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On Stress Sum Eigenvalues and Stress Sum Energy of Graphs

C. Nalina, P. Siva Kota Reddy, M. Kirankumar and M. Pavithra

ABSTRACT: In this article, we introduce the stress sum matrix $SSM(G)$ for a graph G, which is related to the stress sum index. We explore the properties of this matrix, establish bounds on its eigenvalues, and define the stress sum energy $\mathcal{E}_{SS}(G)$ as the sum of the absolute eigenvalues. Additionally, we discuss its potential chemical relevance by comparing $\mathcal{E}_{SS}(G)$ with the π-electron energy of polyaromatic hydrocarbons.

Key Words: Graph, Stress of a vertex, Energy, Stress Sum Eigenvalues, Stress Sum Energy.

Contents

1. Introduction

In this article, we will be focusing on finite, unweighted, simple, and undirected graphs. Let $G = (V, E)$ denote a graph. The degree of a vertex v in G is denoted by $d(v)$. The distance between two vertices u and v in G, denoted $d(u, v)$, is the number of edges in the shortest path (or geodesic) connecting them. A geodesic path P is said to pass through a vertex v if v is an internal vertex of P, meaning v lies on P but is not an endpoint of P. For standard terminology and notion in graph theory, we follow the text-book of Harary [8].

Gutman [6] defined the energy of a graph G as the sum of the absolute values of its eigenvalues, denoted by $\mathcal{E}(G)$. Eigenvalues are crucial in understanding graphs because they relate closely to almost every major graph invariant and extreme property. Consequently, graph energy, a specific type of matrix norm, has attracted attention from both pure and applied mathematicians. Spectral graph theory focuses on matrices associated with graphs, including their eigenvalues and energies, and is vital for analyzing graph matrices through matrix theory and linear algebra. Graph energy provides valuable insights into various structural and dynamic properties of graphs. It is a measure that captures the collective influence of a graph's eigenvalues, linking to diverse applications from chemical graph theory to network analysis. Different graph energies associated with topological indices have been introduced and extensively studied in the literature, highlighting their significance in understanding complex systems. Numerous matrices can be related to a graph, and their spectrums provide certain helpful information about the graph [1,3,5,7,9,14,15,16,17,25].

In 1953, Alfonso Shimbel [26] introduced the notion of vertex stress for graphs as a centrality measure. Stress of a vertex v in a graph G is the number of shortest paths (geodesics) passing through v. This concept has many applications including the study of biological and social networks. Many stress related concepts in graphs and topological indices have been defined and studied by several authors [2,4,10,11,

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12,13,18,19,20,21,22,23,24,27,28]. A graph G is k-stress regular [4] if $str(v) = k$ for all $v \in V(G)$. The stress-sum index $SS(G)$ [19] of a graph $G(V, E)$ is defined by

$$SS(G) = \sum_{uv \in E(G)} \left[str(u) + str(v)\right].$$

The square stress sum index $SSS(G)$ [23] of a graph $G(V, E)$ is defined by

$$SSS(G) = \sum_{uv \in E(G)} \left[str(u)^2 + str(v)^2\right].$$

The second stress index $S_2(G)$ [20] of a graph $G(V, E)$ is defined by

$$S_2(G) = \sum_{uv \in E(G)} str(u)str(v).$$

Motivated by advancements in topological indices and their associated matrices, as well as eigenvalue bounds, we introduce a new matrix and energy measure related to the stress sum index for a graph G. We define the stress sum matrix $SSM(G)$ to encapsulate vertex stress contributions and derive the stress sum energy $\mathcal{E}_{SS}(G)$ from its eigenvalues. Bounds for $\mathcal{E}_{SS}(G)$ in connected graphs are established, elucidating the relationships between the stress sum index and other graph invariants. This research enriches the theoretical framework of topological indices and extends their applicability within graph theory.

In this paper, we introduce the stress sum matrix of a graph G and define the stress sum energy $\mathcal{E}_{SS}(G)$ based on its eigenvalues. This new approach extends the concept of graph energy to incorporate stress-related measures, offering a fresh perspective on graph invariants. We also establish bounds for $\mathcal{E}_{SS}(G)$ in relation to other graph invariants and explore the correlation between the stress sum energy of molecules with heteroatoms and their respective π-electron energy. This work aims to deepen our understanding of graph energy and its implications for molecular and structural analysis.

2. Stress sum matrix and stress sum energy

The stress sum matrix of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $SSM(G) = (x_{ij})$, where

$$x_{ij} = \begin{cases} str\,(v_i) + str\,(v_j), & \text{if} \quad v_iv_j \in E(G); \\ 0, & \text{otherwise}. \end{cases}$$

The stress sum polynomial of a graph G is defined as

$$P_{SSM(G)}(s_\lambda) = |s_\lambda I - SSM(G)|,$$

where I is an $n \times n$ unit matrix.

