MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **89** (2023) 467–477
ISSN: 0340–6253
doi: 10.46793/match.89-2.467R

A Note on Energy and Sombor Energy of Graphs

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(Received July 24, 2022)

Abstract

For a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$ and degree sequence $(d_{v_1}, d_{v_2}, \ldots, d_{v_n})$, the adjacency matrix $A(G)$ of G is a $(0, 1)$ square matrix of order n with ij-th entry 1, if v_i is adjacent to v_j and 0, otherwise. The Sombor matrix $S(G) = (s_{ij})$ is a square matrix of order n, where $s_{ij} = \sqrt{d_{v_i}^2 + d_{v_j}^2}$, whenever v_i is adjacent to v_j, and 0, otherwise. The sum of the absolute values of the eigenvalues of $A(G)$ is the energy, while the sum of the absolute eigenvalues of $S(G)$ is the Sombor energy of G. In this note, we provide counter examples to the upper bound of Theorem 18 in [13] and Theorem 1 in [16].

1 Introduction

We consider only simple, finite and undirected graphs. A graph $G(V, E)$ (shortly G) consists of vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set E of unordered pairs of vertices. The cardinality of V is the order n and that of E is the size m of G. The *degree* of a vertex v in G is the number of edges incident with v and is denoted by d_v. A vertex is said to be pendent (pendent edge), if it has degree one. We follow the standard terminology,

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K_n, $K_{a,b}$, and $S_n \cong K_{1,n-1}$, respectively, denote the compete graph, the complete bipartite graph, the star graph. For other undefined notations, we follow [1].

The adjacency matrix of G is a real symmetric matrix, defined by

$$A(G) = (a_{ij})_{n\times n} = \begin{cases} 1 & \text{if } v_i \sim v_j \\ 0 & \text{otherwise} \end{cases},$$

where $\sim$ represents the adjacency relation of vertices v_i and v_j.

The set of all eigenvalues of $A(G)$ is known as the *adjacency spectrum* (spectrum) of G and are indexed from largest to smallest as:

$$\lambda_1(A(G)) \geq \lambda_2(A(G)) \geq \cdots \geq \lambda_{n-1}(A(G)) \geq \lambda_n(A(G)),$$

where $\lambda_1(A(G))$ is the knows as the *spectral radius* of G. In addition for a connected graph, the Perron Frobenius theorem says that $\lambda_1(A(G))$ is unique and its associated eigenvector has positive components. Also, it is easy to see that $\lambda_1^2(A(G)) + \lambda_2^2(A(G)) + \cdots + \lambda_n^2(A(G)) = 2m$. From now onwards, we simply write λ_i instead of $\lambda_i(A(G))$. The absolute sum of the eigenvalues of $A(G)$ is known as the energy [8] of G, that is

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

The energy $\mathcal{E}(G)$ has its origin in theoretical chemistry and it helps in approximating the π-electron energy of unsaturated hydrocarbons. There is a wealthy literature about the energy and its related topics, see [3, 6, 13, 14].

The Sombor matrix of G is defined by

$$S(G) = (s_{ij})_{n\times n} = \begin{cases} \sqrt{d_u^2 + d_v^2} & \text{if } u \sim v \\ 0 & \text{otherwise.} \end{cases}$$

We denote the eigenvalues of $S(G)$ by μ_i's and order them as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. The multiset of all eigenvalues of $S(G)$ is known as the *Sombor* *spectrum* of $S(G)$ and μ_1 is the *Sombor spectral radius* of G. The Sombor energy [11, 15] of G, is defined by

$$\mathcal{E}_{SO}(G) = \sum_{i=1}^{n} |\mu_i|.$$

The square sum of the eigenvalues of $S(G)$ satisfies (see, [15])

$$\mu_1^2 + \mu_2^2 + \cdots + \mu_n^2 = 2F,$$

where $F = F(G) = \sum_{i=1}^{n} d_{v_i}^3 = \sum_{v_i \sim v_j} (d_{v_i}^2 + d_{v_j}^2)$ is the forgotten topological index of G. Various paper on spectral properties of Sombor matrix, like properties of Sombor eigenvalues, Sombor spectral radius, Sombor energy, Sombor Estrada index, relation of energy with Sombor energy and Sombor index and others can be found in [7, 11, 15, 16, 18].

The Sombor matrix has its origin from the recently introduced topological index called known as Sombor index [9], denoted by $SO(G)$, defined as

$$SO(G) = \sum_{v_i \sim v_j} \sqrt{d_{v_i}^2 + d_{v_j}^2}.$$

Several interesting properties of $SO(G)$ can be seen in [2, 4, 5, 17] and the references cited therein.

In the next section, we give some examples of graph classes whose actual energy (Sombor energy) exceed the upper bound of Theorem 18, in [13] (Theorem 1 in [16]).

