Signless Laplacian Energy of a Graph with Self-Loops

Harshitha A, Sabitha D'Souza, Swati Nayak, and Gowtham H J

***Abstract*—Let G_S be a graph obtained by adding a self-loop to each vertex of $S \subseteq V$ in a graph $G(V,E)$. The signless Laplacian matrix of a graph G_S containing $|S| = \sigma$ self-loops is, $Q(G_S) = A(G_S) + D(G)$, where $A(G_S)$, $D(G)$ are the adjacency matrix of G_S and diagonal matrix of G respectively. The signless Laplacian energy of a graph $G_S(n,m)$ containing σ self-loops and having q_i, $i = 1,2,\ldots,n$, as signless Laplacian eigenvalues is defined as $QE(G_S) = \left|q_i - \frac{2m+\sigma}{n}\right|$. In this paper, the signless Laplacian matrix of a graph with self-loops is considered. Some basic spectral properties and bounds for signless Laplacian energy are studied. The signless Laplacian spectral properties of complete graph, complete bipartite graph, and star graph with self-loops are also obtained. Correlation between Signless Laplacian energy and total $\pi-$electron energy of hetero-molecules is obtained.**

***Index Terms*—Energy, Graph with self-loops, signless Laplacian matrix.**

I. Introduction

Let $G(V,E)$ be a simple graph of order $|V| = n$, size $|E| = m$, and let $S \subseteq V$ with $|S| = \sigma$. The graph G_S is obtained by attaching a self-loop to each vertex of S.

Energy of a simple graph was defined in the year 1978 as sum of the absolute eigenvalues of the adjacency matrix of a graph. Several researchers have worked on spectra of simple graphs since it has various applications in chemical graph theory. The adjacency matrix $A(G)$ of the graph G with n vertices is a square matrix of order n with elements 1, if the corresponding vertices are adjacent and it is 0, if the corresponding vertices are non-adjacent. The diagonal matrix $D(G)$ of G is also a square matrix of order n whose all non-diagonal elements are zero and the diagonal elements are the vertex degrees of respective vertices. The Laplacian matrix of a simple graph G is $L(G) = D(G) - A(G)$. The signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$. Major studies on signless Laplacian energy and relation between energy and signless Laplacian energy can be seen in [1], [2], [3], [4], [5], [6].

Manuscript received October 01, 2024; revised February 12, 2025

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Recently, I. Gutman et al., [10] introduced the concept of energy of graphs with self-loops and they conjectured that, for a simple graph G of order n and for any subset S of set of vertices of G with $1 \le |S| \le n-1$, $E(G_S) > E(G)$. I. Jovanović et al., [7] have disproved this conjecture by providing a counterexample. D. V. Anchana et al.,[8] introduced and characterized Laplacian energy of graphs with self-loops. A. Harshitha et al.,[9] introduced and characterized Seidel energy of a graph with self-loops. In this paper, the concept of signless Laplacian energy of graphs with self-loops is considered and characterized the same.

II. Preliminaries

Definition 1: [10] The adjacency matrix $A(G_S)$ of a graph G_S of order n with σ self-loops is an $n \times n$ square matrix with elements,

$$(a_{ij})_S = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{if } v_i \text{ and } v_j \text{ are non-adjacent,} \\ 1 & \text{if } i = j \text{ and } v_i \in S, \\ 0 & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

If $\lambda_i,\ 1 \le i \le n$, are the eigenvalues of the graph G_S, then energy of G_S is,

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

Definition 2: The diagonal matrix $D(G_S)$ of a graph G_S of order n is an $n \times n$ square matrix with elements,

$$(d_{ij})_S = \begin{cases} \deg_G\ v_i + 2 & \text{if } i = j \text{ and } v_i \in S, \\ \deg_G\ v_i & \text{if } i = j \text{ and } v_i \notin S, \\ 0 & \text{if } i \ne j. \end{cases}$$

Definition 3: The Laplacian matrix of a graph G_S is, $L(G_S) = D(G_S) - A(G_S)$.