All the roots of the equation $P_{SSM(G)}(s_\lambda) = 0$ are real because the matrix $SSM(G)$ is real and symmetric. Therefore, these roots can be ordered as $s_{\lambda_1} \geq s_{\lambda_2} \geq \cdots \geq s_{\lambda_n}$, with s_{λ_1} being the largest and s_{λ_n} being the smallest eigenvalue. The stress sum energy $\mathcal{E}_{SS}(G)$ of a graph G is defined by

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

3. Preliminary results

In this section, we will document the necessary results to support our main findings in section 4.

Theorem 3.1 *Let c_i and d_i, for $1 \leq i \leq n$, be non-negative real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} c_id_i\right)^2,$$

where $M_1 = \max_{1\leq i\leq n}\{c_i\}\,; M_2 = \max_{1\leq i\leq n}\{d_i\}\,; m_1 = \min_{1\leq i\leq n}\{c_i\}$ *and* $m_2 = \min_{1\leq i\leq n}\{d_i\}$*.*

Theorem 3.2 *Let* c_i *and* d_i*, for* $1 \leq i \leq n$ *be positive real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} c_i d_i\right)^2 \leq \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2,$$

where $M_1 = \max_{1\leq i\leq n}\{c_i\}\,; M_2 = \max_{1\leq i\leq n}\{d_i\}\,; m_1 = \min_{1\leq i\leq n}\{c_i\}$ *and* $m_2 = \min_{1\leq i\leq n}\{d_i\}$*.*

Theorem 3.3 *(BPR Inequality) Let* c_i *and* $d_i, for 1 \leq i \leq n$ *be non-negative real numbers. Then*

$$\left| n\sum_{i=1}^{n} c_i d_i - \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i \right| \leq \alpha(n)(A-a)(B-b),$$

where a, b, A *and* B *are real constants, that for each* $i, 1 \leq i \leq n, a \leq c_i \leq A$ *and* $b \leq d_i \leq B$*. Further,* $\alpha(n) = n\left\lceil \frac{n}{2}\right\rceil\left(1 - \frac{1}{n}\left\lceil\frac{n}{2}\right\rceil\right)$*.*

Theorem 3.4 *(Diaz–Metcalf Inequality) If* c_i *and* $d_i, 1 \leq i \leq n$*, are nonnegative real numbers. Then*

$$\sum_{i=1}^{n} d_i^2 + rR\sum_{i=1}^{n} c_i^2 \leq (r+R)\left(\sum_{i=1}^{n} c_i d_i\right),$$

where r *and* R *are real constants, so that for each* $i, 1 \leq i \leq n$*, holds* $rc_i \leq d_i \leq Rc_i$*.*

Theorem 3.5 *(The Cauchy-Schwarz inequality) If* $c = (c_1, c_2, \ldots, c_n)$ *and* $d = (d_1, d_2, \ldots, d_n)$ *are real* n*-vectors, then*

$$\left(\sum_{i=1}^{n} c_i d_i\right)^2 \leq \left(\sum_{i=1}^{n} c_i^2\right)\left(\sum_{i=1}^{n} d_i^2\right).$$

4. Bounds for the stress sum eigenvalues and stress sum energy

Lemma 4.1 *Let* $s_{\lambda_1} \geq s_{\lambda_2} \geq \ldots \geq s_{\lambda_n}$ *be the eigenvalues of the stress sum matrix* $SSM(G)$*. Then*

(i) $\sum_{i=1}^{n} s_{\lambda_i} = 0$

(ii) $\sum_{i=1}^{n} s_{\lambda_i}^2 = 2SSS(G) + 4S_2(G)$*.*

Proof:

(i) The first equality is a direct consequence of $SSM(G)_{ii} = 0$ for all $1, 2, \ldots, n$.

(ii) We have

$$\begin{aligned}
\sum_{i=1}^{n} s_{\lambda_i}^2 &= Trace\left(SSM(G)^2\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} SSM(i,j)SSM(j,i) \\
&= 2\sum_{uv\in E(G)} SSM(u,v)SSM(v,u) \\
&= 2\sum_{uv\in E(G)} (str(u)+str(v))(str(v)+str(u)) \\
&= 2\sum_{uv\in E(G)} (str(u)+str(v))^2 \\
&= 2\sum_{uv\in E(G)} (str(u)^2+str(v)^2) + 4\sum_{uv\in E(G)} (str\,(u)\,str\,(v)) \\
&= 2SSS(G) + 4S_2(G).
\end{aligned}$$

□

Lemma 4.2 *Let $G=(V,E)$ be a graph with $P_{SSM}(G) = s_\lambda^n + c_1 s_\lambda^{n-1} + c_2 s_\lambda^{n-2} + \cdots + c_n$ being the characteristic polynomial of $SSM(G)$. Then*

(i) $c_1 = 0$,

(ii) $c_2 = -[SSS(G) + 2S_2(G)]$,

(iii) $c_3 = -2\sum_\Delta \prod_{uv\in E(\Delta)} str(u) + str(v)$,

where the summation is taken over all cycles $\triangle$ *of length 3 in* G.

