Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2023.252770.1707
Vol. 14, No. 4, 2023, pp. 225–241
Research Paper

Quantization of Sombor Energy for Complete Graphs with Self-Loops of Large Size

Johnny Lim[1⋆], Zheng Kiat Chew[1], Macco Zhi Pei Lim[1] and Kai Jie Thoo[1]

[1]School of Mathematical Sciences, Universiti Sains Malaysia, Malaysia

Keywords:
Euclidean metric,
Sombor energy,
Sombor spectrum,
Graphs with self-loops

AMS Subject Classification (2020):

05C50; 05C90

Article History:

Received: 8 April 2023

Accepted: 13 August 2023

Abstract

A self-loop graph G_S is a simple graph G obtained by attaching loops at $S \subseteq V(G)$. To such G_S an Euclidean metric function is assigned to its vertices, forming the so-called Sombor matrix. In this paper, we derive two summation formulas for the spectrum of the Sombor matrix associated with G_S, for which a Forgotten-like index arises. We explicitly study the Sombor energy $\mathcal{E}_{SO}$ of complete graphs with self-loops $(K_n)_S$, as the sum of the absolute value of the difference of its Sombor eigenvalues and an averaged trace. The behavior of this energy and its change for a large number of vertices n and loops σ is then studied. Surprisingly, the constant $4\sqrt{2}$ is obtained repeatedly in several scenarios, yielding a quantization of the energy change of 1 loop for large n and σ. Finally, we provide a McClelland-type and determinantal-type upper and lower bounds for $\mathcal{E}_{SO}(G_S)$, which generalizes several bounds in the literature.

1 Introduction

Let $G = (V(G), E(G))$ be a simple undirected graph where $V(G)$ is the set of vertices of G and $E(G)$ is the set of edges of G. If $|V(G)| = n$ and $|E(G)| = m$, we call G as a graph of order n and size m. Let $V(G) = \{v_1, \ldots, v_n\}$. For $i = 1, 2, \ldots, n$, denote by d_{v_i} the degree of v_i. The adjacency matrix $A(G) = (a_{ij})$ associated to G is a matrix whose entry is $a_{ij} = 1$ if v_i and v_j are adjacent ($v_i \sim v_j$) and $a_{ij} = 0$ otherwise. Since $A(G)$ is a real symmetric matrix, all eigenvalues $\lambda_i(G)$ of G are real and can be ordered as $\lambda_1(G) \geq \ldots \geq \lambda_n(G)$, where $\lambda_1(G)$ and $\lambda_n(G)$ are the largest and the smallest eigenvalues of G, respectively. We denote the spectrum of graph G as the multiset

$$\mathrm{Spec}(G) = \begin{bmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_k \\ a_1 & a_2 & \ldots & a_k \end{bmatrix}, \tag{1}$$

*Corresponding author
E-mail addresses: johnny.lim@usm.my (J. Lim), zhengkiat.chew@gmail.com (Z. K. Chew), lzp.macco@gmail.com (M. Z. P. Lim), kjthoo@gmail.com (K. J. Thoo)
Academic Editor: Gholam Hossein Fath-Tabar

where a_i is the algebraic multiplicity of λ_i. Then, the *energy* [1] of graph G is defined by

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i(G)|. \tag{2}$$

In general, if M is a real symmetric matrix associated to G of order n with eigenvalues $\lambda_1(M) \geq \ldots \geq \lambda_n(M)$, then the M-*energy* [2] of G can be defined to be

$$\mathcal{E}_M(G) = \sum_{i=1}^{n} \left| \lambda_i(M) - \frac{\mathrm{Tr}(M)}{n} \right|, \tag{3}$$

where $\mathrm{Tr}(M)$ is the trace of M. The M-energy allows us to consider a variety of energies associated with certain matrices.

Let $S \subseteq V(G)$ with $|S| = \sigma$. A self-loop graph G_S over S is obtained from G by attaching a self-loop at each vertex in S. In the case where $\sigma = 0$ or *no loop*, G_S is the simple graph G. In the case of $\sigma = n$ or *full loops*, that is, there is a self-loop at every vertex of G, we write $\widehat{G}$. The adjacency matrix of G_S is $A(G_S) = J_S + A(G)$, where $(J_S)_{i,j} = 1$ if $i = j$ and $v_i \in S$, and $(J_S)_{i,j} = 0$ otherwise. Thus, the eigenvalues of G_S are the eigenvalues of $A(G_S)$. The energy [3] of G_S of order n with $|S| = \sigma$ is defined by

$$\mathcal{E}(G_S) = \sum_{i=1}^{n} \left| \lambda_i(G_S) - \frac{\sigma}{n} \right|.$$

For more details on the energy of self-loop graphs, readers are referred to some recent works [3–5].

Recently in 2021, Gutman [6] has introduced a new vertex-degree-based topological index called *Sombor index* $SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$, for which each summand corresponds to an Euclidean metric function associated to a pair of adjacent vertices in G. The *Sombor matrix* $S(G)$ of G is the matrix associated with $SO(G)$, and is explicitly given by $S(G) = (s_{ij})$ whose entry is $s_{ij} = \sqrt{d_{v_i}^2 + d_{v_j}^2}$ if v_i is adjacent to v_j, $i \neq j$, and $s_{ij} = 0$ otherwise. To distinguish the eigenvalues of the associated adjacency matrix and Sombor matrix, we denote them by λ_i and μ_i, respectively. Since $S(G)$ is also real symmetric, the eigenvalues are real and can be ordered as $\mu_1 \geq \mu_2 \ldots \geq \mu_n$. Thus, we write the *Sombor spectrum* of G as

$$\mathrm{SSpec}(G) = \begin{bmatrix} \mu_1 & \mu_2 & \ldots & \mu_k \\ a_1 & a_2 & \ldots & a_k \end{bmatrix}.$$

If G_S is a self-loop graph with $S \subseteq V(G)$, then its associated Sombor matrix is denoted by $S(G_S)$. More precisely, let $\hat{d}_{v_i}$ be the degree of v_i in G_S given by

$$\hat{d}_{v_i} = \begin{cases} d_{v_i} + 2, & \text{if } v_i \in S, \\ d_{v_i}, & \text{if } v_i \notin S, \end{cases}$$

where d_{v_i} is the degree of v_i in G. Then, the Sombor matrix $S(G_S)$ is given by $S(G_S) = (\hat{s}_{ij})$ whose entry is

$$\hat{s}_{ij} = \begin{cases} \sqrt{\hat{d}_{v_i}^2 + \hat{d}_{v_j}^2}, & \text{if } v_i \sim v_j, \\ 0, & \text{otherwise.} \end{cases}$$