Let $\mu_i,\ i = 1,2,\ldots,n$, be the Laplacian eigenvalues of the graph G_S. The Laplacian energy of G_S is,

$$LE(G_S) = \sum_{i=1}^{n} \left|\mu_i - \frac{2m+\sigma}{n}\right|.$$

Definition 4: [11] The signless Laplacian matrix $Q(G_S)$ of a graph G_S is a square matrix with elements,

$$(q_{ij})_S = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{if } v_i \text{ and } v_j \text{ are non-adjacent,} \\ \deg_G\ v_i + 1 & \text{if } i = j \text{ and } v_i \in S, \\ \deg_G\ v_i & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

Note that

$$\begin{aligned} Q(G_S) &= A(G) + D(G) + J_S \\ &= Q(G) + J_S. \end{aligned}$$

Here, J_S is a square matrix whose non-diagonal elements are all zeros, diagonal elements are 1, if $v_i \in S$ and 0 otherwise. Since $Q(G_S)$ is symmetrically diagonally dominant matrix, it is positive semi-definite.

Let $q_i,\ i = 1, 2, \ldots, n$, be the signless Laplacian eigenvalues of the graph G_S. Each q_i is a real number since $Q(G_S)$ is a symmetric matrix. Also

$$\sum_{i=1}^{n} q_i = 2m + \sigma.$$

Therefore, the signless Laplacian energy of G_S is defined as

$$QE(G_S) = \sum_{i=1}^{n} \left| q_i - \frac{2m+\sigma}{n} \right|.$$

Note that $\mu_i(G_S) = q_i - \frac{2m+\sigma}{n}$, $1 \leq i \leq n$, is called the auxiliary eigenvalues of the matrix $Q(G_S)$.

Remark 1: If $\mu_1, \mu_2, \ldots, \mu_n$ are the auxiliary eigenvalues of $Q(G_S)$, then $\sum_{i=1}^{n} \mu_i(G_S) = 0$.

Definition 5: The first Zagreb index of a graph G, $M_1(G) = \sum_{i=1}^{n} (\deg_G v_i)^2$.

Theorem 1: [12] Let X, Y, and Z be a square matrices of order n such that $X+Y = Z$. Then, $\sum_{i=1}^{n} s_i(X) + \sum_{i=1}^{n} s_i(Y) \geq \sum_{i=1}^{n} s_i(Z)$, where $s_i(M)$ is the singular values of the matrix M. Equality holds if and only if there exists an orthogonal matrix P such that PX and PY are both positive semi-definite.

Theorem 2: If $\overline{a} = (a_1, \ldots, a_n)$, $\overline{b} = (b_1, \ldots, b_n)$ are sequences of real numbers and $\overline{c} = (c_1, \ldots, c_n)$, $\overline{d} = (d_1, \ldots, d_n)$ are non-negative, then

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} c_i a_i^2 + \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i b_i^2 \geq 2 \sum_{i=1}^{n} c_i a_i \sum_{i=1}^{n} d_i b_i. \quad (1)$$

If c_i and d_i $(i = 1, \ldots, n)$ are positive, then equality holds in 1 if and only if $\overline{a} = \overline{b} = \overline{k}$ where $\overline{k} = (k, k, \ldots, k)$ is a constant sequence.

III. Results

Lemma 1: For a graph G_S with $|S| = \sigma$ self-loops, $QE(G_S) = QE(G)$ if $\sigma = 0$ and $\sigma = n$.

Proof: If $\sigma = 0$, then $G_S \cong G$ and $QE(G_S) = \sum_{i=1}^{n} \left| q_i(G) - \frac{2m}{n} \right|$. This implies, $QE(G_S) = QE(G)$.
If $\sigma = n$, then $q_i = q_i(G) + 1$ since $Q(G_S) = Q(G) + I_n$. Therefore,

$$\begin{aligned} QE(G_S) &= \sum_{i=1}^{n} \left| q_i(G) + 1 - \frac{2m}{n} - 1 \right| \\ &= \sum_{i=1}^{n} \left| q_i(G) - \frac{2m}{n} \right| \\ &= QE(G). \end{aligned}$$

■

Remark 2: The graph G_S on n vertices, m edges, and $|S| = \sigma$ self-loops is regular if and only if

- G is regular and σ is either zero or n or
- G_S is obtained from a graph G by adding a self-loop to each vertices of degree r of G, where G is a bi-regular graph with regularities r and $r + 2$.

Remark 3: For a simple regular graph, $E(G) = LE(G) = QE(G)$. In case of the graph with self-loops, $E(G_S) = LE(G_S)$ but $E(G_S)$ need not be equal to $QE(G_S)$.

The graph G_S is regular in only two cases.

