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Research Article

On Spectral Radius and Energy of a Graph with Self-Loops

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The spectral radius of a square matrix is the maximum among absolute values of its eigenvalues. Suppose a square matrix is nonnegative; then, by Perron–Frobenius theory, it will be one among its eigenvalues. In this paper, Perron–Frobenius theory for adjacency matrix of graph with self-loops $A(G_S)$ will be explored. Specifically, it discusses the nontrivial existence of Perron–Frobenius eigenvalue and eigenvector pair in the matrix $A(G_S)-\frac{\sigma}{n}I$, where σ denotes the number of self-loops. Also, Koolen–Moulton type bound for the energy of graph G_S is explored. In addition, the existence of a graph with self-loops for every odd energy is proved.

1. Introduction

Let $G=(V,K)$ be a simple undirected graph of order n and size m. Let $A(G)$ be its adjacency matrix with eigenvalues denoted by $\lambda_1(G),\lambda_2(G),\ldots,\lambda_n(G)$. Then, the energy $E(G)$ [1] is defined as follows:

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

Let G_S be a graph with self-loops obtained from G by adding σ self-loops to each vertices in $S\subseteq V(G)$ and $|S|=\sigma$. Let $d_i(G_S)$ represent the degree of ith vertex in the graph G_S. The adjacency matrix $A(G_S)$ is the square matrix of order n whose (i,j)th element is defined as follows:

$$A(G_S)_{ij}=\begin{cases}1 & \text{if the vertices } v_i\sim v_j \text{ or } i=j \text{ and } v_i\in S,\\ 0 & \text{if the vertices } v_i\nsim v_j \text{ or } i=j \text{ and } v_i\notin S.\end{cases} \tag{2}$$

Let $\lambda_1(G_S),\lambda_2(G_S),\ldots,\lambda_n(G_S)$, be the eigenvalues of $A(G_S)$. Then, the energy $E(G_S)$ [2] of graph G_S defined as follows:

$$E(G_S)=\sum_{i=1}^{n}\left|\lambda_i(G_S)-\frac{\sigma}{n}\right|. \tag{3}$$

Also, from the literature [2], it is observed that eigenvalues of $A(G_S)$ satisfy the following relations:

$$\sum_{i=1}^{n}\lambda_i(G_S)=\sigma \text{ and } \sum_{i=1}^{n}\lambda_i^2(G_S)=2m+\sigma. \tag{4}$$

Let $t_i=\lambda_i(G_S)-\frac{\sigma}{n}$, $i=1,2,\ldots,n$, be the auxiliary eigenvalues of $A(G_S)$. Then, the following relations are satisfied:

$$\sum_{i=1}^{n}t_i=0 \text{ and } \sum_{i=1}^{n}t_i^2=N, \tag{5}$$

where $N=2m+\sigma-\frac{\sigma^2}{n}$.

Chemically, some graphs are associated with a molecular structure of conjugated hydrocarbons, and the sum of absolute values of the adjacency eigenvalues is the total π-electron energy of that molecule [1]. A graph with self-loops is used to represent a hetero-conjugated system [3], in which self-loops are used to distinguish hetero atoms present in the molecule. In the existing literature, studies have predominantly been focused on simple graphs, the matrices characterized by a zero diagonal. However, adding self-loops to a graph alters the zero diagonal entries of the adjacency matrix of a simple graph, which subsequently affects its spectral properties. Motivated by this, we investigate the spectral changes that occur with the inclusion of self-loops. For additional terminologies, one can refer to [4, 5].

The paper is organized as follows: in Section 2, we discuss Perron–Frobenius theory and bounds for the spectral radius of $A(G_S)$. In Section 3, we present Koolen–Moulton type bound for the energy of the graph with self-loops. In Section 4, we discuss the existence of graphs with self-loops having odd energy.

2. On Perron–Frobenius Theory and Spectral Radius

Perron–Frobenius theory is a fundamental theory in the field of linear algebra. It is mainly focused on the properties of nonnegative square matrices in terms of their eigenvalues and eigenvectors. The spectral radius of a matrix is the maximum among absolute values of its eigenvalues, which is not always an eigenvalue of the matrix. However, it will be an eigenvalue that is more dominant in the case of nonnegative matrices. It is stated in the following lemma:

Lemma 1. *If $B \in M_n$ is a nonnegative square matrix, then spectral radius $\rho(B)$ is an eigenvalue of B and there is a nonnegative non-zero vector X such that $BX = \rho(B)X$ (Perron–Frobenius property). Moreover, if the matrix $B \in M_n$ is nonnegative, irreducible, and $n \geq 2$. Then, $\rho(B)$ is algebraically simple, and the corresponding eigenvector X is positive (strong Perron–Frobenius property) [4].*

The adjacency matrix of the graph with self-loops being nonnegative assures the existence of Perron–Frobenius property. If a graph is connected, then the corresponding adjacency matrix of the graph with self-loops $A(G_S)$ is irreducible, and it also satisfies strong Perron–Frobenius property, which is of not much interest. The existence of this property is also studied in the case of some nonpositive matrices, and the same can be referred in [6, 7].