Proof: Since each coefficient $c_i, i = 1, 2, \cdots, \mathrm{n}, (-1)^i c_i$ corresponds to the sum of all the principal minors of $SSM(G)$ with i rows and i columns, we have the following:

(i) $c_1 = 0$ as all the principal diagonal elements of $SSM(G)$ are zero.

(ii) We have

$$\begin{aligned}
c_2 &= \sum_{1\le i<j\le n} \begin{vmatrix} 0 & b_{\mathrm{ij}} \\ \mathrm{b}_{\mathrm{ji}} & 0 \end{vmatrix} \\
&= -\sum_{1\le i<j\le n} \mathrm{b}_{\mathrm{ij}}^2 \\
&= -\sum_{1\le i<j\le n} (str(v_i)+str(v_j))^2 \\
&= -[SSS(G) + 2S_2(G)].
\end{aligned}$$

(iii) From the definition of $P_{SSM(G)}(\lambda)$, we have

$$(-1)^3 c_3 = \text{ sum of all } 3\times 3 \text{ principal minors of } SSM(G),$$

which implies

$$\begin{aligned}
c_3 &= (-1)^3 \sum_{1\le i<j<k\le n} \begin{vmatrix} b_{ii} & b_{ij} & b_{ik} \\ b_{ji} & b_{jj} & b_{jk} \\ b_{ki} & b_{kj} & b_{kk} \end{vmatrix} \\
&= -\sum_{1\le i<j<k\le n} \left[b_{ii}\left(b_{jj}b_{kk} - b_{kj}b_{jk}\right) - b_{ij}\left(b_{ji}b_{kk} - b_{ki}b_{jk}\right) + b_{ik}\left(b_{ji}b_{kj} - b_{ki}b_{jj}\right)\right] \\
&= -\sum_{1\le i<j<k\le n} b_{ii}a_{jj}b_{kk} + \sum_{1\le i<j<k\le n} \left(b_{ii}b_{jk}^2 + b_{jj}b_{ik}^2 + b_{kk}b_{ij}^2\right) \\
&- \sum_{1\le i<j<k\le n} b_{ij}b_{jk}b_{ki} - \sum_{1\le i<j<k\le n} b_{ik}b_{kj}b_{ji} \\
&= -2\sum_{\Delta}\prod_{uv\in E(\Delta)} (str(u)+str(v)).
\end{aligned}$$

□

Theorem 4.1 *Let G be any graph with n-vertices. Then*

$$s_{\lambda_1} \le \sqrt{\frac{(2SSS(G)+4S_2(G))(n-1)}{n}}.$$

Proof:
Setting $c_i = 1, d_i = s_{\lambda_i}$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we have

$$\left(\sum_{i=2}^{n} s_{\lambda_i}\right)^2 \le (n-1)\sum_{i=2}^{n} s_{\lambda_i}^2. \tag{4.1}$$

From Lemma 4.1, we find that

$$\sum_{i=2}^{n} s_{\lambda_i} = -s_{\lambda_1} \text{ and } \sum_{i=2}^{n} s_{\lambda_i}^2 = -s_{\lambda_1}^2 + 2SSS(G) + 4S_2(G).$$

Employing the above in (4.1), we obtain

$$\begin{aligned}
(-s_{\lambda_1})^2 &\le (n-1)\left(2SSS(G) + 4S_2(G) - s_{\lambda_1}^2\right) \\
s_{\lambda_1} &\le \sqrt{\frac{(2SSS(G)+4S_2(G))(n-1)}{n}}.
\end{aligned}$$

□

Theorem 4.2 *Let G be any graph with n-vertices. Then*

$$\mathcal{E}_{SS}(G) \le \sqrt{(2SSS(G)+4S_2(G))n}$$

Proof: Choosing $c_i = 1, d_i = |s_{\lambda_i}|$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we get

$$\left(\sum_{i=1}^{n} |s_{\lambda_i}|\right)^2 \le n\sum_{i=1}^{n} s_{\lambda_i}^2$$

$$\implies (\mathcal{E}_{SS}(G))^2 \le n(2SSS(G)+4S_2(G))$$

$$\implies \mathcal{E}_{SS}(G) \le \sqrt{n(2SSS(G)+4S_2(G))}.$$

□

Theorem 4.3 *If G is a graph with n vertices and $\mathcal{E}_{SS}(G)$ be the stress sum energy of G, then*

$$\sqrt{2SSS(G) + 4S_2(G)} \leq \mathcal{E}_{SS}(G).$$

Proof: By the definition of $\mathcal{E}_{SS}(G)$, we have

$$[\mathcal{E}_{SS}(G)]^2 = \left(\sum_{i=1}^{n} |s_{\lambda_i}|\right)^2 \geq \sum_{i=1}^{n} |s_{\lambda_i}|^2 = 2SSS(G) + 4S_2(G).$$
$$\implies \quad \sqrt{2SSS(G) + 4S_2(G)} \leq \mathcal{E}_{SS}(G).$$