Note that this definition allows the possibility of $i = j$. Alternatively, we can rewrite $S(G_S) = \widetilde{S}(G_S) + D_S$ where $\widetilde{S}(G_S) = (\tilde{s}_{ij})$ and

$$\tilde{s}_{ij} = \begin{cases} \sqrt{\hat{d}_{v_i}^2 + \hat{d}_{v_j}^2}, & \text{if } v_i \sim v_j \text{ and } i \neq j, \\ 0, & \text{otherwise,} \end{cases}$$

and $D_S = (\delta_{ij})$ where $\delta_{ii} = \sqrt{2}\hat{d}_{v_i}$ for $v_i \in S$, and $\delta_{ij} = 0$ for $i \neq j$. The Sombor eigenvalues of G_S are the eigenvalues of $S(G_S)$, which will still be denoted as $\mu_i(G_S)$. Using (3), the *Sombor energy* $S(G_S)$ *of a self-loop graph* G_S is defined by

$$\mathcal{E}_{SO}(G_S) = \sum_{i=1}^{n} \left| \mu_i(G_S) - \frac{\text{Tr}(S(G_S))}{n} \right|. \tag{4}$$

In Section 2, we derive the explicit summation formula of μ_i and μ_i^2 of G_S, respectively, which will be crucial ingredients throughout. A term that is closely related to the well-known Forgotten index $F(G)$ arises in the formula. This relation will be described by a difference formula. In Section 3, we review the Sombor spectrum of (simple) complete graphs K_n via a simpler and direct approach. They serve as the "base case" throughout. Then, we provide a description of Sombor spectrum and energy for edgeless graphs with self-loops $(\overline{K}_n)_S$ and complete graphs with self-loops $(K_n)_S$.

In Section 4, we study the behaviour of the Sombor energy $\mathcal{E}_{SO}((K_n)_S)$ with respect to n and σ. It is surprising that $\mathcal{E}_{SO}((K_n)_S)$ behaves 'tamely' despite a convoluted formula. Moreover, we compute the energy difference of 1 loop explicitly in several cases, all of which are converging to a constant $4\sqrt{2}$ for large n and σ. Lastly, in Section 5, we prove a McClelland-type bound and determinantal-type upper and lower bounds for $\mathcal{E}_{SO}(G_S)$, for which we recover several known bounds for $\mathcal{E}_{SO}(G)$ in [6–8].

2 Some identities of Sombor eigenvalues for self-loop graphs

In the following, we first derive the summation formula by using

$$\sum \mu_i^r(G_S) := \text{Tr}(S(G_S)^r), \quad \text{for } r = 1, 2. \tag{5}$$

By the definition of $S(G_S)$, one can no longer interpret $\sum \mu_i^r$ as the *number of closed walks of length* r, unlike the case of adjacency matrix, cf. [9, Lemma 2.5 & Result 2h]. Despite this, (5) still makes sense: since $S(G_S)$ is real and symmetric, by (real) Schur's Triangularization Theorem [10, Theorem 10.1.1], there exists an orthogonal U such that $S(G_S) = U\Lambda U^T$ where Λ is real upper-triangular with diagonal entries $\mu_i(G_S)$. Then, (5) follows from polynomial functional calculus and the trace commutation property.

Lemma 2.1. *Let* G_S *be a self-loop graph of order* n. *Let* $\mu_i(G_S)$, *for* $i = 1, ..., n$, *be the Sombor eigenvalues of* G_S. *Then,*

(i) $\displaystyle\sum_{i=1}^{n} \mu_i(G_S) = \sqrt{2} \sum_{v_i \in S} \hat{d}_{v_i}$,

(ii) $\displaystyle\sum_{i=1}^{n} \mu_i^2(G_S) = 2\widetilde{F}(G_S) + \sum_{v_i \in S} 2\hat{d}_{v_i}^2$, *where* $\displaystyle\widetilde{F}(G_S) = \frac{1}{2} \sum_{i=1}^{n} \sum_{\substack{v_i \sim v_j \\ i \neq j}} (\hat{d}_{v_i}^2 + \hat{d}_{v_j}^2)$.

Proof. Part (i) follows from

$$\sum_{i=1}^{n}\mu_i(G_S)=\mathrm{Tr}(S(G_S))=\sum_{v_i\in S}\sqrt{\hat{d}_{v_i}^2+\hat{d}_{v_i}^2}=\sum_{v_i\in S}\sqrt{2\hat{d}_{v_i}^2}=\sqrt{2}\sum_{v_i\in S}\hat{d}_{v_i}.$$

For part (ii), let $S(G_S)=\widetilde{S}(G_S)+D_S$. Then, by (5), we have

$$\sum_{i=1}^{n}\mu_i^2(G_S)=\sum_{i=1}^{n}\left[(\widetilde{S}(G_S)+D_S)^2\right]_{ii}=\sum_{i=1}^{n}\left[\widetilde{S}(G_S)^2+\widetilde{S}(G_S)D_S+D_S\widetilde{S}(G_S)+D_S^2\right]_{ii}. \quad (6)$$

One verifies that $\sum_{i=1}^{n}\left[\widetilde{S}(G_S)D_S\right]_{ii}=\sum_{i=1}^{n}\left[D_S\widetilde{S}(G_S)\right]_{ii}=0$. By the definition of D_S,

$$[D_S^2]_{ij}=\begin{cases}2\hat{d}_{v_i}^2, & \text{if } i=j \text{ and } v_i\in S,\\ 0, & \text{otherwise.}\end{cases}$$

So, $\sum_{i=1}^{n}\left[D_S^2\right]_{ii}=\sum_{v_i\in S}2\hat{d}_{v_i}^2$. On the other hand,

$$\sum_{i=1}^{n}\left[\widetilde{S}(G_S)^2\right]_{ii}=\sum_{i=1}^{n}\sum_{\substack{v_i\sim v_j\\ i\neq j}}(\hat{d}_{v_i}^2+\hat{d}_{v_j}^2).$$

Thus, (6) reduces to

$$\sum_{i=1}^{n}\mu_i^2(G_S)=\sum_{i=1}^{n}\sum_{\substack{v_i\sim v_j\\ i\neq j}}(\hat{d}_{v_i}^2+\hat{d}_{v_j}^2)+\sum_{v_i\in S}2\hat{d}_{v_i}^2. \quad (7)$$

■

From [6, Lemma 1], it is known that for any simple graph G,

$$\sum_{i=1}^{n}\mu_i^2(G)=2F(G),$$

where $F(G)$ is the Forgotten topological index of G. One observes that when $\sigma=0$, $\widetilde{F}(G_S)=F(G)$ and the second summand of (7) vanishes. Thus, we shall call $\widetilde{F}(G_S)$ the *Forgotten-like index* of G_S. In fact, upon further investigation, we establish an explicit difference formula that depends only on the degrees of vertices with self-loops deleted.