Case(i): If G is a $r-$regular and σ is either zero or n, then

$$LE(G_S) = LE(G) = E(G) = E(G_S)$$

and

$$QE(G_S) = QE(G) = E(G) = E(G_S).$$

Case(ii): If G_S is obtained from a graph G by adding a self-loop to each vertices of degree r of G, where G is a bi-regular graph with regularities r and $r + 2$. Then

$$L(G_S) = (r + 2)I - A(G_S)$$

and

$$2m = \sigma r + (n - \sigma)(r + 2) = rn + 2n - 2\sigma.$$

If $q_i,\ 1 \leq i \leq n$ are the eigenvalues of $A(G_S)$, Then,

$$\begin{aligned} LE(G_S) &= \left| (r + 2) - q_i - \frac{2m + \sigma}{n} \right| \\ &= \left| (r + 2) - q_i - \frac{rn + 2n - 2\sigma + \sigma}{n} \right| \\ &= \left| \frac{\sigma}{n} - q_i \right| = E(G_S). \end{aligned}$$

The theorem 3 is a Nordhaus-Gaddum type inequality for the spectral radius of signless Laplacian matrix of a graph with σ self-loops.

Theorem 3: Let G_S be a graph with σ self-loops and $\overline{G_S}$ be the complement of G_S with $n - \sigma$ self-loops. If ρ and $\overline{\rho}$ are the spectral radius of G_S and $\overline{G_{\overline{S}}}$ respectively, then

$$2n - 1 \leq \rho + \overline{\rho} \leq \sqrt{2n(2n - 1)}.$$

Proof: Let ρ and $\overline{\rho}$ be the spectral radius of G_S and $\overline{G_{\overline{S}}}$ respectively. Then

$\rho \geq \frac{4m+\sigma}{n}$ and $\overline{\rho} \geq \frac{4\overline{m}+(n-\sigma)}{n}$.

By noting the fact $m + \overline{m} = \binom{n}{2}$, we have

$$\rho + \overline{\rho} \geq \frac{4\binom{n}{2} + n}{n} = 2n - 1.$$

Also, we have $\rho \leq \sqrt{4m + \sigma}$ and $\overline{\rho} \leq \sqrt{4\overline{m} + (n - \sigma)}$. And therefore,

$$\begin{aligned} \rho + \overline{\rho} &\leq 2 \left(\sqrt{m + \frac{\sigma}{4}} + \sqrt{\overline{m} + \frac{(n - \sigma)}{4}} \right) \\ &= 2 \left(\sqrt{m + \frac{\sigma}{4}} + \sqrt{\binom{n}{2} - m + \frac{(n - \sigma)}{4}} \right) \\ &= 2 \left(\sqrt{m + \frac{\sigma}{4}} + \sqrt{\frac{2n^2 - n}{4} - \left(m + \frac{\sigma}{4} \right)} \right). \end{aligned}$$

But $\sqrt{m+\frac{\sigma}{4}}+\sqrt{\frac{2n^2-n}{4}-\left(m+\frac{\sigma}{4}\right)}$ is maximum when $m+\frac{\sigma}{4}=\frac{2n^2-n}{8}$. Therefore

$$\begin{aligned}\rho+\overline{\rho} &\leq 4\sqrt{\frac{2n^2-n}{8}}\\ &=\sqrt{2n(2n-1)}.\end{aligned}$$

■

Lemma 2: If $q_1, q_2, \ldots, q_n$ are the signless Laplacian eigenvalues of the graph $G_S(n,m)$ with σ, then

$$\sum_{i=1}^{n} q_i^2(G_S)=2m+\sigma+M_1(G)+2d.$$

Where, $M_1(G)$ is the first Zagreb index of G and d is the sum of the degrees of the vertices of S.

Proof: Consider,

$$\begin{aligned}\sum_{i=1}^{n} q_i^2 &= \sum_{i=1}^{n}\left(A(G_S)+D(G)\right)_{ii}^2\\ &= \sum_{i=1}^{n}\left(A(G)+D(G)+J_S\right)_{ii}^2\\ &= \sum_{i=1}^{n}(A(G))_{ii}^2+\sum_{i=1}^{n}(D(G))_{ii}^2+\sum_{i=1}^{n}(J_S)_{ii}^2\\ &\quad+\sum_{i=1}^{n}(A(G)D(G))_{ii}+\sum_{i=1}^{n}(D(G)A(G))_{ii}\\ &\quad+\sum_{i=1}^{n}(A(G)J_S)_{ii}+\sum_{i=1}^{n}(J_SA(G))_{ii}\\ &\quad+\sum_{i=1}^{n}(D(G)J_S)_{ii}+\sum_{i=1}^{n}(J_SD(G))_{ii}\end{aligned}$$