□

Theorem 4.4 *Let G be any graph with n-vertices and Φ be the absolute value of the determinant of the stress sum matrix $SSM(G)$. Then*

$$\sqrt{(2SSS(G) + 4S_2(G)) + n(n-1)\Phi^{2/n}} \leq \mathcal{E}_{SS}(G).$$

Proof: By the definition of stress sum energy, we find that

$$(\mathcal{E}_{SS}(G))^2 = \left(\sum_{i=1}^{n} |s_{\lambda_i}|\right)^2 = \sum_{i=1}^{n} |s_{\lambda_i}|^2 + 2\sum_{i<j} |s_{\lambda_i}||s_{\lambda_j}|$$
$$= (2SSS(G) + 4S_2(G)) + \sum_{i \neq j} |s_{\lambda_i}||s_{\lambda_j}|.$$

Since for non-negative numbers, the Arithmetic mean is greater than Geometric mean, we have

$$\frac{1}{n(n-1)} \sum_{i \neq j} |s_{\lambda_i}||s_{\lambda_j}| \geq \left(\prod_{i \neq j} |s_{\lambda_i}||s_{\lambda_j}|\right)^{\frac{1}{n(n-1)}}$$
$$= \left(\prod_{i=1}^{n} |s_{\lambda_i}|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}$$
$$= \prod_{i=1}^{n} |s_{\lambda_i}|^{2/n}$$
$$= \Phi^{2/n}.$$

Therefore,

$$\sum_{i \neq j} |s_{\lambda_i}| \left|s_{\lambda_j}\right| \geq n(n-1)\Phi^{\frac{2}{n}}$$
$$\implies [\mathcal{E}_{SS}(G)]^2 \geq 2SSS(G) + 4S_2(G) + n(n-1)\Phi^{2/n}$$
$$\implies \mathcal{E}_{SS}(G) \geq \sqrt{2SSS(G) + 4S_2(G) + n(n-1)\Phi^{2/n}}.$$

Equality in AM-GM inequality is attained if and only if all $s_{\lambda_i}; i = 1, 2, \ldots, n$ are equal. □

Lemma 4.3 *Let $c_1, c_2, \ldots, c_n$ be non-negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right] \leq n\sum_{i=1}^{n} c_i - \left(\sum_{i=1}^{n} \sqrt{c_i}\right)^2 \leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right].$$

Theorem 4.5 *Let G be a connected graph with n vertices. Then*

$$\sqrt{(2SSS(G)+4S_2(G))+n(n-1)\Phi^{2/n}} \leq$$
$$\mathcal{E}_{SS}(G) \leq \sqrt{(2SSS(G)+4S_2(G))(n-1)+n\Phi^{2/n}}.$$

Proof: Let $c_i = |s_{\lambda_i}|^2, i = 1, 2, \ldots, n$ and

$$\begin{aligned} V &= n\left[\frac{1}{n}\sum_{i=1}^{n}|s_{\lambda_i}|^2 - \left(\prod_{i=1}^{n}|s_{\lambda_i}|^2\right)^{1/n}\right] \\ &= n\left[\frac{(2SSS(G)+4S_2(G))}{n} - \left(\prod_{i=1}^{n}|s_{\lambda_i}|\right)^{2/n}\right] \\ &= n\left[\frac{(2SSS(G)+4S_2(G))}{n} - \Phi^{2/n}\right] \\ &= (2SSS(G)+4S_2(G)) - n\Phi^{2/n}. \end{aligned}$$

By Lemma 4.3, we obtain

$$V \leq n\sum_{i=1}^{n}|s_{\lambda_i}|^2 - \left(\sum_{i=1}^{n}|s_{\lambda_i}|\right)^2 \leq (n-1)V.$$

Upon simplification of the above equation, we find that

$$\sqrt{(2SSS(G)+4S_2(G))+n(n-1)\Phi^{2/n}} \leq$$
$$\mathcal{E}_{SS}(G) \leq \sqrt{(2SSS(G)+4S_2(G))(n-1)+n\Phi^{2/n}}.$$

□

Theorem 4.6 *Let G be a graph of order n. Then*

$$\mathcal{E}_{SS}(G) \geq \sqrt{(2SSS(G)+4S_2(G))n - \frac{n^2}{4}\left(s_{\lambda_1} - s_{\lambda\,\min}\right)^2},$$

where $s_{\lambda_1} = s_{\lambda\,\max} = \max\limits_{1\leq i\leq n}\{|s_{\lambda_i}|\}$ and $S_{\lambda\,\min} = \min\limits_{1\leq i\leq n}\{|s_{\lambda_i}|\}$.

