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On Bounds of Energy of a Graph with Self-Loops

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Abstract

The energy of a graph G_S with n vertices and σ self-loops is defined as $\varepsilon(G_S) = \sum_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|$, where the eigenvalues of the adjacency matrix of G_S are $\lambda_1, \lambda_2, \ldots, \lambda_n$. In this article, we have established some upper and lower bounds for the energy of such a graph. Those new bounds involve parameters like number of vertices (n), number of edges (m), number of self-loops (σ), maximum vertex degree (Δ), and minimum vertex degree (δ). We show that for $1 \leq \sigma < n$, the quantity $|\lambda_i - \frac{\sigma}{n}|$ is always greater than 0, and using that fact we establish a lower bound. We have compared and concluded that the new bounds are either better than the existing bounds or incomparable to a few bounds obtained by some researchers recently.

1 Introduction

A graph is considered simple if it has no parallel edges or has no self-loops. If a graph contains m edges and n vertices, then the graph will be called (n, m)-graph. The number of edges and vertices in a graph G determines its size and order, respectively. Without loss of generality, let us suppose that the vertices of G are labelled according to their degree in decreasing

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order, i.e., $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$, where d_i is the degree of the ith vertex v_i, Δ is the maximum degree and δ is the minimum degree. If there is an edge between v_i and v_j, we'll use the notation $i \sim j$ or $v_i \sim v_j$.

For a simple graph G with n vertices, the (i,j)-th element of the $n \times n$ adjacency matrix A(G) equals 1 if $i \sim j$ and 0 otherwise. Let $\varrho_1 \geq \varrho_2 \geq \cdots \geq \varrho_n$ are the eigenvalues of A(G). Gutman defined (see [9], also you can see [5, 6, 12]) the energy of a simple G. Let $\varepsilon(G)$ represent the energy of graph G, which is the sum of the absolute values of the eigenvalues of $A(G)$. Mathematically, $\varepsilon(G) = \sum_{i=1}^{n} |\varrho_i|$.

A lot of work has been done in the last few decades involving the study of the energy of graphs and its several variants (see [4–6, 8–10, 12]).

Let S be any σ-element subset of $V(G)$, the vertex set of graph G, and G_S be the graph that is created by joining a self-loop to every vertex $v \in S$ in the simple graph G. In this paper, we will consistently use these notations. The $n \times n$ real symmetric matrix representing the adjacency matrix of graph G_S is denoted as $A(G_S)$ or simply A_S, with its (i,j)-th element specified by

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

The eigenvalues of the graph G_S mean the eigenvalues of the matrix $A(G_S)$, just like the eigenvalues of simple graphs.

Let $B = A(G_S) - \frac{\sigma}{n} I_n$. Furthermore, consider that the eigenvalues of $A(G_S)$ and B are, respectively, λ_i and μ_i for $i = 1, 2, \ldots, n$ with decreasing order, i.e., $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. The energy of the graph G_S was defined by Gutman et al. [7] as

$$\varepsilon(G_S) = \sum_{i=1}^{n} \left| \lambda_i - \frac{\sigma}{n} \right| = \sum_{i=1}^{n} |\mu_i|. \tag{2}$$

Readers are referred to [2, 14, 15] for studies on the energy of a graph with self-loops. The following Lemmas will be helpful in our present work.

Lemma 1. *Let $a_1 \geq \cdots \geq a_n$ be any n positive real numbers. Then*

$$a_1 + \cdots + a_n \leq a_1 + \sqrt{(n-1)(a_2^2 + \cdots + a_n^2)} \leq \sqrt{n(a_1^2 + \cdots + a_n^2)}.$$