Lemma 2.2. *Let G be a graph of order n. Let $W\subseteq S\subseteq V(G)$. Then,*

$$\widetilde{F}(G_W)-\widetilde{F}(G_{W\setminus\{v_0\}})=4d_{v_0}(d_{v_0}+1), \quad (8)$$

where v_0 is any element of W. Consequently,

$$\widetilde{F}(G_S)=F(G)+\sum_{v\in S}4d_v(d_v+1). \quad (9)$$

Proof. Let $v_0 \in W$. Since $\hat{d}^2_{v_0} = (d_{v_0} + 2)^2$, we have $\hat{d}^2_{v_0} - d^2_{v_0} = 4(d_{v_0} + 1)$. This is the difference in degree when a loop at v_0 is deleted from G_W. Since there are a total of d_{v_0} edges that incident with v_0, by symmetry and by Lemma 2.1,

$$\widetilde{F}(G_W) - \widetilde{F}(G_{W\setminus\{v_0\}}) = \frac{1}{2}\left(2\left(\sum_{\substack{v_i \sim v_0 \\ v_i \neq v_0}} (\hat{d}^2_{v_i} + \hat{d}^2_{v_0}) - \sum_{\substack{v_i \sim v_0 \\ v_i \neq v_0}} (\hat{d}^2_{v_i} + d^2_{v_0})\right)\right)$$
$$= \frac{1}{2}(8d_{v_0}(d_{v_0} + 1)) = 4d_{v_0}(d_{v_0} + 1).$$

The second equation (9) follows immediately by induction on the number of vertices with deleted loops. ■

3 Sombor spectrum and energy of complete graphs with self-loops

When $\sigma = 0$, $(K_n)_S$ is the ordinary complete graph K_n. We shall call this the *base case* in what follows. Recently, Ghanbari [11] has studied the Sombor spectrum and Sombor energy of K_n, which heavily uses Sombor characteristic polynomials. Here, we give an alternate treatment for the base case without characteristic polynomials. Before that, let us state two useful lemmas.

Lemma 3.1. *([10, (3.4.7)]). If A is a non-singular square matrix, then*

$$\det\left(\begin{bmatrix} A & B \\ C & D \end{bmatrix}\right) = \det(A)\det(D - CA^{-1}B).$$

Lemma 3.2. *([10, Lemma 8.3.2]). Let A be an $n \times n$ matrix with eigenvalues $\lambda_1, ..., \lambda_n$. Then,*

(i) For $m \in \mathbb{N}$, the eigenvalues of A^m are $\lambda_1^m, ..., \lambda_n^m$.

(ii) For $k \in \mathbb{R}$, the eigenvalues of kA are $k\lambda_1, ..., k\lambda_n$.

(iii) For $k \in \mathbb{R}$, the eigenvalues of $A + kI$ are $\lambda_1 + k, ..., \lambda_n + k$.

Theorem 3.3. *For natural number $n \geq 2$, let K_n be the complete graph of order n.*

(i) Let $A(K_n)$ and $S(K_n)$ be the adjacency matrix and Sombor matrix of K_n, respectively. Then, we have

$$S(K_n) = \sqrt{2}(n-1)A(K_n).$$

(ii) The Sombor spectrum of K_n is

$$\mathrm{SSpec}(K_n) = \begin{bmatrix} \sqrt{2}(n-1)^2 & -\sqrt{2}(n-1) \\ 1 & n-1 \end{bmatrix}. \quad (10)$$

(iii) The Sombor energy of K_n is $\mathcal{E}_{SO}(K_n) = 2\sqrt{2}(n-1)^2$.

Proof. The Sombor matrix of K_n is an $n \times n$ matrix of the form

$$S(K_n) = \begin{bmatrix} 0 & \sqrt{2}(n-1) & \cdots & \sqrt{2}(n-1) \\ \sqrt{2}(n-1) & 0 & \cdots & \sqrt{2}(n-1) \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{2}(n-1) & \sqrt{2}(n-1) & \cdots & 0 \end{bmatrix},$$

where the entries are all $\sqrt{2}(n-1)$ except the diagonal. Thus, $S(K_n) = \sqrt{2}(n-1)A(K_n)$. Recall that the ordinary spectrum of K_n is given by $\begin{bmatrix} n-1 & -1 \\ 1 & n-1 \end{bmatrix}$. By Lemma 3.2, the Sombor spectrum of K_n is

$$\begin{bmatrix} \sqrt{2}(n-1)^2 & -\sqrt{2}(n-1) \\ 1 & n-1 \end{bmatrix}.$$

It follows from (2) that the Sombor energy of K_n is $2\sqrt{2}(n-1)^2$. ■

Theorem 3.4. *Let $\left(\overline{K}_n\right)_S$ be the edgeless graph with self-loops of order n. Let $|S| = \sigma$ with $0 \leq \sigma \leq n$. Then,*

$$\mathcal{E}_{SO}((\overline{K}_n)_S) = 4\sqrt{2}\sigma\left(1 - \frac{\sigma}{n}\right). \tag{11}$$

Moreover, $\mathcal{E}_{SO}((\overline{K}_n)_S)$ is maximum when $\sigma = \frac{1}{2}n$ for even n, and $\sigma = \frac{1}{2}(n \pm 1)$ for odd n.

Proof. Let $S((\overline{K}_n)_S) = \mathrm{Diag}(a_1, a_2, ..., a_n)$ be the Sombor matrix of $(\overline{K}_n)_S$, where $a_1 = a_2 = \cdots = a_\sigma = 2\sqrt{2}$ and the remaining $a_i = 0$. Since the eigenvalues of a diagonal matrix are the diagonal entries, thus the eigenvalues of $S((\overline{K}_n)_S)$ are $2\sqrt{2}$ and 0 with multiplicities of σ and $n-\sigma$, respectively. Thus, $\mathcal{E}_{SO}((\overline{K}_n)_S) = 4\sqrt{2}\sigma\left(1 - \frac{\sigma}{n}\right)$. Since the Sombor energy is a quadratic polynomial in σ for fixed n, by elementary analysis, one finds that $\mathcal{E}_{SO}((\overline{K}_n)_S)$ is maximum when $\sigma = \frac{1}{2}n$ for even n and $\sigma = \frac{1}{2}(n \pm 1)$ for odd n. ■

Theorem 3.5. *Let $(K_n)_S$ be the self-loop graph of K_n. Let $|S| = \sigma$ with $0 \leq \sigma \leq n$ and $n \geq 2$. Then, $\mathrm{SSpec}((K_n)_S)$ are characterized in the following three cases.*

(i) For $\sigma = 0$,

$$\mathrm{SSpec}((K_n)_S) = \begin{bmatrix} \sqrt{2}(n-1)^2 & -\sqrt{2}(n-1) \\ 1 & n-1 \end{bmatrix}, \text{ and } \mathcal{E}_{SO}(K_n)_S = 2\sqrt{2}(n-1)^2.$$

(ii) For $\sigma = n$,

$$\mathrm{SSpec}((K_n)_S) = \begin{bmatrix} \sqrt{2}n(n+1) & 0 \\ 1 & n-1 \end{bmatrix}, \text{ and } \mathcal{E}_{SO}(K_n)_S = 2\sqrt{2}(n+1)(n-1).$$

(iii) For $0 < \sigma < n$,

$$\mathrm{SSpec}((K_n)_S) = \begin{bmatrix} \frac{k_1}{2} + \frac{1}{2}\sqrt{2k_3 - k_1^2 - 2k_2} & 0 & -\sqrt{2}(n-1) & \frac{k_1}{2} - \frac{1}{2}\sqrt{2k_3 - k_1^2 - 2k_2} \\ 1 & \sigma - 1 & n-\sigma-1 & 1 \end{bmatrix},$$

where

– $k_1 = \sqrt{2}(\sigma(n+1) + (n-1)(n-\sigma-1))$,

– $k_2 = (n-\sigma-1)(2(n-1)^2)$,
– $k_3 = 2\sigma^2(n+1)^2 + 2\sigma(n-\sigma)((n+1)^2+(n-1)^2) + 2((n-\sigma)^2-(n-\sigma))(n-1)^2$.