2 Modified Sombor energy of graphs

The upper bound (1) on the energy of G was given in [13]. For some graphs, like the complete graph, the complete bipartite graph, the complete multipartite complete graphs and some other small graphs, the upper bound (1) is true. While in general, the result fails and the proof of Theorem 1 [13] violates the monotonic property of the function considered there. Here, we state the result of [13].

Theorem 1 (Theorem 18, [13])**.** *Let G be a non-empty graph with n vertices, m edges and degree sequence $d_{v_1} \geq d_{v_2} \geq \cdots \geq d_{v_n}$. Then*

$$\mathcal{E}(G) \leq \sqrt{\frac{2m(n-1)}{n}}. \tag{1}$$

Equality holds if and only if $G \cong K_n$.

Following the similar technique as in the proof of Theorem 18 of [13], the authors in [16] gave the upper bound (2) for the Sombor energy of G. Next, The result is stated and like Theorem 1, it is not valid.

Theorem 2 (Theorem 1, [16])**.** *Let G be a graph of order n with forgotten topological index F. Then*

$$\mathcal{E}_{SO}(G) \leq 2\sqrt{\frac{2F(n-1)}{n}}, \tag{2}$$

equality occurs if and only if $G \cong K_n$.

The brief outline of the proof of Theorem 1 (Theorem 18 [13]) is given below:
By using Cauchy-Schwartz inequality, and $\sum\limits_{i=1}^{n} \lambda_i^2 = 2m$, we have

$$\sum_{i=2}^{n} |\mu_i| \leq \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^2} = \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) = \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \leq \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Note that the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{1}{2n}} \leq x \leq \sqrt{2m}$. By Lemma 1 [13], $\lambda_1 \leq \sqrt{\frac{2m(n-1)}{n}}$. Clearly, $\sqrt{\frac{2m(n-1)}{n}} \leq \sqrt{2m}$. Thereby,

$$\lambda_1 \leq \sqrt{\frac{2m(n-1)}{n}} \leq \sqrt{2m}.$$

So $F(\lambda_1) \leq F\left(\sqrt{\frac{2m(n-1)}{n}}\right)$, which implies that

$$\begin{aligned} \mathcal{E}(G) \leq & \sqrt{\frac{2m(n-1)}{n}} + \sqrt{(n-1)\left(2m - \left(\sqrt{\frac{2m(n-1)}{n}}\right)^2\right)} \\ = & 2\sqrt{\frac{2m(n-1)}{n}}. \end{aligned} \tag{3}$$

The following are the defects of proof.

- $F(x)$ decreases for x in $\left[\sqrt{\frac{1}{2n}}, \sqrt{2m}\right]$ and $F(\lambda_1) \leq F\left(\sqrt{\frac{2m(n-1)}{n}}\right)$ must be $F(\lambda_1) \geq F\left(\sqrt{\frac{2m(n-1)}{n}}\right)$, that is, it must be used for lower bound rather than the upper bound of the energy of G.
- For suppose, if $F(\lambda_1) \geq F\left(\sqrt{\frac{2m(n-1)}{n}}\right)$ is used for lower bound for the energy, that lower bound may or may not hold, since in the beginning of proof, we use Cauchy-Schwartz inequality for establishing the upper bound for the energy of G.
- Thus, in this way, any lower bound (not the upper bound) of λ_1 along with Cauchy-Schwartz inequality and $F(x)$ can be used to obtain the upper bound for the energy of G.

Let $a \geq 1$ be a positive integer. The tree Su_a of order $n = 2a + 1$, containing a pendent vertices, each attached to a vertex of degree 2, and a vertex of degree a, will be called the a-sun (see, [10]), see Figure 1. This tree can be viewed as obtained by inserting a new vertex on each edge of the star S_{a+1}. Note that $Su_0 \cong P_1,\ Su_1 \cong P_3,\ Su_2 \cong P_5$ where as for $a \geq 3$, the a-sun is not a path graph.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. The union $G_1 \cup G_2$ of graphs G_1 and G_2 is the graph $G = (V, E)$ for which $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$. The complete product $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph obtained from $G_1 \cup G_2$ by joining every vertex of G_1 with every vertex of G_2. For $a \geq 1,\ b \geq 1$ and $c \geq 1$, the extended complete split type graph $ECS_a^{b,c}$ (see, [12] and Figure 1) is defined by $ECS_a^{b,c} \cong \overline{K}_a \vee \big(K_b \cup K_c\big)$.

For $a = 2,\ b = c = 1$, $ECS_2^{1,1} \cong \overline{K}_2 \vee (K_1 \cup K_1) = K_{2,2}$, otherwise $ECS_a^{b,c}$ is not the complete bipartite graph.