But, $\sum_{i=1}^{n}(A(G))_{ii}^2=2m$, $\sum_{i=1}^{n}(D(G))_{ii}^2=M_1(G)$, $\sum_{i=1}^{n}(J_S)_{ii}^2=\sigma$, $\sum_{i=1}^{n}(A(G)D(G))_{ii}=\sum_{i=1}^{n}(D(G)A(G))_{ii}=\sum_{i=1}^{n}(A(G)J_S)_{ii}=\sum_{i=1}^{n}(J_SA(G))_{ii}=0$, and $\sum_{i=1}^{n}(D(G)J_S)_{ii}=\sum_{i=1}^{n}(J_SD(G))_{ii}=d$. Therefore,

$$\sum_{i=1}^{n} q_i^2=2m+\sigma+M_1(G)+2d.$$

■

Lemma 3: If $q_1, q_2, \ldots, q_n$ are the signless Laplacian eigenvalues of the graph $G_S(n,m)$ with $|S|=\sigma$, then

$$\begin{aligned}\sum_{i=1}^{n}\left|q_i-\left(\frac{2m+\sigma}{n}\right)\right|^2 &= 2m+\sigma+M_1(G)+2d\\ &\quad-\frac{(2m+\sigma)^2}{n}.\end{aligned}$$

Where, $M_1(G)$ is the first Zagreb index of G and d is the sum of the degrees of the vertices of S.

Proof: Consider,

$$\begin{aligned}\sum_{i=1}^{n}\left|q_i-\left(\frac{2m+\sigma}{n}\right)\right|^2 &= \sum_{i=1}^{n}q_i^2+\sum_{i=1}^{n}\left(\frac{2m+\sigma}{n}\right)^2\\ &\quad-2\left(\frac{2m+\sigma}{n}\right)\sum_{i=1}^{n}q_i.\end{aligned}$$

But, from Lemma 2,

$$\sum_{i=1}^{n} q_i^2(G_S)=2m+\sigma+M_1(G)+2d.$$

Where, $M_1(G)$ is the first Zagreb index of a graph and d is the sum of the degrees of the vertices of S and from remark 1, $\sum_{i=1}^{n} q_i=2m+\sigma$. Therefore,

$$\begin{aligned}\sum_{i=1}^{n}\left|q_i-\left(\frac{2m+\sigma}{n}\right)\right|^2 &= 2m+\sigma+M_1(G)+2d\\ &\quad-\frac{(2m+\sigma)^2}{n}.\end{aligned}$$

■

Theorem 4: Let $G_S(n,m)$ be a graph with σ self-loops. Then,

$$QE(G_S)\leq E(G_S)+\sqrt{nM_1(G)-4m^2}.$$

Where $M_1(G)$ is the first Zagreb index of G.

Proof: Consider $Q(G_S)=A(G_S)+D(G)$. Now subtract $\frac{2m+\sigma}{n}I_n$ on both the sides, where I_n is the $n\times n$ identity matrix. Now,

$$Q(G_S)-\frac{2m+\sigma}{n}I_n=D(G)+A(G_S)-\frac{2m+\sigma}{n}I_n.$$

By Theorem 1,

$$\begin{aligned}s_i\left(Q(G_S)-\frac{2m+\sigma}{n}I_n\right) &\leq s_i(A(G_S)-\frac{\sigma}{n}I_n)\\ &\quad+s_i\left(D(G)-\frac{2m}{n}I_n\right).\end{aligned}$$

This implies,

$$QE(G_S)\leq E(G_S)+\sum_{i=1}^{n}\left|d_i(G)-\frac{2m}{n}\right|.$$

By Cauchy-Schwarz inequality,

$$\begin{aligned}\sum_{i=1}^{n}\left|d_i(G)-\frac{2m}{n}\right| &\leq \sqrt{n\sum_{i=1}^{n}\left(d_i(G)-\frac{2m}{n}\right)^2}\\ &=\sqrt{nM_1(G)-4m^2}.\end{aligned}$$

Therefore,

$$QE(G_S)\leq E(G_S)+\sqrt{nM_1(G)-4m^2}.$$

■

Theorem 5: Let $G_S(n,m)$ be a graph with σ self-loops and $\overline{G_{\overline{S}}}$ be a graph obtained by attaching a self-loop to the vertices of $V\backslash S$ in $\overline{G}$. Then

$$QE(G_S)+QE(\overline{G_{\overline{S}}})\geq 2(n-1).$$

Equality holds if $G_S\cong(K_n)$ or $G_S\cong(K_n)_n$.