Moreover, the explicit Sombor energy of $(K_n)_S$ is given by

$$\begin{aligned}\mathcal{E}_{SO}(K_n)_S = \frac{1}{\sqrt{2}}\Bigg(& 2\sigma(\sigma-1)(1+\frac{1}{n})\\ &+\left|1+n(n-2)-\frac{2\sigma}{n}-\sqrt{(n-1)^4+8n^2\sigma-4\sigma^2}\right|\\ &+\left|1+n(n-2)-\frac{2\sigma}{n}+\sqrt{(n-1)^4+8n^2\sigma-4\sigma^2}\right|\\ &+2(n-\sigma-1)\left|n+\sigma+\frac{\sigma}{n}-1\right|\Bigg).\end{aligned} \tag{12}$$

Proof. The base case (i) is essentially Theorem 3.3. For (ii), when $\sigma = n$, for all vertices v_i, $\hat{d}_{v_i} = n+1$. Since $S((K_n)_S) = \left[\sqrt{2}(n+1)\right]_{n\times n} = \sqrt{2}(n+1)J_n$ where J_n is a $n\times n$ matrix whose all entries are 1, and the spectrum of J_n is $\begin{bmatrix} n & 0 \\ 1 & n-1\end{bmatrix}$. By Lemma 3.2, we have

$$\mathrm{SSpec}((K_n)_S) = \begin{bmatrix}\sqrt{2}n(n+1) & 0\\ 1 & n-1\end{bmatrix}.$$

By Lemma 2.1 and (4), the Sombor energy can be computed to be

$$\begin{aligned}\mathcal{E}_{SO}((K_n)_S) &= \left|\sqrt{2}n(n+1) - \frac{\sqrt{2}n(n+1)}{n}\right| + (n-1)\left|-\frac{\sqrt{2}n(n+1)}{n}\right|\\ &= 2\sqrt{2}(n+1)(n-1).\end{aligned}$$

Lastly, we will prove (iii) when $0<\sigma<n$. Note that $\hat{d}_{v_i} = n+1$ when $v_i \in S$ and $\hat{d}_{v_i} = n-1$ when $v_i \notin S$. Thus, we have an explicit Sombor matrix

$$S((K_n)_S) = \left[\begin{array}{c|c}(S_1)_{\sigma\times\sigma} & (S_2)_{\sigma\times(n-\sigma)}\\ \hline (S_2^T)_{(n-\sigma)\times\sigma} & (S_3)_{(n-\sigma)\times(n-\sigma)}\end{array}\right] = \left[\begin{array}{c} B\\ \hline C\end{array}\right],$$

where entries of $(S_1)_{\sigma\times\sigma}$ are all $\sqrt{2}(n+1)$; entries of $(S_2)_{\sigma\times(n-\sigma)}$ are all $\sqrt{(n+1)^2+(n-1)^2}$; and $(S_3)_{(n-\sigma)\times(n-\sigma)} = \left[\sqrt{2}(n-1)\right]_{(n-\sigma)\times(n-\sigma)} - \sqrt{2}(n-1)I_{n-\sigma}$. First, we determine the nullity $\mathrm{null}(S((K_n)_S))$, which is the multiplicity of eigenvalue 0. Clearly, $\mathrm{rank}(B) = 1$ since all rows in B are identical. Since $(S_3)_{(n-\sigma)\times(n-\sigma)} = \sqrt{2}(n-1)A(K_{n-\sigma})$, and $A(K_{n-\sigma})$ has no zero eigenvalue, this implies that $(S_3)_{(n-\sigma)\times(n-\sigma)}$ also has no zero eigenvalue. Thus, $(S_3)_{(n-\sigma)\times(n-\sigma)}$ is invertible and $\mathrm{rank}(C) = n-\sigma$.

Next, we show that any row in B is linearly independent of all rows of C, which would imply that $\mathrm{rank}(S((K_n)_S)) = n-\sigma+1$. Since all rows above and all columns to the left of S_3 are repeated, it suffices to consider S_3 with a row above and a column on the left. Denote this matrix as A_0. Let $x = \sqrt{2}(n+1), y = \sqrt{(n+1)^2+(n-1)^2}, z = \sqrt{2}(n-1)$. Then, A_0, as a matrix of size $(n-\sigma+1)\times(n-\sigma+1)$ can be written in the following form:

$$A_0 = \left[\begin{array}{c|cccc} x & y & \cdots & & y \\ \hline & 0 & z & \cdots & z \\ y & z & 0 & \cdots & z \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y & z & z & \cdots & 0 \end{array}\right].$$

It suffices to determine the rank of A_0 by showing that the determinant of A_0 is non-zero. By Lemma 3.1,

$$\begin{aligned} \det(A_0) =& \det([x]) \det \left(\begin{bmatrix} 0 & z & \cdots & z \\ z & 0 & \cdots & z \\ \vdots & \vdots & \ddots & \vdots \\ z & z & \cdots & 0 \end{bmatrix} - \begin{bmatrix} y \\ \vdots \\ y \end{bmatrix} [x]^{-1} \begin{bmatrix} y & \cdots & y \end{bmatrix} \right) \\ =& x \det \begin{bmatrix} -\frac{y^2}{x} & z-\frac{y^2}{x} & \cdots & z-\frac{y^2}{x} \\ z-\frac{y^2}{x} & -\frac{y^2}{x} & \cdots & z-\frac{y^2}{x} \\ \vdots & \vdots & \ddots & \vdots \\ z-\frac{y^2}{x} & z-\frac{y^2}{x} & \cdots & -\frac{y^2}{x} \end{bmatrix}. \end{aligned}$$