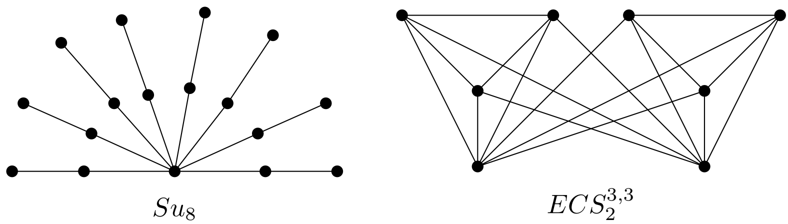

Figure 1. a-sun tree Su_8 and extended complete split type graph $ECS_2^{3,3}$.

Theorem 1 states that the energy of any non-empty graph is at most $2\sqrt{\frac{2m(n-1)}{n}}$, while in reality, the actual value of the energy of majority of graphs is above the bound of (1). Next, we consider two such family of graphs which discards the bound given in (1).

Proposition 3. *For $a \geq 2$, the energy of Su_a is strictly greater than the upper bound* (1) *given in Theorem 1.*

Proof. Let $G \cong Su_a$ be a graph of order $n = 2a + 1$ with size $m = 2a$ and let

$$\{u, u_1, u_2, \ldots, u_{a-1}, u_a, v_1, v_2, \ldots, v_{a-1}, v_a\}$$

be the vertex labelling of G, where u is a vertex of degree a, u_i's are vertices of degree 2 and v_i's are vertices (pendent) of degree 1. Under this labelling, the adjacency matrix of G can be written as:

$$A(G) = \begin{pmatrix} 0 & J_{1\times a} & \mathbf{0}_{1\times a} \\ J_{a\times 1} & \mathbf{0}_{a\times a} & I_{a\times a} \\ \mathbf{0}_{a\times 1} & I_{a\times a} & \mathbf{0}_{a\times a} \end{pmatrix}, \tag{4}$$

where I is the identity matrix, $\mathbf{0}$ is the zero matrix and J is the matrix with all entries equal to one. Choosing

$$X_1^T = \Big(a, \underbrace{\sqrt{a+1}, \sqrt{a+1}, \ldots, \sqrt{a+1}}_{a}, \underbrace{1, 1, \ldots, 1, 1}_{a}\Big),$$

then we have

$$\begin{aligned} A(G)X_1 &= \Big(a\sqrt{a+1}, \underbrace{a+1, a+1, \dots, a+1}_{a}, \underbrace{1, 1, \dots, 1}_{a}\Big) \\ &= \sqrt{a+1}\Big(a, \underbrace{\sqrt{a+1}, \sqrt{a+1}, \dots, \sqrt{a+1}}_{a}, \underbrace{1, 1, \dots, 1}_{a}\Big) \\ &= \sqrt{a+1}X_1. \end{aligned}$$

By Perron Frobenious theorem, $\sqrt{a+1}$ is the spectral radius of (4) with its Perron eigenvector X_1. Proceeding as above, it can be verified that

$$X_2^T = \Big(a, \underbrace{-\sqrt{a+1}, -\sqrt{a+1}, \dots, -\sqrt{a+1}}_{a}, \underbrace{1, 1, \dots, 1}_{a}\Big)$$

is the eigenvector corresponding to the eigenvalue $-\sqrt{a+1}$. Next, for $i = 2, 3, \dots, a$, let

$$Y_{i-1}^T = \Big(0, 1, x_{22}, x_{33}, \dots, x_{(a-1)(a-1)}, x_{aa}, -1, y_{22}, y_{33}, \dots, y_{(a-1)(a-1)}, y_{aa}\Big),$$

where $x_{ij} = \begin{cases} -1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$, and $y_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$. It is easy to see that $Y_1, Y_2, \dots, Y_{a-1}$ are linearly independent vectors. For $Y_1 = \big(0, 1, -1, 0, 0, \dots, 0, -1, 1, 0, 0, \dots, 0\big)$, we have

$$A(G)Y_1 = \Big(1-1, -1, 1, 0, 0, \dots, 0, 1, -1, 0, 0, \dots, 0\Big) = -1Y_1.$$