It is observed that the auxiliary eigenvalues of matrix $A(G_S)$, i.e., $t_i = \lambda_i(G_S) - \frac{\sigma}{n}, i = 1, 2, \ldots, n$ are the eigenvalues of matrix $A(G_S) - \frac{\sigma}{n}I$. It has at least one and at most $n-1$ negative entries in the diagonal, if $1 \leq \sigma < n$. It serves as a potential example of a matrix having some negative entries. Moreover, it is of the form $A(G_S) - cI$, where c is any scalar and if $\lambda_i(G_S)$ is an eigenvalue of $A(G_S)$ then $\lambda_i(G_S) - c$ is the eigenvalue of $A(G_s) - cI$. Suppose Y_i be the eigenvector corresponding to eigenvalue $\lambda_i(G_S)$, then $A(G_S)Y_i = \lambda_i(G_S)Y_i$. We know that $A(G_S)$ has Perron–Frobenius eigenpair say $(\rho(A(G_S)) = \lambda_1(G_S), X = Y_1)$ i.e., $A(G_S)X = \rho(A(G_S))X$, implying $(A(G_S) - cI)X = (\rho(A(G_S)) - c)X$ which proves the existence of nonnegative eigenvector in matrix $A(G_S) - cI$. Note that the resulting eigenvalue $\rho(A(G_S)) - c$ need not be a spectral radius. For example, consider cycle C_4 with one self-loop with $c = 0.3$.

$$A(G_S) - 0.3I = \begin{bmatrix} 1-0.3 & 1 & 0 & 1 \\ 1 & -0.3 & 1 & 0 \\ 0 & 1 & -0.3 & 1 \\ 1 & 0 & 1 & -0.3 \end{bmatrix}. \quad (6)$$

The eigenvalues of $A(G_S)$ are $-1.8136, 0, 0.4707, 2.3429$, inferring $\rho(A(G_S)) = 2.3429$. The eigenvalues of $A(G_S) - 0.3I$ are $-2.1136, -0.3, 0.1707, 2.0429$ imply $\rho(A(G_S) - 0.3I) = 2.1136 \neq \rho(A(G_S)) - 0.3$. If we take $c = 0.25$, which being the average of eigenvalues satisfy $\rho(A(G_S) - 0.25I) = \rho(A(G_S)) - 0.25$, it inherits Perron–Frobenius eigenpair from the original matrix $A(G_S)$. But in general, this is not true for all graphs with self-loops. For instance, consider a complete bipartite graph $K_{5,2}$ with one self-loop to a vertex in the partite set of order 5; its eigenvalues are -3.0839, $0.7868, 3.2971, 0, 0, 0, 0$. Then, $\rho(A(K_{(5,2)_S}) - \frac{1}{7}I) = 3.22675 \neq \rho(A(K_{(5,2)_S})) - \frac{1}{7}$. This observation leads us to prove Theorem 1.

Lemma 2. *Let a square matrix $A \in \mathbf{M_n}$ be Hermitian, and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the ordered eigenvalues of* A. *Then $\lambda_n y^* y \leq y^* A y \leq \lambda_1 y^* y$ for all $y \in \mathbf{C}^n$ [4].*

Theorem 1. *Let G_S be a connected graph with $1 \leq \sigma < n$ self-loops. Let $(\rho(A(G_S)), X)$ be Perron–Frobenius eigenpair of matrix $A(G_S)$, with $\|X\| = 1$. Then, $(\rho(A(G_S)) - \frac{\sigma}{n}, X)$ is Perron–Frobenius eigenpair of matrix $A(G_S) - \frac{\sigma}{n}I$, if and only if the sum of smallest and spectral radius of $A(G_S)$ is greater than or equal to $\frac{2\sigma}{n}$.*

Proof. Let G_S be a connected graph with $1 \leq \sigma < n$ self-loops. Let $(\rho(A(G_S)), X)$ be Perron–Frobenius eigenpair of matrix $A(G_S)$, with $\|X\| = 1$. Let $(\rho(A(G_S)) - \frac{\sigma}{n}, X)$ be Perron–Frobenius eigenpair of matrix $A(G_S) - \frac{\sigma}{n}I$. Let $\lambda_n(G_S)$ be smallest eigenvalue. Suppose, $\rho(A(G_S)) + \lambda_n(G_S) < \frac{2\sigma}{n}$. Then, $X^t A(G_S) X - \frac{\sigma}{n} < |\lambda_n(G_S) - \frac{\sigma}{n}|$. Implying $\rho(A(G_S) - \frac{\sigma}{n}I) = |\lambda_n(G_S) - \frac{\sigma}{n}|$, a contradiction to the fact that $\rho(A(G_S)) - \frac{\sigma}{n}$ is spectral radius.