Proof: Consider,

$$Q(G_S) + Q(\overline{G_{\overline{S}}}) = Q((K_n)_n)$$

. Where $(K_n)_n$ is a complete graph on n vertices with a self-loop attached on each vertex. Now subtract $\left(\frac{2m+\sigma+2\overline{m}+n-\sigma}{n}\right) I_n$ on both the sides. Noting $\left(\frac{2m+\sigma+2\overline{m}+n-\sigma}{n}\right) I_n = nI_n$, we have

$$Q(G_S) - \left(\frac{2m+\sigma}{n}\right) I_n + Q(\overline{G_{\overline{S}}}) - \left(\frac{2\overline{m}+n-\sigma}{n}\right) I_n = Q((K_n)_n) - nI_n.$$

But

$$Q((K_n)_n) - nI_n = A(K_n).$$

Now by using Theorem 1, we get

$$QE(G_S) + QE(\overline{G_{\overline{S}}}) \geq E(K_n) = 2(n-1).$$

If $G_S \cong K_n$, then $\overline{G}_{\overline{S}} \cong (\overline{K_n})_n$. Therefore, $QE(G_S) + QE(\overline{G_{\overline{S}}}) = 2(n-1) + 0 = 2(n-1)$.

If $G_S \cong (K_n)_n$, then $\overline{G}_{\overline{S}} \cong \overline{K_n}$. Therefore, $QE(G_S) + QE(\overline{G_{\overline{S}}}) = 2(n-1) + 0 = 2(n-1)$. ■

Theorem 6: For a graph $G_S(n, m)$ with σ self-loops,

$$QE(G_S) \leq \sqrt{n\left(2m + \sigma + M_1(G) + 2d\right) - \frac{(2m+\sigma)^2}{n}},$$

where $M_1(G)$ is the first Zagreb index of G.

Proof: Consider,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\left|q_i - \frac{2m+\sigma}{n}\right| - \left|q_j - \frac{2m+\sigma}{n}\right|\right)^2 \geq 0$$

This implies,

$$n\sum_{i=1}^{n}\left(\left|q_i - \frac{2m+\sigma}{n}\right|^2\right) + n\sum_{j=1}^{n}\left(\left|q_j - \frac{2m+\sigma}{n}\right|^2\right) \geq 2\sum_{i=1}^{n}\left|q_i - \frac{2m+\sigma}{n}\right|\sum_{j=1}^{n}\left|q_j - \frac{2m+\sigma}{n}\right|.$$

$$\implies 2n\left\{(2m + \sigma + M_1(G) + 2d) - \left(\frac{2m+\sigma}{n}\right)^2\right\} \geq 2(QE(G_S))^2$$

This implies,

$$QE(G_S) \leq \sqrt{n\left(2m + \sigma + M_1(G) + 2d\right) - \frac{(2m+\sigma)^2}{n}}.$$

■

Theorem 7: Let G_S be a graph on n vertices, m edges, and σ self-loops. Then

$$QE(G_S) \leq \frac{2m + n + \sigma + M_1(G) + 2d - \frac{(2m+\sigma)^2}{n}}{2}.$$

Where, $M_1(G)$ is the first Zagreb index of G and d is the sum of the degrees of the vertices of S.

Proof: By substituting $a_i = \left|q_i - \frac{2m+\sigma}{n}\right|$, $b_i = c_i = d_i = 1$ in equation 1, we get

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n}\left|q_i - \frac{2m+\sigma}{n}\right|^2 + \sum_{i=1}^{n} 1 \sum_{i=1}^{n} 1 \geq 2\sum_{i=1}^{n}\left|q_i - \frac{2m+\sigma}{n}\right|\sum_{i=1}^{n} 1.$$

But from Lemma 3,

$$\sum_{i=1}^{n}\left|q_i - \left(\frac{2m+\sigma}{n}\right)\right|^2 = 2m + \sigma + M_1(G) + 2d - \frac{(2m+\sigma)^2}{n}.$$