Let $Q = \begin{bmatrix} -\frac{y^2}{x} & z-\frac{y^2}{x} & \cdots & z-\frac{y^2}{x} \\ z-\frac{y^2}{x} & -\frac{y^2}{x} & \cdots & z-\frac{y^2}{x} \\ \vdots & \vdots & \ddots & \vdots \\ z-\frac{y^2}{x} & z-\frac{y^2}{x} & \cdots & -\frac{y^2}{x} \end{bmatrix}$. Since Q is of size $(n-\sigma) \times (n-\sigma)$, it can be rewritten as $Q = (z - \frac{y^2}{x})A(K_{n-\sigma}) - (\frac{y^2}{x})I_{n-\sigma}$. Then, the spectrum of Q can be obtained by using Lemma 3.2 and the spectrum of $K_{n-\sigma}$:

$$\begin{aligned} \operatorname{Spec}(Q) &= \begin{bmatrix} (z-\frac{y^2}{x})(n-\sigma-1) - \frac{y^2}{x} & -(z-\frac{y^2}{x}) - \frac{y^2}{x} \\ 1 & n-\sigma-1 \end{bmatrix} \\ &= \begin{bmatrix} (n-\sigma-1)z - (n-\sigma)\frac{y^2}{x} & -z \\ 1 & n-\sigma-1 \end{bmatrix}. \end{aligned}$$

Since the determinant of Q is equal to the product of its eigenvalues,

$$\det(Q) = \left((n-\sigma-1)z - (n-\sigma)\frac{y^2}{x} \right) (-z)^{n-\sigma-1},$$

one can verify that $\det(Q) \neq 0$ for our case.

Therefore, $\det(A_0) = x \det(Q) \neq 0$. This implies that A_0 is invertible and $\operatorname{rank}(A_0) = n-\sigma+1$. Thus, any row in B is linearly independent to all rows of C and $\operatorname{rank}(S((K_n)_S)) = n-\sigma+1$. By Rank-Nullity theorem, we conclude that $\operatorname{null}(S((K_n)_S)) = \sigma - 1$.

Next, we consider the matrix $S((K_n)_S) + \sqrt{2}(n-1)I_n$ and determine its nullity, which is the multiplicity of eigenvalue $-\sqrt{2}(n-1)$. We write

$$S((K_n)_S) + \sqrt{2}(n-1)I_n = \left[\begin{array}{c|c} (T_1)_{\sigma\times\sigma} & (T_2)_{\sigma\times(n-\sigma)} \\ \hline (T_2^T)_{(n-\sigma)\times\sigma} & (T_3)_{(n-\sigma)\times(n-\sigma)} \end{array}\right] = \left[\begin{array}{c} D \\ \hline E \end{array}\right],$$

where $(T_1)_{\sigma\times\sigma} = \left[\sqrt{2}(n+1)\right]_{\sigma\times\sigma} + \sqrt{2}(n-1)I_\sigma$; entries of $(T_2)_{\sigma\times(n-\sigma)}$ are all $\sqrt{(n+1)^2+(n-1)^2}$; and entries of $(T_3)_{(n-\sigma)\times(n-\sigma)}$ are all $\sqrt{2}(n-1)$. By a similar argument to the case of $S((K_n)_S)$ above, we get $\operatorname{rank}(E) = 1$ and $\operatorname{rank}(D) = \sigma$. One can also show that all rows in D are linearly independent of any row in E. Thus, we have $\operatorname{rank}(S((K_n)_S)+\sqrt{2}(n-1)I_n) = \sigma+1$ and $\operatorname{null}(S((K_n)_S)+\sqrt{2}(n-1)I_n) = n-\sigma-1$.

Note that there are $n-(\sigma-1)-(n-\sigma-1) = 2$ eigenvalues left to be determined. By Lemma 2.1, we obtain the following equations:

$$\mu_1+\mu_2+(n-\sigma-1)(-\sqrt{2}(n-1)) = \sqrt{2}(\sigma(n+1)), \tag{13}$$

$$\mu_1^2+\mu_2^2+(n-\sigma-1)(2(n-1)^2) = \sum_{i=1}^{n}\sum_{\substack{v_i\sim v_j\\ i\neq j}}(d_{v_i}^2+d_{v_j}^2)+2\sigma(n+1)^2. \tag{14}$$

More precisely, the nested summation terms in (14) can be written explicitly as

$$\begin{aligned}&\mu_1^2+\mu_2^2+(n-\sigma-1)(2(n-1)^2) = \\ &\qquad 2\sigma^2(n+1)^2+2\sigma(n-\sigma)((n+1)^2+(n-1)^2)+2((n-\sigma)^2-(n-\sigma))(n-1)^2.\end{aligned} \tag{15}$$

Now, let $k_1 = \sqrt{2}(\sigma(n+1)+(n-1)(n-\sigma-1))$, $k_2 = (n-\sigma-1)(2(n-1)^2)$ and $k_3 = 2\sigma^2(n+1)^2+2\sigma(n-\sigma)((n+1)^2+(n-1)^2)+2((n-\sigma)^2-(n-\sigma))(n-1)^2$. Then, (13) and (15) can be simplified into:

$$\mu_1+\mu_2 = k_1, \tag{16}$$

$$\mu_1^2+\mu_2^2 = k_3-k_2. \tag{17}$$

Solving (16) and (17), we have

$$\mu_{1,2} = \frac{k_1}{2} \pm \frac{1}{2}\sqrt{2k_3-k_1^2-2k_2}.$$

By applying (4) and with some simplification, we obtain the desired Sombor energy formula. This completes the proof. ∎

4 Behaviour of the Sombor energy of complete graphs with loops

Once the explicit formula for $\mathcal{E}_{SO}(K_n)_S$ is obtained in (12), it is natural to study its behavior, especially on how the energy changes with respect to increasing n and σ. Whilst (12) is complicated to compare in symbolic terms, it is still possible to plot as in Figure 1.

It is surprising to see that $\mathcal{E}_{SO}(K_n)_S$ is 'tamed' and appears to be increasing consistently and almost linearly for large n and σ. This leads us to further investigate the *Sombor energy change* on several occasions.

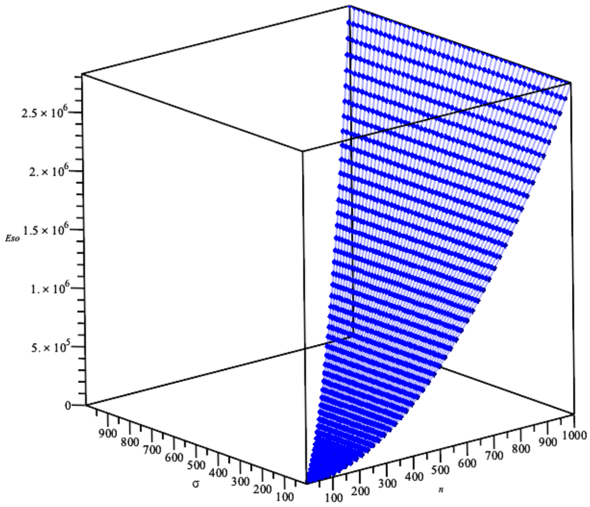

Figure 1: Sombor Energy of $(K_n)_S$ with $n = 2, ..., 1000$ and $\sigma = 1, ..., 999$.