Now, let $\rho(A(G_S)) + \lambda_n(G_S) \geq \frac{2\sigma}{n}$. To prove the converse, it is enough to show $\rho(A(G_S) - \frac{\sigma}{n}I) = \rho(A(G_S)) - \frac{\sigma}{n}$. Suppose, $\rho(A(G_S) - \frac{\sigma}{n}I) \neq \rho(A(G_S)) - \frac{\sigma}{n}$, then there exists an eigenvalue and eigenvector pair $(\lambda_j(G_S), Y_j)$, $2 \leq j \leq n$, with $\|Y\| = 1$, satisfying $X^t(A(G_S) - \frac{\sigma}{n}I)X < |Y_j^t(A(G_S) - \frac{\sigma}{n}I)Y_j|$, which further implies the following:

$$X^t A(G_S) X - \frac{\sigma}{n} < \left| Y_j^t A(G_S) Y_j - \frac{\sigma}{n} \right|. \quad (7)$$

We discuss four possible cases and arrive at a contradiction to our assumption.

Case 1: Suppose $Y_j^t A(G_S) Y_j > \frac{\sigma}{n}$. Then, by Equation (7), we write the following:

$$\begin{gathered} X^t A(G_S) X - \frac{\sigma}{n} < Y_j^t A(G_S) Y_j - \frac{\sigma}{n}, \\ \text{implies } \rho(A(G_S)) < \lambda_j(G_S), \text{ a contradiction,} \end{gathered} \quad (8)$$

since $\rho(A(G_S))$ is spectral radius of $A(G_S)$.

Case 2: Suppose $Y_j^t A(G_S) Y_j = \frac{\sigma}{n}$. Then, by Equation (7), we get $\rho(A(G_S)) < 0$, which is again a contradiction.

Case 3: Suppose $Y_j^t A(G_S) Y_j < \frac{\sigma}{n}$ and $Y_j^t A(G_S) Y_j \geq 0$. Then, by Equation (7), we get $X^t A(G_S) X - \frac{\sigma}{n} < - Y_j^t A(G_S) Y_j + \frac{\sigma}{n} < \frac{\sigma}{n}$, it implies $X^t A(G_S) X < \frac{2\sigma}{n}$. By using Lemma 2 we write, $\frac{2m+\sigma}{n} \leq X^t A(G_S) X < \frac{2\sigma}{n} \implies \frac{2m}{n} < \frac{\sigma}{n} \implies 2m < \sigma$, a contradiction to $2m \geq n > \sigma$.

Case 4: Suppose $Y_j^t A(G_S) Y_j < \frac{\sigma}{n}$ and $Y_j^t A(G_S) Y_j < 0$. Then, by Equation (7), we get the following:

$$\begin{aligned} X^t A(G_S) X - \frac{\sigma}{n} &< - Y_j^t A(G_S) Y_j + \frac{\sigma}{n} \\ &\leq - Y_n^t A(G_S) Y_n + \frac{\sigma}{n} \\ &= -\lambda_n(G_S) + \frac{\sigma}{n}. \end{aligned} \tag{9}$$

Therefore, $\rho(A(G_S)) + \lambda_n(G_S) < \frac{2\sigma}{n}$, a contradiction to our assumption. Hence, if $\rho(A(G_S)) + \lambda_n(G_S) \geq, \frac{2\sigma}{n}$, then $\rho(A(G_S) - \frac{\sigma}{n} I) = \rho(A(G_S)) - \frac{\sigma}{n}$. □

Remark 1. For a disconnected graph, Theorem 1 fails. For example, consider the graph $C_4 \cup K_1$ with one self-loop in C_4. Then, $\frac{\sigma}{n} = 0.2$.

$$A(G_S) - 0.2I = \begin{bmatrix} 1-0.2 & 1 & 0 & 1 & 0 \\ 1 & -0.2 & 1 & 0 & 0 \\ 0 & 1 & -0.2 & 1 & 0 \\ 1 & 0 & 1 & -0.2 & 0 \\ 0 & 0 & 0 & 0 & -0.2 \end{bmatrix}.$$

The eigenvalues of $A(G_S)$ are $-1.8136, 0, 0.4707, 1, 2.3429$, $\rho(A(G_S)) = 2.3429$ and $\lambda_n(G_S) = -1.8136$. Then, $\rho(A(G_S)) + \lambda_n(G_S) = 0.5293 > 2 \times 0.2 = 0.4$. But the eigenvalues of $A(G_S) - 0.2I$ are $-2.2136, -0.4, 0.0707, 0.6, 1.9429$. Therefore, $\rho(A(G_S) - 0.4I) = 2.2136 \neq \rho(A(G_S)) - 0.4$.