Therefore,

$$E(G_S) \leq \frac{n\left(2m + \sigma + M_1(G) + 2d - \frac{(2m+\sigma)^2}{n}\right) + n^2}{2n} = \frac{2m + n + \sigma + M_1(G) + 2d - \frac{(2m+\sigma)^2}{n}}{2}$$

■

Theorem 8: Let $(K_n)_S$ be a complete graph with σ self-loops. Then characteristic polynomial of $Q((K_n)_S)$ is,

$$Ch(Q((K_n)_S)) = (q - n + 1)^{\sigma-1}(q - n + 2)^{n-\sigma-1} q^2 + (3 - 3n)q + 2n^2 - 4n + 2 - \sigma.$$

Proof: The signless Laplacian matrix of $(K_n)_S$ with σ self-loops is given by, $Q((K_n)_S) = \left(\begin{array}{c|c} (nI+J)_{\sigma\times\sigma} & J_{\sigma\times n-\sigma} \\ \hline J_{n-\sigma\times\sigma} & ((n-1)I+J)_{n-\sigma\times n-\sigma}\end{array}\right)$.

Where, I and J are identity matrix and all one matrix. By elementary row and column operation, $\det(Q((K_n)_S) - qI)$ is reduced to

$$(n-q)^{\sigma-1}(n-2-q)^{n-\sigma-1}\begin{vmatrix} n-1-q & 1 \\ \sigma & 2n-2-q\end{vmatrix}.$$

On reduction, one can get the characteristic polynomial of $Q((K_n)_S)$ as,

$$Ch(Q((K_n)_S)) = (q - n + 1)^{\sigma-1}(q - n + 2)^{n-\sigma-1} q^2 + (3 - 3n)q + 2n^2 - 4n + 2 - \sigma.$$

■

Theorem 9: Let $(K_{m,n})_S$ be a complete bipartite graph with $\sigma_1 + \sigma_2$ self-loops and $m + n = p$. Let V_1 and V_2 be partition of $(K_{m,n})_S$ and $S_1 \in V_1$ and $S_2 \in V_2$ with $|S_1| = \sigma_1$ and $|S_2| = \sigma_2$. Then the characteristic polynomial of signless Laplacian matrix of $(K_{m,n})_S$ is, $(q - n - 1)^{\sigma_1-1}(q - m - 1)^{\sigma_2-1}(q - n)^{m-\sigma_1-1}(q - m)^{n-\sigma_2-1}(\sigma_1(\sigma_2 + n(q - m - 1)) - (q - n - 1)(m\sigma_2 - (q - m - 1)(q - m - n)q))$.

Proof: The signless Laplacian matrix of $(K_{m,n})_S$ with $\sigma_1 + \sigma_2$ self-loops is, $Q((K_{m,n})_S) = \left(\begin{array}{c|c|c|c} (n+1)I_{\sigma_1} & 0_{\sigma_1\times m-\sigma_1} & J_{\sigma_1\times\sigma_2} & J_{\sigma_1\times n-\sigma_2} \\ \hline 0_{m-\sigma_1\times\sigma_1} & nI_{m-\sigma_1} & J_{m-\sigma_1\times\sigma_2} & J_{m-\sigma_1\times n-\sigma_2} \\ \hline J_{\sigma_2\times\sigma_1} & J_{\sigma_2\times m-\sigma_1} & (m+1)I_{\sigma_2} & 0_{\sigma_2\times n-\sigma_1} \\ \hline J_{n-\sigma_2\times\sigma_1} & J_{n-\sigma_2\times m-\sigma_1} & 0_{n-\sigma_2\times\sigma_1} & mI_{n-\sigma_2}\end{array}\right)$.

By elementary row and column operation, $\det(Q((K_{m,n})_S) - qI)$ is reduced to

$$(n+1-q)^{\sigma_1-1}(m+1-q)^{\sigma_2-1}(n-q)^{m-\sigma_1-1}(m-q)^{n-\sigma_2-1}\begin{vmatrix} m+1-q & 1 & 0 & 0 \\ 0 & m-q & \sigma_1 & m \\ 0 & 0 & n+1-q & 1 \\ \sigma_2 & n & 0 & n-q\end{vmatrix}.$$

By expanding the determinant, the characteristic polynomial of $Q((K_{m,n})_S)$ is, $(q - n - 1)^{\sigma_1-1}(q - m - 1)^{\sigma_2-1}(q - n)^{m-\sigma_1-1}(q - m)^{n-\sigma_2-1}(\sigma_1(\sigma_2 + n(q - m - 1)) - (q - n - 1)(m\sigma_2 - (q - m - 1)(q - m - n)q))$. ■