Proof: Suppose $s_{\lambda_1}, s_{\lambda_2}, \ldots, s_{\lambda_n}$ are the eigenvalues of $SSM(G)$. We choose $c_i = 1$ and $d_i = |s_{\lambda_i}|$, which by Theorem 3.2 implies

$$\sum_{i=1}^{n}1^2\sum_{i=1}^{n}|s_{\lambda_i}|^2 - \left(\sum_{i=1}^{n}|s_{\lambda_i}|\right)^2 \leq \frac{n^2}{4}\left(s_{\lambda_1} - S_{\lambda\,\min}\right)^2$$

$$\text{i.e.,}\quad (2SSS(G)+4S_2(G))n - (\mathcal{E}_{SS}(G))^2 \leq \frac{n^2}{4}\left(s_{\lambda_1} - S_{\lambda\,\min}\right)^2$$

$$\implies \mathcal{E}_{SS}(G) \geq \sqrt{(2SSS(G)+4S_2(G))n - \frac{n^2}{4}\left(s_{\lambda_1} - S_{\lambda\,\min}\right)^2}.$$

□

Theorem 4.7 *Suppose zero is not an eigenvalue of $SSM(G)$, then*

$$\mathcal{E}_{SS}(G) \geq \frac{2\sqrt{s_{\lambda_1}s_{\lambda\,\min}}\sqrt{(2SSS(G)+4S_2(G))n}}{s_{\lambda_1} + s_{\lambda\,\min}},$$

where $s_{\lambda_1} = s_{\lambda\,\max} = \max\limits_{1\leq i\leq n}\{|s_{\lambda_i}|\}$ and $s_{\lambda\,\min} = \min\limits_{1\leq i\leq n}\{|s_{\lambda_i}|\}$.

Proof: Suppose $s_{\lambda_1}, s_{\lambda_2}, \ldots, s_{\lambda_n}$ are the eigenvalues of $SSM(G)$.
Setting $c_i = |s_{\lambda_i}|$ and $d_i = 1$ in Theorem 3.1, we have

$$\sum_{i=1}^{n} |s_{\lambda_i}|^2 \sum_{i=1}^{n} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{s_{\lambda_1}}{s_{\lambda \min}}} + \sqrt{\frac{s_{\lambda \min}}{s_{\lambda_1}}}\right)^2 \left(\sum_{i=1}^{n} |s_{\lambda_i}|\right)^2$$

$$\text{i.e.,} \quad (2SSS(G) + 4S_2(G))n \leq \frac{1}{4}\left(\frac{(s_{\lambda_1} + s_{\lambda \min})^2}{s_{\lambda_1} s_{\lambda \min}}\right)(\mathcal{E}_{SS}(G))^2$$

$$\implies \mathcal{E}_{SS}(G) \geq \frac{2\sqrt{s_{\lambda_1} s_{\lambda \min}}\sqrt{(2SSS(G) + 4S_2(G))n}}{s_{\lambda_1} + s_{\lambda \min}}.$$

□

Theorem 4.8 *Let G be a graph of order n and $s_{\lambda_1} \geq s_{\lambda_2} \geq \ldots \geq s_{\lambda_n}$ be the eigenvalues of $SSM(G)$. Then*

$$\mathcal{E}_{SS}(G) \geq \frac{(2SSS(G) + 4S_2(G)) + n s_{\lambda_1} s_{\lambda \min}}{s_{\lambda_1} + s_{\lambda \min}},$$

where $s_{\lambda_1} = s_{\lambda \max} = \max_{1 \leq i \leq n} \{|s_{\lambda_i}|\}$ and $s_{\lambda \min} = \min_{1 \leq i \leq n} \{|s_{\lambda_i}|\}$.

Proof: Assigning $d_i = |s_{\lambda_i}|, c_i = 1, R = |s_{\lambda_1}|$ and $r = |s_{\lambda \min}|$ in Theorem 3.4, we get

$$\sum_{i=1}^{n} |s_{\lambda_i}|^2 + s_{\lambda_1} s_{\lambda \min} \sum_{i=1}^{n} 1^2 \leq (s_{\lambda_1} + s_{\lambda \min}) \sum_{i=1}^{n} |s_{\lambda_i}|$$

$$(2SSS(G) + 4S_2(G)) + n s_{\lambda_1} s_{\lambda \min} \leq (s_{\lambda_1} + s_{\lambda \min})\, \mathcal{E}_{SS}(G)$$

After simplifying and using the definition of $\mathcal{E}_{SS}(G)$, we obtain

$$\mathcal{E}_{SS}(G) \geq \frac{(2SSS(G) + 4S_2(G)) + n s_{\lambda_1} s_{\lambda \min}}{s_{\lambda_1} + s_{\lambda \min}}.$$

□

Theorem 4.9 *Let G be a graph of order n and $s_{\lambda_1} \geq s_{\lambda_2} \geq \ldots \geq s_{\lambda_n}$ be the eigenvalues of $SSM(G)$. Then*

$$\mathcal{E}_{SS}(G) \geq \sqrt{(2SSS(G) + 4S_2(G))n - \alpha(n)\,(s_{\lambda_1} - s_{\lambda \min})^2}$$

where $s_{\lambda_1} = s_{\lambda \max} = \max_{1 \leq i \leq n} \{|s_{\lambda_i}|\}$ and $s_{\lambda \min} = \min_{1 \leq i \leq n} \{|s_{\lambda_i}|\}$ and $\alpha(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$.