In 1987, Stanley [8] obtained the bound for the spectral radius $\rho(A(G))$ of adjacency matrix $A(G)$ as follows:

$$\rho(A(G)) \leq \frac{1}{2}\left(-1 + \sqrt{1+8m}\right). \tag{10}$$

The key to its proof lies in adjacency matrix $A(G)$ having diagonal zero and its entries in set $\{0, 1\}$. We now present a bound for the spectral radius of the graph with self-loops, which has a non-zero diagonal.

Theorem 2. *Let G_S be the graph with σ self-loops and $L = \{i / v_i \in S\}$. Then,*
$\rho(A(G_S)) \leq \frac{1}{2}(-1 + \sqrt{1 + 4(2m + \sigma + Q)})$, where $Q = \sum_{i \in L} d_i(G_S) - \sigma$.

Proof. Let G_S be the graph with σ self-loops and $L = \{i / v_i \in S\}$. Let $(\rho(A(G_S)), X)$ be Perron–Frobenius eigenpair, $X = (x_1, x_2, \ldots, x_n)^T$ with $x_1 \geq x_2 \geq \cdots \geq x_n \geq 0$ having $\|X\| = 1$. Let $X(i)$ represent vector having entries as in X except ith co-ordinate of X (i.e., x_i) is replaced by 1 if $v_i \in S$, 0 if $v_i \notin S$. Let $A(G_S)_i$ denote ith row of matrix $A(G_S)$ and r_i be the row sum. Since $X = (x_1, x_2, \ldots, x_n)^T$ with $x_1 \geq x_2 \geq \cdots \geq x_n \geq 0$ having $\|X\| = 1$ imply $x_i \in [0, 1]$ which results in the following:

$$\rho(A(G_S)) x_i = A(G_S)_i X \leq A(G_S)_i X(i). \tag{11}$$

Applying Cauchy–Schwarz inequality [4], we get the following:

$$\rho^2(A(G_S)) x_i^2 \leq |A(G_S)_i X(i)|^2 \leq |A(G_S)_i|^2 |X(i)|^2. \tag{12}$$

Observe that

$$|A(G_S)_i|^2 |X(i)|^2 = \begin{cases} r_i(2 - x_i^2), & \text{if } i \in L, \\ r_i(1 - x_i^2), & \text{otherwise.} \end{cases} \tag{13}$$

Now

$$\begin{aligned} \rho^2(A(G_S)) \sum_{i=1}^n x_i^2 &\leq \sum_{i \in L} r_i(2 - x_i^2) + \sum_{i \notin L} r_i(1 - x_i^2) \\ &= 2\sum_{i \in L} r_i - \sum_{i \in L} r_i x_i^2 + \sum_{i \notin L} r_i - \sum_{i \notin L} r_i x_i^2 \\ &= 2m + \sigma + Q - \sum_{i=1}^n r_i x_i^2 \\ &= 2m + \sigma + Q - \sum_{\substack{i,j=1 \\ i<j}}^n \left(x_i^2 + x_j^2\right) [A(G_S)]_{ij} - \sum_{i=1}^n x_i^2 [A(G_S)]_{ii}. \end{aligned} \tag{14}$$

Since,

$$\begin{aligned} \sum_{\substack{i,j=1 \\ i<j}}^n \left(x_i^2 + x_j^2\right) [A(G_S)]_{ij} + \sum_{i=1}^n x_i^2 [A(G_S)]_{ii} &\geq \sum_{\substack{i,j=1 \\ i<j}}^n 2x_i x_j [A(G_S)]_{ij} + \sum_{i=1}^n x_i^2 [A(G_S)]_{ii} \\ &= X^T A(G_S) X \\ &= \rho(A(G_S)). \end{aligned} \tag{15}$$

Then we write,

$$\begin{aligned}\rho^2(A(G_S))\sum_{i=1}^{n}x_i^2 &\le 2m+\sigma+Q-\rho(A(G_S))\\ \rho^2(A(G_S)) &\le 2m+\sigma+Q-\rho(A(G_S)).\end{aligned} \tag{16}$$

Further simplification results in $\rho(A(G_S))\le\frac{1}{2}(-1+\sqrt{1+4(2m+\sigma+Q)})$. □

Theorem 3. *Let G_S be a connected graph with σ self-loops, $L=\{i/v_i\in S\}$ and the sum of smallest and spectral radius of $A(G_S)$ be greater than or equal to $\frac{2\sigma}{n}$. Then,*
$\rho(A(G_S))\le\frac{1}{2}(-1+\frac{2\sigma}{n}+\sqrt{1+4(2m+\sigma+Q+\frac{\sigma^2}{n^2}(n+\sigma-1)-\frac{2\sigma}{n}(n+\sigma-\frac{1}{2}))})$,
where $Q=\sum_{i\in L}d(G_S)_i-\sigma$.