Corollary 1: The characteristic polynomial of signless Laplacian matrix of star graph $(S_{n+1})_S$ with σ self-loops is (i)

1) $(q-2)^{\sigma-1}(q-1)(q-1)^{n-\sigma}(q^3-nq^2-4q^2+2nq+5q-\sigma-1)$, if the vertex of degree n in S_{n+1} has a self-loop.
2) $(q-2)^{\sigma-1}(q-1)(q-1)^{n-\sigma-1}(q^3-nq^2-3q^2+2nq+2q-\sigma)$, if the vertex of degree n in S_{n+1} does not have a self-loop.

Proof: Let $(S_{n+1})_S$ be a star graph with σ self-loops. Let v be the vertex of degree n in S_{n+1}. (i)

1) Suppose v has a self-loop. Then the characteristic polynomial of $Q((S_{n+1})_S)$ is obtained by substituting $m=1$, $\sigma_1=1$, $\sigma_2=\sigma-1$ in Theorem 9.
2) Suppose v does not have a self-loop. Then the characteristic polynomial of $Q((S_{n+1})_S)$ is obtained by substituting $m=1$, $\sigma_1=0$, $\sigma_2=\sigma$ in Theorem 9.

■

IV. Chemical Applicability of Signless Laplacian Energy of a Graph with Self-Loops

In this section, Signless Laplacian energy of the hetero-molecules listed in 1 is calculated and compared with the total $\pi-$electron energy of those hetero-molecules, where each hetero-atom is replaced by a self-loop. For hetero-molecules, the total $\pi-$electron energy is calculated for different values of h and k, where h is the Coulomb term of the hetero-atom and k is the resonance integral of the carbon-hetero-atom bond. One can refer [14] for more information regarding total $\pi-$electron energy of hetero-molecules. In this study, the comparison between two energies are done for $h=k=1$, $h=2$, $k=1$ and obtained a strong correlation with correlation coefficient 0.99 and 0.95 respectively.

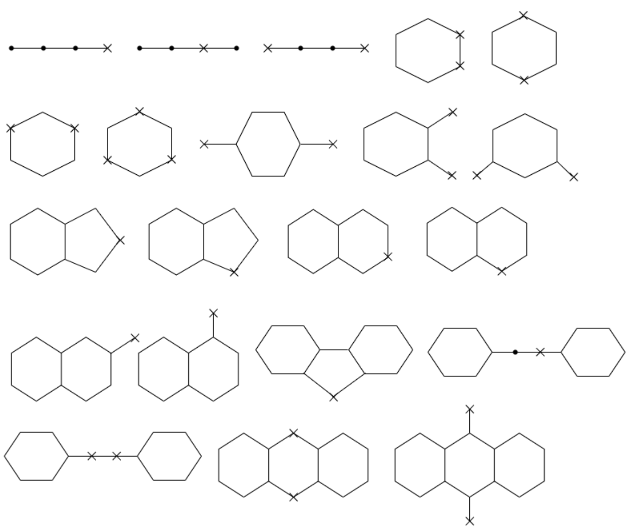

Figure 1. Hetero-molecules.

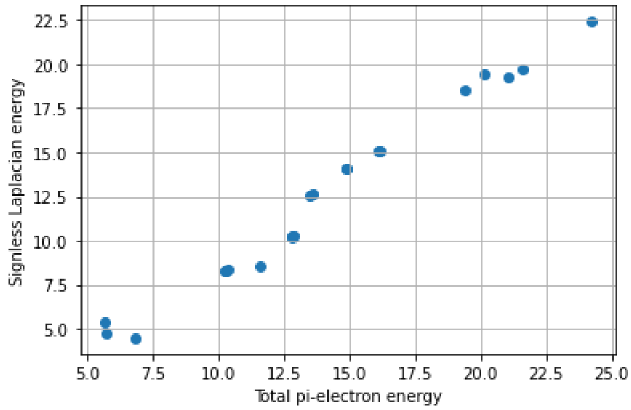

Figure 2. Scatter plot of Signless Laplacian energy of a graph with self-loops and total $\pi-$electron energy of hetero-molecules for $h=k=1$.