Proof: Setting $c_i = |s_{\lambda_i}| = d_i, A \leq |s_{\lambda_i}| \leq B$ and $a \leq |s_{\lambda_n}| \leq b$ in Theorem 3.3, we get

$$\left| n \sum_{i=1}^{n} |s_{\lambda_i}|^2 - \left(\sum_{i=1}^{n} |s_{\lambda_i}|\right)^2 \right| \leq \alpha(n)\,(s_{\lambda_1} - s_{\lambda \min})^2$$

$$\left|(2SSS(G) + 4S_2(G))n - (\mathcal{E}_{SS}(G))^2\right| \leq \alpha(n)\,(s_{\lambda_1} - s_{\lambda \min})^2$$

$$\mathcal{E}_{SS}(G) \geq \sqrt{(2SSS(G) + 4S_2(G))n - \alpha(n)\,(s_{\lambda_1} - s_{\lambda \min})^2}.$$

□

Theorem 4.10 *Let s_{λ_1} be the largest eigen value in the spectrum of stress sum matrix. Then*

$$s_{\lambda_1} \geq \frac{2SS(G)}{n}.$$

Proof: According to the Rayleigh-Ritz variational principle , if ξ is any n-dimensional column vector, then $\frac{\xi^T SS(G)\xi}{\xi^T\xi} \leq s_{\lambda_1}$. Setting ξ=(1,1,. . . ,1), we get

$$\xi^T SSM(G)\xi = \sum_{i=1}^{n}\sum_{j=1}^{n} SSM(G)_{i,j} = 2\sum_{ij\in E(G)} SSM(G)_{i,j}$$

$$= 2\sum_{ij\in E(G)} str(v_i) + str(v_j) = 2SS(G)$$

and

$$\xi^T\xi = n$$

$\Longrightarrow$

$$s_{\lambda_1} \geq \frac{2SS(G)}{n}.$$

□

Theorem 4.11 *(Koolen-Moulton-type bound for the stress sum energy) Let G be a graph on n vertices. Suppose G has second stress and square stress sum indices denoted by $S_2(G)$ and $SSS(G)$, respectively. Then*

$$\mathcal{E}_{SS}(G) \leq \frac{2SS(G)}{n} + \sqrt{(n-1)\left[(2SSS(G)+4S_2(G)) - \left(\frac{2SS(G)}{n}\right)^2\right]}$$

which is the analogue of the Koolen-Moulton bound (Koolen & Moulton, 2001), namely

$$\mathrm{En}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

Proof:

$$\sum_{i=2}^{n}\sum_{j=2}^{n}\left(|s_{\lambda_i}| - |s_{\lambda_j}|\right)^2 \geq 0$$

from which it follows

$$\sum_{i=2}^{n}|s_{\lambda_i}| \leq \sqrt{2(n-1)S^*(G)}$$

where

$$2S^*(G) = \sum_{i=2}^{n} s_{\lambda_i}^2 = (2SSS(G)+4S_2(G)) - s_{\lambda_1}^2$$

$$\mathcal{E}_{SS}(G) - |s_{\lambda_i}| \leq \sqrt{(n-1)\left[(2SSS(G)+4S_2(G)) - s_{\lambda_i}^2\right]}$$

and

$$\mathcal{E}_{SS}(G) \leq s_{\lambda_i} + \sqrt{(n-1)\left[(2SSS(G)+4S_2(G)) - s_{\lambda_i}^2\right]}.$$

Consider the function

$$\psi(x) \leq x + \sqrt{(n-1)\left[(2SSS(G)+4S_2(G)) - x^2\right]}$$

It monotonically decreases in the interval (a, b) where

$$a = \sqrt{\frac{(2SSS(G) + 4S_2(G))}{n}} \quad \text{and} \quad b = \sqrt{(2SSS(G) + 4S_2(G))}$$

From Theorem 4.10 result follows. □

Theorem 4.12 *Let G be a bipartite graph on n vertices. The graph has second stress and square stress sum indices denoted by $S_2(G)$ and $SSS(G)$, respectively. Then*

$$\mathcal{E}_{SS}(G) \leq \tfrac{4SS(G)}{n} + \sqrt{(n-2)\left[(2SSS(G) + 4S_2(G)) - 2\left(\tfrac{2SS(G)}{n}\right)^2\right]}$$

which, again is analogous to another Koolen-Moulton bound (Koolen & Moulton, 2003):

$$\mathcal{E}_{SS}(G) \leq \frac{4m}{n} + \sqrt{2(n-2)\left[m - \left(\frac{2m}{n}\right)^2\right]}.$$

Proof:

The theorem above is valid for bipartite graphs and it starts with

$$\sum_{i=2}^{n-1}\sum_{j=2}^{n-1}\left(|s_{\lambda_i}| - |s_{\lambda_j}|\right)^2 \geq 0$$

and by considering that for bipartite graphs $|s_{\lambda_i}| = |s_{\lambda_n}|$. □