Proof. Let G_S be the connected graph with σ self-loops, $L=\{i/v_i\in S\}$ and the sum of the smallest and spectral radius of $A(G_S)$ be greater than or equal to $\frac{2\sigma}{n}$. Let $(\rho(A(G_S)),X)$ be Perron–Frobenius eigenpair. By Theorem 1, $(\rho(A(G_S))-\frac{\sigma}{n},X)$ will be Perron–Frobenius eigenpair of $A(G_S)-\frac{\sigma}{n}I$. That is, $(A(G_S)-\frac{\sigma}{n}I)X=(\rho(A(G_S)-\frac{\sigma}{n})X$, where X is chosen as $X=(x_1,x_2,\ldots,x_n)^T$ with $x_1\ge x_2\ge\cdots\ge x_n\ge 0$ having $\|X\|=1$. Let $X(i)$ represent vector having entries as in X except ith co-ordinate of X (i.e., x_i) being replaced by 1 if $v_i\in S$, 0 if $v_i\notin S$. Let $\left[A(G_S)-\frac{\sigma}{n}I\right]_i$ denote ith row of matrix $A(G_S)-\frac{\sigma}{n}I$. Since $X=(x_1,x_2,\ldots,x_n)^T$ with $x_1\ge x_2\ge\cdots\ge x_n\ge 0$ having $\|X\|=1$ imply $x_i\in[0,1]$ which results in,

$$\begin{aligned}\left(\rho(A(G_S))-\frac{\sigma}{n}\right)x_i &= \left[A(G_S)-\frac{\sigma}{n}I\right]_i X\\ &\le \left[A(G_S)-\frac{\sigma}{n}I\right]_i X(i).\end{aligned} \tag{17}$$

Applying Cauchy–Schwarz inequality [4], we get the following:

$$\begin{aligned}\left(\left(\rho(A(G_S))-\frac{\sigma}{n}\right)x_i\right)^2 &\le \left|\left[A(G_S)-\frac{\sigma}{n}I\right]_i X(i)\right|^2\\ &\le \left|\left[A(G_S)-\frac{\sigma}{n}I\right]_i\right|^2|X(i)|^2\\ &= \left(|[A(G_S)]_i|^2+\left|\left[\frac{\sigma}{n}I\right]_i\right|^2-2|[A(G_S)]_i|\left|\left[\frac{\sigma}{n}I\right]_i\right|\right)|X(i)|^2\\ &\le \begin{cases}\left(r_i+\left(\frac{\sigma}{n}\right)^2-\frac{2\sigma}{n}\right)(1-x_i^2), & \text{if } i\in L,\\ \left(r_i+\left(\frac{\sigma}{n}\right)^2-\frac{2\sigma}{n}\right)(2-x_i^2), & \text{otherwise.}\end{cases}\end{aligned} \tag{18}$$

Now

$$\begin{aligned}\left(\rho(A(G_S))-\frac{\sigma}{n}\right)^2\sum_{i=1}^{n}x_i^2 &\le \sum_{i\in L}\left(r_i+\left(\frac{\sigma}{n}\right)^2-\frac{2\sigma}{n}\right)(1-x_i^2)+\sum_{i\notin L}\left(r_i+\left(\frac{\sigma}{n}\right)^2-\frac{2\sigma}{n}\right)(2-x_i^2)\\ &= 2m+\sigma+Q-\sum_{i=1}^{n}r_ix_i^2+\left(\frac{\sigma^2}{n^2}-\frac{2\sigma}{n}\right)(n+\sigma-1)\\ &= 2m+\sigma+Q-\sum_{\substack{i,j=1\\ i<j}}^{n}\left(x_i^2+x_j^2\right)[A(G_S)]_{ij}-\sum_{i=1}^{n}x_i^2[A(G_S)]_{ii}\\ &\quad+\left(\frac{\sigma^2}{n^2}-\frac{2\sigma}{n}\right)(n+\sigma-1).\end{aligned} \tag{19}$$