Proposition 4.1. *(i) For $n \geq 2$, the Sombor energy change between complete graphs with 1-loop and no loop is given by*

$$\mathcal{E}_{SO}(K_n)_{|S|=1} - \mathcal{E}_{SO}(K_n) = -\frac{\sqrt{2}(n^3 - 2n^2 + n + 2)}{n}$$
$$+ \left| \frac{-\sqrt{2n^4 - 8n^3 + 28n^2 - 8n - 6}\, n + \sqrt{2}\,(n-2)\left(n^2+1\right)}{2n} \right|$$
$$+ \left| \frac{\sqrt{2n^4 - 8n^3 + 28n^2 - 8n - 6}\, n + \sqrt{2}\,(n-2)\left(n^2+1\right)}{2n} \right|. \tag{18}$$

(ii) For $n \geq 2$, the Sombor energy change between complete graphs with $(n-1)$-loops and full n-loops is given by

$$\mathcal{E}_{SO}(\widehat{K}_n) - \mathcal{E}_{SO}(K_n)_{|S|=n-1} = \frac{\sqrt{2}(n^2-1)(n+2)}{n}$$
$$- \left| \frac{\sqrt{2}\,\sqrt{(n-1)\,(n^3+5n^2-n+3)}\, n + \sqrt{2}\,(n-1)\,(n-2)\,(n+1)}{2n} \right|$$
$$- \left| \frac{-\sqrt{2}\,\sqrt{(n-1)\,(n^3+5n^2-n+3)}\, n + \sqrt{2}\,(n-1)\,(n-2)\,(n+1)}{2n} \right|. \tag{19}$$

When $n \to \infty$,

$$\lim_{n\to\infty} (\mathcal{E}_{SO}(K_n)_{|S|=1} - \mathcal{E}_{SO}(K_n)) = 4\sqrt{2} = \lim_{n\to\infty} (\mathcal{E}_{SO}(\widehat{K}_n) - \mathcal{E}_{SO}(K_n)_{|S|=n-1}). \tag{20}$$

Proposition 4.1 tells us that for sufficiently large n, the energy change due to 1 loop near the boundary cases is consistent and converging to $4\sqrt{2}$. Surprisingly, this phenomenon remains true even for the *non-boundary* cases with the difference of 1 loop!

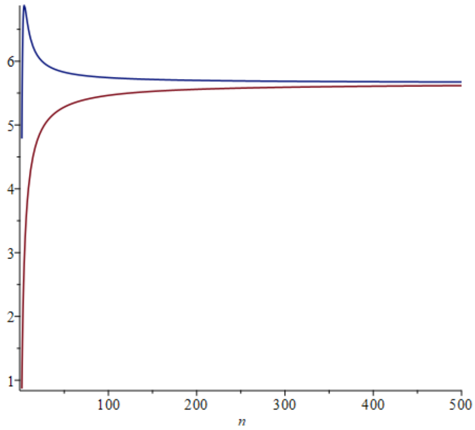

Figure 2: The top curve is $\mathcal{E}_{SO}(K_n)_{|S|=1} - \mathcal{E}_{SO}(K_n)$; The bottom curve is $\mathcal{E}_{SO}(\widehat{K}_n) - \mathcal{E}_{SO}(K_n)_{|S|=n-1}$, both for $n = 2, ..., 500$.

Proposition 4.2. *For $n \geq 2$ and $0 < \sigma < n$, then*

$$\begin{aligned}
&\mathcal{E}_{SO}(K_n)_{|S|=\sigma} - \mathcal{E}_{SO}(K_n)_{|S|=\sigma-1} \\
= \; & -\frac{2\sqrt{2}}{n} + \left|\frac{\sqrt{2}\left(-n^3+2n^2+2\sigma-n\right) - \sqrt{2n^4-8n^3+(16\sigma+12)\,n^2-8n-8\sigma^2+2}\,n}{2n}\right| \\
+ \; & \left|\frac{\sqrt{2}\left(-n^3+2n^2+2\sigma-n\right) + \sqrt{2n^4-8n^3+(16\sigma+12)\,n^2-8n-8\sigma^2+2}\,n}{2n}\right| \\
- \; & \left|\frac{\sqrt{2}\left(-n^3+2n^2+2\sigma-n-2\right) - \sqrt{2n^4-8n^3+(16\sigma-4)\,n^2-8n-8\sigma^2+16\sigma-6}\,n}{2n}\right| \\
- \; & 7\left|\frac{\sqrt{2}\left(-n^3+2n^2+2\sigma-n-2\right) + \sqrt{2n^4-8n^3+(16\sigma-4)\,n^2-8n-8\sigma^2+16\sigma-6}\,n}{2n}\right|.
\end{aligned} \tag{21}$$

Moreover,

$$\lim_{\substack{n\to\infty \\ \sigma\to\infty}} \left(\mathcal{E}_{SO}(K_n)_{|S|=\sigma} - \mathcal{E}_{SO}(K_n)_{|S|=\sigma-1}\right) = 4\sqrt{2}.$$

Example 4.3. For simplicity, if we write $D\mathcal{E}_{SO}(n,\sigma,\sigma-1)$ as $\mathcal{E}_{SO}(K_n)_{|S|=\sigma} - \mathcal{E}_{SO}(K_n)_{|S|=\sigma-1}$, then one can compare the following with $4\sqrt{2} \approx 5.65685$:

$$\begin{aligned}
&D\mathcal{E}_{SO}(100,50,49) \approx 5.60029,\; D\mathcal{E}_{SO}(1000,50,49) \approx 5.66395, \\
&D\mathcal{E}_{SO}(10000,50,49) \approx 5.65769,\; D\mathcal{E}_{SO}(10000,500,499) \approx 5.65120, \\
&D\mathcal{E}_{SO}(10000,5000,4999) \approx 5.65629.
\end{aligned}$$

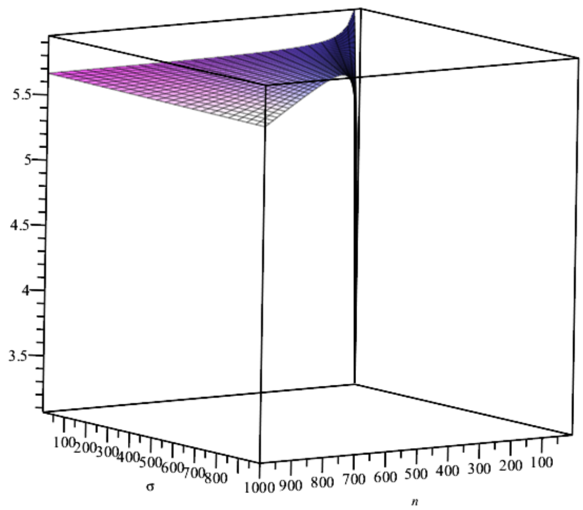

Figure 3: The vertical axis represents $\mathcal{E}_{SO}(K_n)_{|S|=\sigma} - \mathcal{E}_{SO}(K_n)_{|S|=\sigma-1}$ for $n = 2, ..., 1000$ and $\sigma = 1, ..., 999$, which shows a fluctuation for small n and σ but consistent for large n and σ.