Lemma 4.4 *(Abel's inequality) Let $c_1, c_2, \ldots, c_n$ and $d_1, d_2, \ldots, d_n$ be real numbers such that $d_n \geq d_{n+1} \geq 0$ for all n, then*

$$|c_1d_1 + c_2d_2 + \cdots + c_nd_n| \leq Ad_1,$$

where

$$A = \max\{|c_1|, |c_1 + c_2|, \ldots, |c_1 + c_2 + \cdots + c_n|\}.$$

Theorem 4.13 *Let G be any graph with $n \geq 2$ vertices. Then*

$$\mathcal{E}_{SS(G)} \geq \frac{2SSS(G) + 4S_2(G)}{|s_{\lambda_1}|}$$

where $|s_{\lambda_1}| \geq |s_{\lambda_2}| \geq \ldots \geq |s_{\lambda_n}|$ be the sequence of modulus value of eigenvalues of $SSM(G)$. Equality holds if and only if $|s_{\lambda_1}| = |s_{\lambda_2}| = \cdots = |s_{\lambda_n}|$ or $|s_{\lambda_1}| = |s_{\lambda_l}|, 2 \leq l \leq n$ and $|s_{\lambda_k}| = 0$ where $k \neq l, 2 \leq k \leq n$.

Proof: Consider $c_i = |s_{\lambda_i}|$ and $d_i = |s_{\lambda_i}|$ for all $1 \leq i \leq n$. Clearly, $d_1 \geq d_2 \geq \cdots \geq d_n \geq 0$.Then by Lemma 4.4, we have

$$|s_{\lambda_1}|^2 + |s_{\lambda_2}|^2 + \cdots + |s_{\lambda_n}|^2 \leq \mathcal{E}_{SS}(G)\,|s_{\lambda_1}|.$$

Since,

$$A = \max\{|s_{\lambda_1}|, |s_{\lambda_1}| + |s_{\lambda_2}|, \ldots, |s_{\lambda_1}| + |s_{\lambda_2}| + \cdots + |s_{\lambda_n}|\} = \mathcal{E}_{SS}(G)$$

Thus

$$Tr\left(SS(G)^2\right) \leq \mathcal{E}_{SS}(G)\,|s_{\lambda_1}|$$

$$\implies \frac{Tr\left(SS(G)^2\right)}{|s_{\lambda_1}|} \leq \mathcal{E}_{SS}(G).$$

Using Lemma 4.1 in the above inequality, we find that

$$\mathcal{E}_{SS(G)} \geq \frac{2SSS(G) + 4S_2(G)}{|s_{\lambda_1}|}.$$

Further,

$$\begin{aligned}\mathcal{E}_{SS}(G) = \frac{Tr\left(SSM(G)^2\right)}{|s_{\lambda_1}|} &\iff |s_{\lambda_1}|\left(|s_{\lambda_1}| + |s_{\lambda_2}| + \cdots + |s_{\lambda_n}|\right) = \sum_{i=1}^{n} |s_{\lambda_i}|^2 \\ &\iff |s_{\lambda_1}|\left(|s_{\lambda_2}| + \cdots + |s_{\lambda_n}|\right) = \sum_{i=2}^{n} |s_{\lambda_i}|^2.\end{aligned}$$

This is possible if and only if $|s_{\lambda_1}| = |s_{\lambda_2}| = \cdots = |s_{\lambda_n}|$ or $|s_{\lambda_1}| = |s_{\lambda_l}|, 2 \leq l \leq n$ and $|s_{\lambda_k}| = 0$ where $k \neq l, 2 \leq k \leq n$. □