By using a similar argument as in the proof of Theorem 2, we write the following:

$$\begin{aligned}&\left(\rho(A(G_S))-\frac{\sigma}{n}\right)^2\sum_{i=1}^{n}x_i^2\le 2m+\sigma+Q-\rho(A(G_S))+\left(\frac{\sigma^2}{n^2}-\frac{2\sigma}{n}\right)(n+\sigma-1)\\ &\rho^2(A(G_S))+\frac{\sigma^2}{n^2}-2\rho(A(G_S))\frac{\sigma}{n}\le 2m+\sigma+Q-\rho(A(G_S))+\left(\frac{\sigma^2}{n^2}-\frac{2\sigma}{n}\right)(n+\sigma-1).\end{aligned} \tag{20}$$

Further simplification results in, $\rho(A(G_S)) \leq \frac{1}{2}(-1+\frac{2\sigma}{n}+\sqrt{(1+4(2m+\sigma+Q+\frac{\sigma^2}{n^2}(n+\sigma-1)-\frac{2\sigma}{n}(n+\sigma-\frac{1}{2}))}$. □

Remark 2. It is observed that in a few cases, the bound in Theorem 2 is more sharper than the bound in Theorem 3. For example, consider K_4 with three self-loops, then the observed spectral radius is 2.3429. The upper bounds obtained by Theorem 2 and 3 are 4.7201 and 4.8189, respectively.

In some other cases, the bound in Theorem 3 is more sharper than the bound in Theorem 2. For example, consider cycle C_4 with one self-loop, then the observed spectral radius is 2.3429. The upper bound obtained by Theorems 3 and 2 are 2.9515 and 3, respectively.

3. Koolen–Moulton Bound for a Graph G_S

In 2001, Koolen and Moulton [9] derived the sharp, well-known bound for graph energy called Koolen–Moulton bound for a graph G with $2m \geq n$ as follows:

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}. \quad (21)$$

In 2007, Nikiforov [10], using matrix norms generalized Koolen–Moulton type bound for energy of $m \times n$ $(n \geq m)$ nonnegative complex matrix, say M whose (i, j)th − element is represented as m_{ij}, with maximum element α and $||M||_1 \geq n\alpha$ as follows:

$$\varepsilon(M) \leq \frac{||M||_1}{\sqrt{mn}} + \sqrt{(m-1)\left(||M||_2^2 - \frac{||M||_1^2}{mn}\right)}, \quad (22)$$

where $\varepsilon\ (M) = \sigma_1(M) + \sigma_2(M) + \cdots + \sigma_n(M)$ is the energy of M having σ_i, $1 \leq i \leq n$ as its singular values (for $M_{n\times n}$ Hermitian matrix, singular values are just the moduli of its eigenvalues), $||M||_1 = \sum_{i=1}^{n}\sum_{j=1}^{m}|m_{ij}|$ and $||M||_2 = (\sum_{i=1}^{n}\sum_{j=1}^{m}|m_{ij}|^2)^{\frac{1}{2}}$.

Let M be any graph based $n \times n$ real symmetric adjacency type matrix having the eigenvalues $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$. Suppose $trace(M) = \sum_{i=1}^{n}\theta_i = k$, then the energy of M [11] is defined as follows:

$$E_M = \sum_{i=1}^{n}\left|\theta_i - \frac{k}{n}\right|. \quad (23)$$

Let $b_i = \theta_i - \frac{k}{n}$ for $1 \leq i \leq n$, be the auxiliary eigenvalues of M. Then, Equation (23) is written as follows:

$$E_M = \sum_{i=1}^{n}|b_i|. \quad (24)$$

For a real symmetric matrix M with non-zero trace, it is observed that $\varepsilon\ (M)$ being the sum of absolute values of eigenvalues of M is not equal to E_M, i.e., to conclude the definition of $\varepsilon\ (M)$ given by V. Nikiforov in Equation (22), coincides with the graph energies in Equation (23) only when the matrix has trace zero. But there are many graph-based matrices studied in literature [2, 12–14] which has non-zero traces. Motivated by this, we use a few more properties of matrices and discuss Koolen–Moulton type bound for graph energy in the presence of self-loops. More on Koolen–Moulton type bound refers to [10, 15–17].

Remark 3. Let G be a graph with n vertices, then

(1) $||M||_2^2 = \sum_{i=1}^{n}\theta_i^2 = 2\sum_{i<j}^{n}m_{ij}^2 + \sum_{i=1}^{n}m_{ii}^2$.

(2) $||M - \frac{k}{n}I||_2^2 = \sum_{i=1}^{n}b_i^2 = B$, where $B = 2\sum_{i<j}^{n}m_{ij}^2 + \sum_{i=1}^{n}m_{ii}^2 - \frac{k^2}{n}$.

