n+126+28(n-3)\sqrt{2}+28,\\
(n-1-\mathit{null}(R)) &\le \frac{14n^2-84n+154+28(n-3)\sqrt{2}}{15n-13}.
\end{aligned}$$

Hence,

$$\begin{aligned}
-\mathit{null}(R) &\le \frac{14n^2-84n+154+28(n-3)\sqrt{2}}{15n-13}-n+1,\\
\mathit{null}(R) &\ge -\frac{14n^2-84n+154+28(n-3)\sqrt{2}}{15n-13}+n-1,\\
\mathit{null}(R) &\ge \frac{15n^2-13n-15n+13-14n^2+84n-154-28(n-3)\sqrt{2}}{15n-13},\\
\mathit{null}(R) &\ge \frac{n^2+56n-141-28(n-3)\sqrt{2}}{15n-13}.
\end{aligned}$$

■

In the case of trees, using $R_{-1}(G) \le (15n-1)/56$ and the fact that ± 1 are eigenvalues, Theorem 4.5 can be improved to show that $\mathit{null}(T) \ge \frac{n^2-3n-12}{15n-57}$ implies $RE(T) \le (n-3)\frac{\sqrt{2}}{2}+2$.

A *suspended path* is a path uvw, with $d_u = 1$ and $d_v = 2$, i.e. u is a pendent vertex and its neighbor has degree 2. The next result improves the bound on $R_{-1}(G)$ when G has no suspended paths.

Theorem 4.6. *[3] Let G be a connected graph on $n \ge 3$ vertices. If G has no suspended paths, then*

$$R_{-1}(G) \le \frac{n}{4}$$

If G is bipartite, then we can use that ± 1 are eigenvalues of R, and, hence, 1 is an eigenvalue of multiplicity 2 of R^2 to obtain the following.

Theorem 4.7. *Let G be a connected bipartite graph on $n \ge 3$ vertices. If G has no suspended paths, then*

$$RE(G) \le \sqrt{n-2}\sqrt{n-4}\frac{\sqrt{2}}{2}+2.$$

Notice that $\sqrt{n-2}\sqrt{n-4} = \sqrt{n^2-6n+8} < \sqrt{n^2-6n+9} = (n-3)$. Therefore, if $n = 2p+1$ is odd and G is a connected bipartite graph on $n \ge 3$ vertices that has no suspended paths, then $RE(G) \le RE(S^p)$.

When G is not bipartite, it is better to look at a result using $null(R)$.

Theorem 4.8. *Let G be a connected graph on $n \geq 3$ vertices. If G has no suspended paths, then*

$$RE(G) \leq \sqrt{n-1-null(R)}\sqrt{n-2}\frac{\sqrt{2}}{2}+1.$$

Notice in particular that if $null(R) \geq 1$, then

$$\begin{aligned}
\sqrt{n-1-null(R)}\sqrt{n-2}\frac{\sqrt{2}}{2}+1 \leq & \sqrt{n-2}\sqrt{n-2}\frac{\sqrt{2}}{2}+1 \\
= & (n-2)\frac{\sqrt{2}}{2}+1 \\
= & (n-3)\frac{\sqrt{2}}{2}+\frac{\sqrt{2}}{2}+1 \\
< (n-3)\frac{\sqrt{2}}{2}+2. &
\end{aligned}$$

Hence, if $n = 2p+1$ is odd and G is a connected graph on $n \geq 3$ vertices that has no suspended paths, and $null(R) \geq 1$, then $RE(G) < RE(S^p)$.

5 TB graphs

In the previous section we showed how finding good bounds for $tr(R^2)$ yields good bounds for $RE(G)$. In this section we study $tr(R^2)$ for a particular family of bipartite graphs, and use it to show that their randić energy is bounded by the randić energy of the sun graph. The family that we consider is bipartite graphs with bipartition A, B, such that $\deg(b) \leq 2$ for every $b \in B$. We denote this graphs as TB graphs. Notice that the family of TB graphs include many important subfamilies of graphs:

- starlike trees, which are trees with exactly one vertex of degree greater than 2;
- basic trees, see [11], which are trees with a unique maximum independent set of size $\lceil n/2 \rceil$ (the importance of this trees is due to their null space);
- a graph obtained by taking a graph G and replacing each edge $e = \{v_1, v_2\}$ by two edges $e_1 = \{v_1, w_e\}$ and $e_2 = \{v_2, w_e\}$.