5. Chemical applicability of $\mathcal{E}_{SS}(G)$

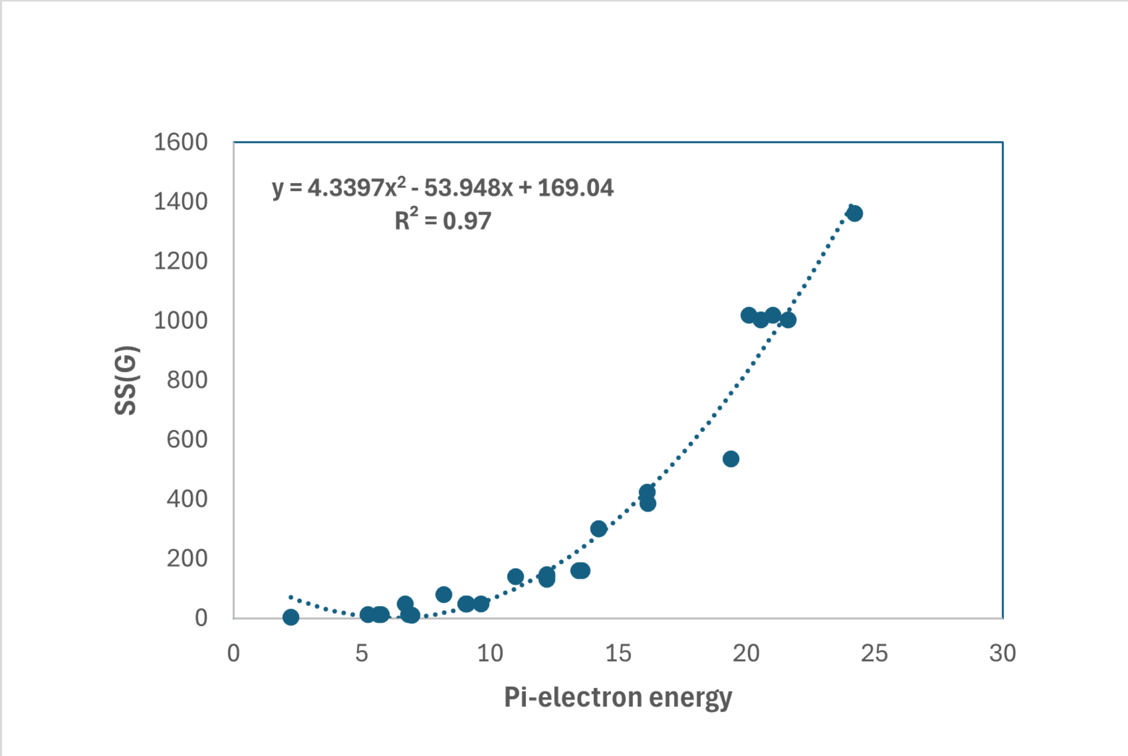
Hückel molecular orbital theory, as initially formulated, was applicable only to conjugated systems composed entirely of carbon atoms. To extend the applicability of this theory to include compounds with heteroatoms, we must adjust the Coulomb integral (α) and the resonance integral (β) for these heteroatoms. This adjustment is achieved using the following relations:

$$\alpha' = \alpha + h\beta \quad \text{and} \quad \beta' = k\beta$$

Here, h and k are correction factors that vary depending on the specific heteroatom present in the conjugated system. Consequently, a heteroatom may have multiple α values depending on how many electrons it contributes to the π-system.

We found that the secular matrix of a heteroatomic molecule closely resembles the stress sum matrix $SSM(G)$ of its corresponding molecular graph G. Testing the $\mathcal{E}_{SS}(G)$ values against a dataset of total π-electron energy values for heteroatom-containing compounds revealed a strong correlation. Specifically, $\mathcal{E}_{SS}(G)$ showed a significant correlation with the total π-electron energy values of these molecules, with $r^2 = 0.9829$. This result highlights the effectiveness of the proposed adjustments for incorporating heteroatoms into Hückel theory.

Molecule	Total π-electron energy	$\mathcal{E}_{SS}(G)$
Venyl chloride like system	2.23	2.828
Acrolein like systems	5.76	11.313
1,1-Dichloro-ethylene like systems	6.96	10.392
Glyoxal like and 1,2-Dichloro-ethylene like systems	6.82	11.312
Butadiene perturbed at C2	5.66	11.313
Pyrrole like systems	5.23	12.944
Pyridine like systems	6.69	48
Pyridazine like systems	9.06	48
Pyrimidine like systems	9.10	48
Pyrazine like systems	9.07	48
S-Triazene like systems	9.65	48
Aniline like systems	8.19	79.6
O-Phenylene-diamine like systems	12.21	140.118
m-Phenylene-diamine like systems	12.22	130.924
p-Phenylene-diamine like systems	12.21	147.470
Benzaldehyde like systems	11.00	139.285
Quinoline like systems	14.23	300.068
Iso-quinoline like systems	14.23	300.068
1-Naphthalein like systems	16.15	385.680
2-Naphthalein like systems	16.12	424.513
Acridine like systems	20.56	1003.898
Phenazine like systems	21.62	1003.898
Iso-indole like systems	13.46	159.725
Indole like systems	13.59	159.725
Azobenzene like systems	21.02	1018.369
Benzylidine-aniline-like systems	20.10	1018.369
9,10-Anthraquinoline structures	24.23	1361.29
Cabazole like structures	19.39	535.627



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C. Nalina
Department of Mathematics
JSS Science and Technology University
Mysuru–570 006, INDIA
E-mail address: `nalinac@jssstuniv.in`

and

P. Siva Kota Reddy (Corresponding author)
Department of Mathematics
JSS Science and Technology University
Mysuru–570 006, INDIA
E-mail address: `pskreddy@jssstuniv.in`

and

M. Kirankumar
Department of Mathematics
Vidyavardhaka College of Engineering
Mysuru-570 002, India.
(Affiliated to Visvesvaraya Technological University, Belagavi-590 018, India)
E-mail address: `kiran.maths@vvce.ac.in`

and

M. Pavithra
Department of Studies in Mathematics
Karnataka State Open University
Mysuru–570 006, INDIA
E-mail address: sampavi08@gmail.com