Lemma 3. *Let A be $n \times n$ matrix and $\lambda, \mu \in \mathbf{C}$. Then, λ is an eigenvalue of A if and only if $\lambda + \mu$ is an eigenvalue of $A + \mu I$ [4].*

Lemma 4. *Let $b_1, b_2, \ldots, b_n$ be the auxiliary eigenvalues of M with trace* k*. Then,*

$$E_M = \varepsilon\left(M - \frac{k}{n}I\right). \quad (25)$$

Proof. Let $b_1, b_2, \ldots, b_n$ be the auxiliary eigenvalues of M with trace k. Let $\theta_1, \theta_2, \ldots, \theta_n$ be the eigenvalues of matrix M. By Lemma 3, θ_i is an eigenvalue of M if and only if $\theta_i - \frac{k}{n}$ is an eigenvalue of $M - \frac{k}{n}I$, i.e., $b_1, b_2, \ldots, b_n$ are the eigenvalues of matrix $M - \frac{k}{n}I$. Then,

$$E_M = \sum_{i=1}^{n}\left|\theta_i - \frac{k}{n}\right| = \sum_{i=1}^{n}|b_i| = \varepsilon\left(M - \frac{k}{n}I\right). \quad (26)$$

□

Remark 4. Let $\rho(M)$ and $\rho(M - \frac{k}{n}I)$ be spectral radii of M and $M - \frac{k}{n}I$, respectively. Suppose $y = 1_n$($n \times 1$ vector having all its entry 1) in Lemma 2, then,

(1) $\frac{1}{n}\sum_{i,j=1}^{n}m_{ij} \leq \rho(M)$.

(2) $\frac{2}{n}\sum_{\substack{i,j=1\\ i<j}}^{n}m_{ij} \leq \rho(M - \frac{k}{n}I)$.

Lemma 5. *Let M be any $n \times n$ real symmetric matrix, $n \geq 2$. Let C be any number satisfying $\rho(M - \frac{k}{n}I) \geq C \geq \frac{||M - \frac{k}{n}I||_2}{\sqrt{n}}$. Then, $E_M \leq C + \sqrt{(n-1)(||M - \frac{k}{n}I||_2^2 - C^2)}$. Moreover, if M is nonnegative matrix with $||M - \frac{k}{n}I||_1 \geq n\alpha$, where α is the maximum element of M, then,*

$$E_M \leq \frac{||M - \frac{k}{n}I||_1}{n} + \sqrt{(n-1)\left(||M - \frac{k}{n}I||_2^2 - \left(\frac{||M - \frac{k}{n}I||_1}{n}\right)^2\right)}.$$

Proof. Let M be any $n \times n$ real symmetric matrix, $n \geq 2$. Let $\rho(M - \frac{k}{n}I) = |b_1|$. Consider,

$$\sum_{i=2}^{n}\sum_{j=2}^{n}\left(|b_i|-|b_j|\right)^2\geq 0$$
$$\sum_{i=2}^{n}\left(\sum_{j=2}^{n}|b_i|^2+\sum_{j=2}^{n}|b_j|^2-2\sum_{j=2}^{n}|b_i||b_j|\right)\geq 0$$
$$2(n-1)(B-|b_1|^2)-2\left(\varepsilon\left(M-\frac{k}{n}I\right)-|b_1|\right)^2\geq 0. \tag{27}$$

Further simplification results in,

$$E_M=\varepsilon\left(M-\frac{k}{n}I\right)\leq|b_1|+\sqrt{(n-1)(B-|b_1|^2)}. \tag{28}$$

The function in Equation (28) is monotonically decreasing in the interval $(\sqrt{\frac{B}{n}},\sqrt{B})$. Thus, by using $\sqrt{\frac{B}{n}}\leq C$ in Equation (28) results in,

$$E_M\leq C+\sqrt{(n-1)(B-C^2)}. \tag{29}$$

i.e.,

$$E_M\leq C+\sqrt{(n-1)\left(\left\|M-\tfrac{k}{n}I\right\|_2^2-C^2\right)}. \tag{30}$$

Let M be nonnegative with $\|M-\frac{k}{n}I\|_1\geq n\alpha$, where α being the maximum element of M. Then, it is followed by Equation (22). □

Theorem 4. *Let $A(G_S)$ be the adjacency matrix of graph G_S with $2m\geq n$. Then, $E(G_S)\leq\frac{2m}{n}+\sqrt{(n-1)(N-(\frac{2m}{n})^2)}$, where $N=2m+\sigma-\frac{\sigma^2}{n}$ (Koolen–Moulton-type bound for E (G_s)).*