5 Bounds for Sombor energy of graphs with loops

5.1 McClelland-type bound for $\mathcal{E}_{SO}(G_S)$

Theorem 5.1. *Let G_S be a self-loop graph of order n. Let $\widetilde{F}(G_S)$ be the Forgotten-like index in (9). Then,*

$$\mathcal{E}_{SO}(G_S) \le \sqrt{2n\left(\widetilde{F}(G_S) + \sum_{v_i \in S} \hat{d}_{v_i}^2 - \frac{1}{n}\left(\sum_{v_i \in S} \hat{d}_{v_i}\right)^2\right)}. \tag{22}$$

The equality holds if and only if (i) $G_S \cong (\overline{K_n})_S$ (edgeless graphs with self-loops) for the boundary cases $\sigma = 0, n$, and the half-loop case $\sigma = \frac{n}{2}$ when n is even; or (ii) $G_S \cong (K_2)_S$ (1-regular graph) with $\sigma = 0, 1, 2$.

Proof. We adopt a similar strategy in [6]. In the following, for simplicity, we write $\mu_i = \mu_i(G_S)$ and $a = \sum_i \mu_i$. Consider

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\left|\mu_i - \frac{a}{n}\right| - \left|\mu_j - \frac{a}{n}\right|\right)^2 \ge 0.$$

This is equivalent to the inequality

$$2n\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2 \ge 2\sum_{i,j=1}^{n}\left|\mu_i - \frac{a}{n}\right|\left|\mu_j - \frac{a}{n}\right|. \tag{23}$$

By direct computation,

$$\sum_{i=1}^{n}\left(\mu_i - \frac{a}{n}\right)^2 = \left(\sum_{i=1}^{n}\mu_i^2\right) - \frac{a^2}{n}. \tag{24}$$

On the other hand, we observe that

$$\mathcal{E}_{SO}^2(G_S) = \left(\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|\right)^2 = \sum_{i,j=1}^{n}\left|\mu_i - \frac{a}{n}\right|\left|\mu_j - \frac{a}{n}\right|.$$

Thus, by Lemma 2.1, equation (23) reduces to the desired inequality

$$2n\widetilde{F}(G_S) + 2n\sum_{v_i\in S}\hat{d}_{v_i}^2 - 2\left(\sum_{v_i\in S}\hat{d}_{v_i}\right)^2 \geq \mathcal{E}_{SO}^2(G_S),$$

and the claim is complete by taking square roots.

The equality holds if and only if $|\mu_1 - \frac{a}{n}| = |\mu_2 - \frac{a}{n}| = \cdots = |\mu_n - \frac{a}{n}|$. Graphs that satisfy this condition are (i) the edgeless graph with certain loops and (ii) the regular graph of degree 1 with all possible loops. More precisely, for (i), by (11), the boundary cases are clear. For $0 < \sigma < n$, it amounts to solve $|n - \sigma| = |\sigma|$, which implies that the equality holds if and only if $\sigma = \frac{n}{2}$ when n is even. For (ii), we apply Theorem 3.5 for all cases below. When $\sigma = 0$, with $\mu_{1,2} = \pm\sqrt{2}$ and $a = 0$, we have $|\mu_1| = |\mu_2|$. When $\sigma = 2$, with $\mu_1 = 6\sqrt{2} = a$, and $\mu_2 = 0$, then $|\mu_1 - a/2| = |\mu_2 - a/2|$. When $\sigma = 1$, the Sombor spectra are $\frac{3}{\sqrt{2}} \pm \sqrt{\frac{29}{2}}$, together with $k_1 = 3\sqrt{2}, k_2 = 0$, and $k_3 = 38$, it follows that the equality holds when $\mathcal{E}_{SO}(K_2)_S = \sqrt{58}$. ■

5.2 Determinantal lower and upper bounds for $\mathcal{E}_{SO}(G_S)$

Lemma 5.2. *([8, Lemma 2.4]). Let $a_1 \geq a_2 \geq \ldots \geq a_n$ be a sequence of non-negative real numbers. Then,*

$$\sum_{i=1}^{n} a_i + n(n-1)\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \leq \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2 \leq (n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}. \tag{25}$$

We will also need the following useful form [7, Lemma 7.2]:

$$n\left(\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2 \leq n(n-1)\left(\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right). \tag{26}$$

Theorem 5.3. *Let G_S be a self-loop graph of order n. Let C be the diagonal matrix with entries $\hat{d}_{v_i}$ if $v_i \in S$ and zero otherwise. Let $a = \sum_i \mu_i$. Then,*

$$\mathcal{E}_{SO}(G_S) \leq \sqrt{n\left(\sum_{i=1}^{n}\mu_i^2\right) - \frac{a^2}{n} - 2n(n-1)\left|\det(C)\right|^{\frac{2}{n}}}, \tag{27}$$

with equality holds if $G_S \cong \widehat{K}_2$.

Proof. By Lemma 5.2, take $a_i = \hat{d}_{v_i}^2$, then we have

$$n\sum_{v_i\in S}\hat{d}_{v_i}^2 - \left(\sum_{v_i\in S}\hat{d}_{v_i}\right)^2 \leq (n-1)\sum_{v_i\in S}\hat{d}_{v_i}^2 - n(n-1)\left(\prod_{v_i\in S}\hat{d}_{v_i}^2\right)^{\frac{1}{n}}.$$

Since $C = \mathrm{Diag}(\hat{d}_{v_i})_{v_i \in S}$ is a diagonal matrix, the determinant of C^2 is the square of the absolute value of the determinant of C. By Cauchy's inequality, $a^2/n \leq 2\sum_{i=1}^{n} \hat{d}_{v_i}^2$. It follows that

$$2n\widetilde{F}(G_S) + 2n \sum_{v_i \in S} \hat{d}_{v_i}^2 - 2\left(\sum_{v_i \in S} \hat{d}_{v_i}\right)^2 \leq n\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n} - 2n(n-1)\left|\det(C)\right|^{\frac{2}{n}}.$$

By Theorem 5.1, we obtain (27). For equality, we apply Theorem 3.5 for $\widehat{K}_2$. Since $\mu_1 = 6\sqrt{2} = a, \mu_2 = 0$, and $\det(C) = \hat{d}_{v_1}\hat{d}_{v_2} = 9$, one verifies that the equality is attainable with both sides of (27) being $6\sqrt{2}$. ■

The next corollary is an immediate consequence when $G_S = G$.