This implies that Y_1 is the eigenvectors corresponding to the eigenvalues -1 of $A(G)$. In a similar way, $Y_2, Y_3, \dots, Y_{a-1}$ are the eigenvectors corresponding to the eigenvalues -1. Consider

$$Z_{i-1}^T = \Big(0, -1, x'_{22}, x'_{33}, \dots, x'_{(a-1)(a-1)}, x'_{aa}, -1, y'_{22}, \dots, y'_{(a-1)(a-1)}, y'_{aa}\Big),$$

where $x'_{ij} = \begin{cases} -1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$, and $y'_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$. Again, it is easy to verify that $Z_1, Z_2, \dots, Z_{a-1}$ are the eigenvectors corresponding to the eigenvalues 1. Finally, for $X = \big(-1, \underbrace{0, 0, \ldots, 0}_{a}, \underbrace{1, 1, \ldots, 1}_{a} \big)$, we have

$$A(G)X = \Big(0, 1-1, 1-1, \ldots, 1-1, 0, 0, \ldots, 0\Big) = 0Y_1.$$

Therefore the spectrum of G is

$$\Big\{ \pm\sqrt{a+1}, 0, (-1)^{[a-1]}, 1^{[a-1]} \Big\}.$$

Now, the energy of G is

$$\mathcal{E}(G) = 2\sqrt{a+1} + 2(a-1).$$

Finally, comparing energy of G with (1) with $n = 2a+1$ and $m = 2a$, we have

$$2\sqrt{\frac{2a(2a+1-1)}{2a+1}} < 2\sqrt{a+1} + 2(a-1),$$

which further gives

$$\frac{2a^3 - 5a^2 + 3a + 2}{2a+1} + 2(a-1)\sqrt{a+1} > 0.$$

Simplifying above expression, we get

$$4a^4 - 36a^3 + 37a^2 + 6a - 7 > 0 \tag{5}$$

Inequality (5) holds for $a \geq 8$. For $a = 2, 3, 4, 5, 6, 7$, the following tables gives the energy of G and the values of bound (1) of Theorem 1.

G	Su_2	Su_3	Su_4	Su_5	Su_6	Su_7
$\mathcal{E}(G)$	5.4641	8	10.4721	12.899	15.2915	17.6569
Thm. 1	5.05964	6.41427	7.54247	8.52803	9.41357	10.2242

Table 1. Energy of Su_a, for $a = 2, 3, 4, 5, 6, 7$ and the approximate values of the upper bound (1) of Theorem 1.

Thus from Table 1 and Inequality 5, it follows that the energy of $Su_a, a \geq 2$ is always greater than the upper bound (1) given in Theorem 1. ∎

Next, we consider another family of graphs for which Theorem 1 is not valid.

Proposition 4. *For $a \geq 2$, the energy of $ECS_2^{a,a} \cong \overline{K}_2 \vee \left(K_a \cup K_a\right)$ is strictly greater than the upper bound* (1) *of Theorem 1.*

Proof. Let $G \cong ECS_2^{a,a}$ be a graph of order $n = 2a + 2$ and size $m = a^2+3a$ and let $\{u_1, u_2, v_1, v_2, \dots, v_a, v_{a+1}, v_{a+2}, \dots, v_{2a}\}$ be the vertex labelling of G, where $d_{u_1} = d_{u_2} = 2a,\ d_{v_i} = a+1,\ i = 1, 2, \dots, 2a$. Under this vertex indexing, the adjacency matrix of G is

$$A(G) = \begin{pmatrix} \mathbf{0}_{2\times 2} & J_{2\times a} & J_{2\times a} \\ J_{a\times 2} & B_{a\times a} & \mathbf{0}_{a\times a} \\ J_{a\times 2} & \mathbf{0}_{a\times a} & B_{a\times a} \end{pmatrix},$$

where $B = J_{a\times a} - I_{a\times a}$. It is not hard to show that the spectrum of $A(G)$ is

$$\left\{0, (-1)^{[2a-2]}, a-1, \frac{1}{2}\left(a - 1 \pm \sqrt{a^2 + 14a + 1}\right)\right\},$$

and its energy is

$$\mathcal{E}(G) = 3(a-1) + \sqrt{a^2 + 14a + 1}.$$

Now, by comparing the energy of G, with the upper bound (1), we obtain the following inequality

$$4\left(2a^6 + 37a^5 - 31a^4 - 82a^3 + 23a^2 + 39a - 4\right) > 0,$$

which is always true for $a \geq 2$. Thus the energy of $ECS_2^{a,a}$ exceeds the upper bound (1) given by Theorem 1. ■

Proceeding as in Proposition 3 and 4, the proof of the following results can be worked out similarly.

Proposition 5. *For $a \geq 2$, the Sombor energy of Su_a is strictly greater than the upper bound* (2) *given in Theorem 2.*

Proposition 6. *For $a \geq 2$, the Sombor energy of $ECS_2^{a,a} \cong \overline{K}_2 \vee \left(K_a \cup K_a\right)$ is strictly greater than the upper bound* (2) *of Theorem 2.*

Hence, in this note, both Theorem 18 of [13] and Theorem 1 of [16] are not valid.

***Acknowledgment*:** The authors are very thankful to the referees for their valuable comments and input to improve the paper. This research is supported by the UPAR Grant of the United Arab Emirates University (UAEU), UAE, via Grant No. G00003739.

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