Proof. Let G be a graph with $2m\geq n$ and G_S be a graph with self-loops obtained from G by adding σ self-loops. Since $2m\geq n$ we get $\|A(G_S)-\frac{\sigma}{n}I\|_1=2m\geq n$. Then, by using Lemma 5, we get $E(G_S)\leq\frac{2m}{n}+\sqrt{(n-1)(N-(\frac{2m}{n})^2)}$. □

4. On Odd Energy of a Graph with Self-Loops

In 2004, Bapat and Pati [18] proved that the energy of a simple graph is never an odd integer. This motivated us to explore whether a graph with self-loops has odd energy. Interestingly, some graphs with self-loops not only have odd energy, but also, for every odd energy, there exists a graph with self-loops. This significant result is discussed in the following theorem:

Theorem 5. *For any odd positive integer α, there exists a graph G_S with self-loops $(\sigma\neq 0,n)$ on even vertices n having energy α.*

Table 1: Pairs of l,n forming perfect square.

α	1	3	5	7	9	11	13
l	0	1	2	3	4	5	6
n	2	8	18	32	50	72	98

Proof. Let α be any odd positive integer. Consider a totally disconnected graph G on $n=2\alpha$ vertices. Let G_S be a graph obtained from G by adding $\sigma=\alpha$ self-loops.

Claim: The totally disconnected graph with self-loops G_S has the energy α.

It is observed that eigenvalues of G_S are 1 and 0 with algebraic multiplicity α and $n-\alpha$, respectively. Then, the energy of G_S is given by the following:

$$\begin{aligned}E(G_S)&=\alpha\left(1-\frac{\alpha}{n}\right)+(n-\alpha)\left(\frac{\alpha}{n}\right)\\&=\frac{2\alpha(2\alpha-\alpha)}{2\alpha}=\alpha.\end{aligned} \tag{31}$$

Therefore, for any odd positive integer α, a totally disconnected graph G_S with self-loops is obtained serving the purpose. □

Remark 5. For any odd $\alpha>1$, the existence of graph G_S need not be unique, i.e., for some wise choice of n,σ, we can construct totally disconnected graph G_S, having energy α.

For the construction of the desired graph, let $\alpha=2l+1$, where $l\in Z^+\cup\{0\}$.

Consider a totally disconnected graph G_S on n vertices with σ self-loops. In order to obtain the condition on n,σ, we look at the energy of totally disconnected graph G_S,

$$\begin{aligned}E(G_S)=\alpha&=\sigma\left(1-\frac{\sigma}{n}\right)+(n-\sigma)\left(\frac{\sigma}{n}\right)\\&=\frac{2\sigma(n-\sigma)}{n}.\end{aligned} \tag{32}$$

By rearranging, we get the quadratic equation as $2\sigma^2-2\sigma n+n\alpha=0$. Therefore,

$$\sigma=\frac{n\pm\sqrt{n^2-2n\alpha}}{2}. \tag{33}$$

Since σ is an integer, we get $n^2-2n\alpha$ must be a perfect square; moreover, even. If $n^2-2n\alpha=0$, then $n=2\alpha$ with $\sigma=\alpha$ which is discussed in the proof of Theorem 5. If $n^2-2n\alpha$ is non-zero, then by observation, we construct the following l,n pairs forming a perfect square for a given α, refer to Table 1.

Let $\{n_l\}$ be the sequence of n corresponding to l. It is observed that sequence $\{x_l\}$ is the difference of adjacent terms of $\{n_l\}$ (i.e., $x_l=n_{l+1}-n_l$), is an arithmetic progression with first term 6 and common difference 4. Then, the lth term of the sequence $\{n_l\}$ is given by $n_l=\sum_{j=1}^{l}x_j+2$, which on further simplification results in $n_l=2(l+1)^2$. For a given l, choice of n can be $n_l=2(l+1)^2$, by substituting in

TABLE 2: Totally disconnected graph on pairs n, σ corresponding to α.

α	1	3		5		7		9		11		13	
n	2	6	8	10	18	14	32	18	50	22	72	26	98
σ	1	3	2, 6	5	3,15	7	4, 28	9	5, 45	11	6, 66	13	7, 91

Equation (33), we get σ as $(l+1)(2l+1)$ and $(l+1)$. Thus, for odd energy $\alpha = (2l+1) > 1$ we find two different graphs G_S on $n = 2(l+1)^2$ vertices with self-loops $(l+1)(2l+1)$ and $(l+1)$. The different pairs of n, σ are observed for given α, as in Table 2.

Remark 6. Graphs G_S other than totally disconnected graphs are found having odd energy.

Example 1: The graph $K_3 \cup (K_1)_S$ has energy 5.

Example 2: The resultant graph G_S obtained from complete graph K_8 by removing one edge and adding self-loops to vertices incident with it has energy 15.

Data Availability

All the data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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