Corollary 5.4. *Let G_S be a self-loop graph of order n. When $\sigma = 0$, both upper bounds (22) and (27) reduces to [6, Theorem 1]:*

$$\mathcal{E}_{SO}(G) \leq \sqrt{2nF(G)}.$$

Theorem 5.5. *Let G_S be a graph with loops of order n. Let $B = S(G_S) - \dfrac{a}{n}I_n$ with $a = \sum_i \mu_i$. Then,*

$$\begin{aligned} \sqrt{\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n} + n(n-1)|\det(B)|^{\frac{2}{n}}} &\leq \mathcal{E}_{SO}(G_S) && (28)\\ &\leq \sqrt{(n-1)\left(\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n}\right) + n|\det(B)|^{\frac{2}{n}}}. \end{aligned}$$

Proof. By taking $a_i = |\mu_i - \frac{a}{n}|^2$ in (26) in Lemma 5.2, on one hand we have

$$n\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2 - \left(\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|\right)^2 \leq (n-1)\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2 - n(n-1)\left(\prod_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2\right)^{\frac{1}{n}}.$$

Notice that the second term of the left side is exactly $\mathcal{E}_{SO}^2(G_S)$. By (24) and since $|\mu_i|^2 = \mu_i^2$, we obtain

$$\begin{aligned} \mathcal{E}_{SO}(G_S) &\geq \sqrt{\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2 + n(n-1)\left(\prod_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2\right)^{\frac{1}{n}}} \\ &= \sqrt{\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n} + n(n-1)\left|\det(B)\right|^{\frac{2}{n}}}. \end{aligned}$$

On the other hand, following a similar approach and by (24) again, we obtain

$$\begin{aligned} \mathcal{E}_{SO}(G_S) &\leq \sqrt{(n-1)\sum_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2 - n\left(\prod_{i=1}^{n}\left|\mu_i - \frac{a}{n}\right|^2\right)^{\frac{1}{n}}} \\ &= \sqrt{(n-1)\left(\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n}\right) - n\left|\det(B)\right|^{\frac{2}{n}}}. \end{aligned}$$

■

Here, we also present an alternate argument for the left side of (28) by adopting a trick of McClelland in [12, §III].

Alternate proof for lower bound of (28). Since $(\sum_{i=1}^{n} |\mu_i - \frac{a}{n}|)^2 = \sum_{i=1}^{n} |\mu_i - \frac{a}{n}|^2 + \sum_{i \neq j} |\mu_i - \frac{a}{n}||\mu_j - \frac{a}{n}|$ with $a = \sum_{i=1}^{n} \mu_i$, by AM-GM inequality,

$$\frac{\sum_{i \neq j} |\mu_i - \frac{a}{n}| \, |\mu_j - \frac{a}{n}|}{n(n-1)} \geq \left(\prod_{i \neq j} \left|\mu_i - \frac{a}{n}\right| \left|\mu_j - \frac{a}{n}\right| \right)^{\frac{1}{n(n-1)}} = \left(\prod_{i=1}^{n} \left|\mu_i - \frac{a}{n}\right| \right)^{\frac{2}{n}} = |\det(B)|^{\frac{2}{n}}.$$

Now, by [12, Theorem 1],

$$\left(\sum_{i=1}^{n} \left|\mu_i - \frac{a}{n}\right| \right)^2 \leq nN^2(B),$$

where $N^2(B) = \sum_{kl} |B_{kl}|^2$ is the square of the Frobenius norm of B. Observe that $N^2(B)$ is the summation of all squares of entries of B, which coincides with the sum of those off-diagonal terms $2\widetilde{F}(G_S)$, those diagonal terms with loops $\sum_{v_i \in S} \left(\sqrt{2}\hat{d}_{v_i} - \frac{a}{n}\right)^2$, and those diagonal terms without loops $(n-\sigma)\frac{a^2}{n^2}$. Thus, by [12, eq (12)],

$$\begin{aligned} \mathcal{E}_{SO}(G_S) &= \sum_{i=1}^{n} \left|\mu_i - \frac{a}{n}\right| \\ &\geq \sqrt{N^2 + n(n-1)|\det(B)|^{\frac{2}{n}}} \\ &= \sqrt{2\widetilde{F}(G_S) + \sum_{v_i \in S} \left(\sqrt{2}\hat{d}_{v_i} - \frac{a}{n}\right)^2 + (n-\sigma)\frac{a^2}{n^2} + n(n-1)|\det(B)|^{\frac{2}{n}}} \\ &= \sqrt{\left(\sum_{i=1}^{n} \mu_i^2\right) - \frac{a^2}{n} + n(n-1)|\det(B)|^{\frac{2}{n}}}. \end{aligned}$$

■

Corollary 5.6. *When* $\sigma = 0$, *that is, when* $G_S = G$, *the inequality* (28) *reduces to*

$$\sqrt{2F(G) + n(n-1)|\det(S(G))|^{\frac{2}{n}}} \leq \mathcal{E}_{SO}(G) \leq \sqrt{2(n-1)F(G) + n|\det(S(G))|^{\frac{2}{n}}}, \qquad (29)$$

which recovers [8, Theorem 4.1] and [7, Theorem 7.3 & 7.6].

6 Significance and further questions

Further remarks:

1. There is a crucial difference between the explicit determination of ordinary and Sombor spectrum (and thus energy) of complete graphs with self-loops. In [5] it was achieved by considering the adjacency matrix associated with G_S, which is *static* with respect to other vertices, i.e. adding or removing a loop does not affect the vertex degrees in its neighborhood. In our case, as a degree-based energy (cf. [13]), the existence of a loop at a vertex will change the vertex degrees in its neighborhood. This dependence results in a more convoluted energy formula.

2. In Section 4, we showed that the Sombor energy of $(K_n)_S$ increases with n and σ. The quantization $4\sqrt{2}$ is obtained for large n or for the large number of edges and σ. We believe this provides new insight into the results in [14], where the ordinary energy of K_n for large n and its various modifications via edge deletions are studied. The upshots of results in Sections 3 and 4 are: (i) they can now be programmed for energy calculation using only n and σ; (ii) for a large fix n and varying σ, only one energy is required as the others can be approximated by a modification by a factor of $4\sqrt{2}$.

3. With the existing role of graphs with loops in the mathematical study of heteroconjugated molecules, as in [15–18], and [6] (and references therein) under the Sombor settings for ordinary graphs, we believe our results have applications in molecular chemistry.

Further open questions:

1. Is there a simpler method or scheme for determining the Sombor spectrum and energy of some families of graphs with loops, such as trees, complete bipartite graphs, cyclic graphs, etc? Is there any quantization of energy similar to that of in Section 4?

2. Is there a novel construction of graphs with loops from simple graphs such that the energy (ordinary, Sombor or variants) does not increase post-construction?

3. What are the effects of edge and loop deletion on energy (ordinary, Sombor or variants) for general graphs with loops?

Conflicts of interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

Acknowledgement: The first author acknowledges the support from the Ministry of Higher Education Malaysia for Fundamental Research Grant Scheme with Project Code: FRGS/1/2021/STG06/USM/02/7. He thanks Prof. Saieed Akbari for introducing him to the topic of self-loop graphs. We thank Dr. Nur Fariha Syaqina Mohd Zulkepli, Dr. Siti Amirah Abd Rahman and Sho Yun Peng for their helpful software and coding assistance. We also thank the referees' valuable feedback that improves the presentation of this paper.

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