The graphs described above satisfy the condition $\deg(b) = 2$ for every $b \in B$. In this section, we give a bound on $tr(R^2)$ for any TB graph. Before doing so, we give a short explanation on how to find $tr(R^2)$ for any bipartite graph. Let G be a bipartite graph. As G is bipartite, the underlying graph of R^2 has two connected components.

Consider a bipartite graph G with $V(G) = A \cup B$. Let R be the Randić matrix of G indexed first with the vertices in A and then in B. As there are no edges between vertices in A and no edges between vertices in B, R is a block anti-diagonal matrix. I.e., R is of the form

$$R = \begin{bmatrix} 0 & C \\ C^t & 0 \end{bmatrix},$$

where C is a $|A| \times |B|$ matrix. Then

$$R^2 = \begin{bmatrix} R_A^2 & 0 \\ 0 & R_B^2 \end{bmatrix}$$

with $R_A^2 = CC^t$ and $R_B^2 = C^tC$. It follows that $tr(R_A^2) = tr(R_B^2)$, and $tr(R^2) = 2tr(R_A^2) = 2tr(R_B^2)$. There is actually a big difference between vertices of degree 1 and vertices of degree 2 in B, hence we partition B into $B_1 = \{b \in B \mid \deg(b) = 1\}$ and $B_2 = \{b \in B \mid \deg(b) = 2\}$.

Lemma 5.1. *Let G be a connected TB graph with $|G| \geq 3$. Then for every $a \in A$,*

$$\frac{1}{2} \leq R_{a,a}^2 \leq \frac{1}{2} + \frac{1}{4}|N(a) \cap B_1|,$$

where $N(a)$ is the neighborhood of a.

Proof: If $\deg(a) \geq 2$, then

$$\begin{aligned}
R_{a,a}^2 &= \sum_{b \in N(a)} \frac{1}{\deg(b)\deg(a)} \\
&= \sum_{b \in N(a) \cap B_1} \frac{1}{\deg(a)} + \sum_{b \in N(a) \cap B_2} \frac{1}{2\deg(a)} \\
&= \sum_{b \in N(a) \cap B_1} \frac{2}{2\deg(a)} + \sum_{b \in N(a) \cap B_2} \frac{1}{2\deg(a)} \\
&= \sum_{b \in N(a) \cap B_1} \frac{1}{2\deg(a)} + \sum_{b \in N(a) \cap B_1} \frac{1}{2\deg(a)} + \sum_{b \in N(a) \cap B_2} \frac{1}{2\deg(a)} \\
&= \sum_{b \in N(a) \cap B_1} \frac{1}{2\deg(a)} + \sum_{b \in N(a)} \frac{1}{2\deg(a)} \\
&= |N(a) \cap B_1| \frac{1}{2\deg(a)} + \deg(a)\frac{1}{2\deg(a)} \\
&= |N(a) \cap B_1| \frac{1}{2\deg(a)} + \frac{1}{2},
\end{aligned}$$

thus

$$\frac{1}{2} \leq R^2_{a,a} \leq |N(a) \cap B_1|\frac{1}{4} + \frac{1}{2},$$

where the second inequality follows from $\deg(a) \geq 2$.

If $\deg(a) = 1$, let b be the only neighbor of a,

$$\begin{aligned} R^2_{a,a} =& \frac{1}{\deg(b)} \\ =& \frac{1}{2} \\ =& |N(a) \cap B_1|\frac{1}{4} + \frac{1}{2}, \end{aligned}$$

because $\deg(b) = 2$, as G is a connected TB graph with at least 3 vertices. ■

Notice that if G is a TB graph, then $E(G) = |B_1| + 2|B_2|$. As G is connected, $E(G) \geq n - 1 = |A| + |B_1| + |B_2| - 1$. Thus $2|B_2| \geq |A| + |B_2| - 1$, or $|A| \leq |B_2| + 1$. We can now bound the trace.

Lemma 5.2. *Let G be a connected TB graph with $|G| \geq 3$. Then $tr(R^2_A) \leq \frac{n+1}{4}$.*

Proof:

$$tr(R^2_A) = \sum_{a \in A} R^2_{a,a} \leq \sum_{a \in A} \left(\frac{1}{2} + \frac{1}{4}|N(a) \cap B_1|\right)$$

but as the vertices in B_1 have degree 1, they each appear in exactly one $N(a) \cap B_1$. Hence

$$\sum_{a \in A} \frac{1}{4}|N(a) \cap B_1| = \sum_{b \in B_1} \frac{1}{4} = \frac{|B_1|}{4}.$$

Then

$$\begin{aligned} tr(R^2_A) \leq& \sum_{a \in A} \left(\frac{1}{2}\right) + \frac{1}{4}|B_1| \\ \leq& \frac{2|A|}{4} + \frac{1}{4}|B_1| \\ \leq& \frac{|A| + |B_2| + 1}{4} + \frac{1}{4}|B_1| \\ \leq& \frac{|A| + |B_2| + 1 + |B_1|}{4} \\ \leq& \frac{n+1}{4}. \end{aligned}$$

■

As a TB graph is bipartite, $tr(R^2) = 2\, tr(R^2_A)$.