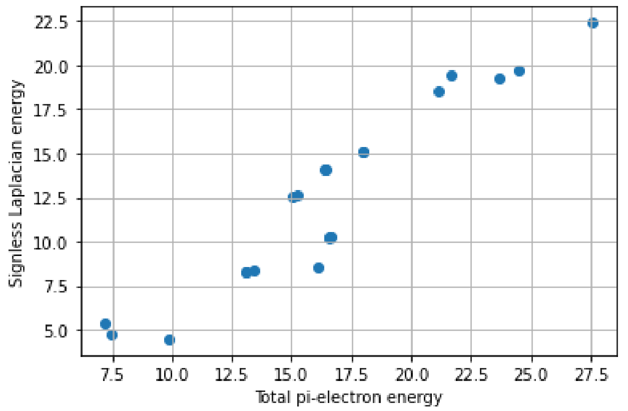

Figure 3. Scatter plot of Signless Laplacian energy of a graph with self-loops and total $\pi-$electron energy of hetero-molecules for $h=2$ and $k=1$.

V. Conclusion

The signless Laplacian energy of a graph with self-loops is introduced and studied some basic properties. Few bounds for the same is obtained in terms of various graph parameters such as number of vertices, edges, first Zagreb index, and number of self-loops. A Nordhaus-Gaddum type inequality for signless Laplacian spectral radius is obtained and signless Laplacian spectral properties of complete and complete bipartite graph is also obtained. As an application, correlation between Signless Laplacian energy and total $\pi-$electron energy of hetero-molecules is obtained.

References

[1] D. Cvetković, New theorems for signless Laplacian eigenvalues, *Bulletin (Académie Serbe Des Sciences et Des Arts. Classe Des Sciences Mathématiques et Naturelles Sciences Mathématiques)*. Vol. 33, pp. 131–146, 2008.

[2] D. Cvetković and S. K. Simić, Towards a spectral theory of graphs based on the signless Laplacian, I, *Publications de l'Institut Mathématique*. Vol. 85, pp. 19–33, 2009.

[3] D. Cvetković and S. K. Simić, Towards a spectral theory of graphs based on the signless Laplacian, II, *Linear Algebra and its Applications*. Vol. 432, pp. 2257–2272, 2010.

[4] D. Cvetković and S. K. Simić, Towards a spectral theory of graphs based on the signless Laplacian, III, *Applicable Analysis and Discrete Mathematics*. Vol. 4, pp. 156–166, 2010.

[5] K. C. Das and S. A. Mojallal, Relation between signless Laplacian energy, energy of graph and its line graph, *Linear Algebra and its Applications*. Vol. 493, pp. 91–107, 2016.

[6] H. A. Ganie, B. A. Chat and S. Pirzada, Signless Laplacian energy of a graph and energy of a line graph, *Linear Algebra and its Applications*. Vol 544, pp. 306–324, 2018.

[7] I. Jovanović, E. Zogic and E. Glogić, On the Conjecture Related to the Energy of Graphs with Self–Loops, *MATCH Communications in Mathematical and in Computer Chemistry*. Vol. 89, pp. 479–488, 2023.

[8] D. V. Anchana, S. D'Souza, H. J. Gowtham and P. G. Bhat, Laplacian Energy of a Graph with Self-Loops, *MATCH Communications in Mathematical and in Computer Chemistry*. Vol. 90, pp. 247–258, 2023.

[9] A. Harshitha, S. D'Souza, S. Nayak, and I. Gutman, Seidel energy of a graph with self-loops, *Communications in Combinatorics and Optimization*. 2024 (article in press).

[10] I. Gutman, I. Redžepović, B. Furtula and A. Sahal, Energy of Graphs with Self-Loops, *MATCH Communications in Mathematical and in Computer Chemistry*. Vol. 87, pp. 645–652, 2022.

[11] S. Akbari, I. M. Jovanović, and J. Lim, Line Graphs and Nordhaus–Gaddum-Type Bounds for Self-Loop Graphs, *Bulletin of the Malaysian Mathematical Sciences Society*. Vol. 47, 117, 2024.

[12] W. So, M. Robbiano, N. M. Maia and I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Linear Algebra and its Applications*. Vol. 432, pp. 2163–2169, 2010.

[13] S. S. Dragomir, A survey on Cauchy-Bunyakovsky-Schwarz type discrete inequalities, *Journal of Inequalities in Pure and Applied Mathematics*. Vol. 4, pp. 1–142, 2003.

[14] C. A. Coulson and A. Streitwieser, *Dictionary of [pi]-electron calculations*, W.H. Freeman, San Francisco, 1965.