Lemma 5.3. *Let G be a connected TB graph, then $tr(R^2) \leq \frac{n+1}{2}$.*

Lemma 5.4. *Let G be a bipartite graph. If $tr(R^2) \leq \frac{n+1}{2}$, then*

$$RE(G) \leq \sqrt{n-2-null(R)}\sqrt{n-3}\frac{\sqrt{2}}{2}+2.$$

Proof: As G is bipartite, Corollary 3.4 yields

$$RE(G) \leq \sqrt{(n-2-null(R))\, tr(R^2-2)}+2.$$

But $tr(R^2)-2 \leq \frac{n+1}{2}-2 = \frac{n-3}{2}$. Thus

$$RE(G) \leq \sqrt{n-2-null(R)}\sqrt{n-3}\frac{\sqrt{2}}{2}+2.$$

■

We can now combine Lemma 5.3 with Lemma 5.4 to obtain the following.

Theorem 5.5. *Let G be a connected TB graph. Then*

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

Even more, if $null(R) \geq 1$, then

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

Notice that bipartite graphs with an odd number of vertices have $null(R) \geq 1$. This shows that the randić energy of TB graphs of odd order is less or equal than the randić energy of the sun graph of that same order.

Acknowledgments: This work was supported by MATHAmSud, grant 18-MATH-01. L. E. Allem thanks CAPES for the support of the MATHAmSud project. G. Molina and A. Pastine acknowledge the support of the Universidad Nacional de San Luis, grant PROICO 03-0918.

References

[1] Ş. Burcu Bozkurt, A. Dilek Güngör, I. Gutman, A. Sinan Çevik, Randić matrix and Randić energy, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 239–250.

[2] R. O. Braga, R. R. Del–Vecchio, V. M. Rodrigues, V. Trevisan, Trees with 4 or 5 distinct normalized Laplacian eigenvalues, *Lin. Algebra Appl.* **471** (2015) 615–635.

[3] M. Cavers, S. Fallat, S. Kirkland, On the normalized Laplacian energy and general Randić index R_{-1} of graphs, *Lin. Algebra Appl.* **433** (2010) 172-–190.

[4] F. R. K. Chung, *Spectral Graph Theory*, AMS, Providence, 1997.

[5] L. H. Clark, J. W. Moon, On the general Randić index for certain families of trees, *Ars Comb.* **54** (2000) 223-–235.

[6] K. C. Das, S. Sorgun, K. Xu, On Randić energy of graphs, in: I. Gutman, X. Li (Eds.), *Energies of Graphs – Theory and Applications*, Univ. Kragujevac, Kragujevac, 2016, pp. 111–122.

[7] E. Fritscher, C. Hoppen, I. Rocha, V. Trevisan, On the sum of the Laplacian eigenvalues of a tree, *Lin. Algebra Appl.* **435** (2011) 371–399.

[8] I. Gutman, Acyclic systems with extremal Hückel π-eletron energy, *Theor. Chim. Acta (Berl)* **45** (1977) 79–87.

[9] I. Gutman, B. Furtula, S. B. Bozkurt, On Randić energy, *Lin. Algebra Appl.* **442** (2014) 50–57.

[10] Y. Hu, X. Li, Y. Yuan, Solutions to two unsolved questions on the best upper bound for the Randić index R_{-1} of trees, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 441–454.

[11] D. A. Jaume, G. Molina, R. Sota, S-trees, *Preprint available as arXiv:1709.03865.*

[12] L. Pavlović, M. Stojanović, X. Li, More on "Solutions to two unsolved questions on the best upper bound for the Randić index R_{-1} of trees", *MATCH Commun. Math. Comput. Chem.* **58** (2007) 117–192.

[13] S. Radenković, I. Gutman, Total π-electron energy and Laplacian energy: How far the analogy goes? *J. Serb. Chem. Soc.* **72** (2007) 1343–1350.

[14] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.