Proof. Using the relation between Arithmetic mean-Quadratic mean on n positive real numbers $a_1 \geq \cdots \geq a_n$ we can write $a_1 + \cdots + a_n \leq \sqrt{n(a_1^2 + \cdots + a_n^2)}$ and equality holds if and only if $a_1 = \cdots = a_n$. Also $a_1 + \cdots + a_n \leq a_1 + \sqrt{(n-1)(a_2^2 + \cdots + a_n^2)}$ with equality holds if and only if $a_2 = \cdots = a_n$. Let $B = a_1 + \sqrt{(n-1)(a_2^2 + \cdots + a_n^2)}$ and $A = \sqrt{n(a_1^2 + \cdots + a_n^2)}$. Then A and B are two upper bounds of the sum $a_1 + \cdots + a_n$. If $a_1 = a_n$, then $a_1 + \cdots + a_n = A = B$. Now for any $a_1 \geq \cdots \geq a_n$ where $a_1 > a_n$, the upper bound A of $a_1 + \cdots + a_n$ is never attained, but for $a_1 > a_2 = \cdots = a_n$, the upper bound B of $a_1 + \cdots + a_n$ is attainable. So, $B \leq A$, i.e.,

$$a_1 + \cdots + a_n \leq a_1 + \sqrt{(n-1)(a_2^2 + \cdots + a_n^2)} \leq \sqrt{n(a_1^2 + \cdots + a_n^2)}.$$

■

Lemma 2. *[7] Assume that G_S is a graph consisting of n vertices, m edges, and σ self-loops. If the adjacency eigenvalues of the graph G_S are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then*

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

Lemma 3. *[7] With the same notation as in Lemma 2,*

$$\sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|^2 = 2m + \sigma - \frac{\sigma^2}{n}\cdot$$

It may be noted that $\sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|^2 = 2m + \sigma - \frac{\sigma^2}{n}$, and we will use the notation $2M_\sigma = 2m + \sigma - \frac{\sigma^2}{n}$.

Lemma 4. *[1] With the same notation as in Lemma 2,*

$$\frac{2m}{n} + \frac{\sigma}{n} \leq \lambda_1.$$

Lemma 5. *With the same notations as in Lemma 2,*

$$\lambda_1 \leq \begin{cases} \Delta + 1, & \textit{if there exists a loop on the vertex with degree } \Delta \\ \Delta, & \textit{if there is no loop on the vertex with degree } \Delta \end{cases}$$

where Δ is the maximum degree in G.

Proof. We have,

$$\begin{aligned} \|A(G_S)\|_1 &= \max_i \sum_{j=1}^{n} (A(G_S)_{ij} \\ &= \begin{cases} \Delta + 1, & \text{if there exists a loop on the vertex with degree } \Delta \\ \Delta, & \text{if there is no loop on the vertex with degree } \Delta. \end{cases} \end{aligned}$$

Since λ_1 is the spectral radius of $A(G_S)$, it is less than or equal to any norm of $A(G_S)$. Then from the fact that $\lambda_1 \leq \|A(G_S)\|_1$, the lemma follows.

■

Lemma 6. *Let $B = A(G_S) - \frac{\sigma}{n} I_n$, and μ_1 is the spectral radius of B. Then,*

$$\frac{2m}{n} \leq \mu_1 \leq \sqrt{\frac{2M_\sigma(n-1)}{n}} \tag{3}$$

where $2M_\sigma = 2m + \sigma - \frac{\sigma^2}{n}\cdot$

Proof. Here, μ_1 is the spectral radius of B. So,

$$\begin{aligned}
\mu_1 = \max_{\substack{x\in\mathbb{R}^n \\ x\neq 0}} \frac{x^T Bx}{x^T x} &\geq \frac{\mathbf{1}^T B\mathbf{1}}{\mathbf{1}^T\mathbf{1}} \qquad \text{where } \mathbf{1} = (1,1,\ldots,1)^T \\
&= \frac{1}{n}\Big(d_1 + d_2 + \cdots + d_n + \sigma(1-\frac{\sigma}{n}) - (n-\sigma)\frac{\sigma}{n}\Big) \\
&= \frac{2m}{n}. \qquad (4)
\end{aligned}$$

Again,

$$\sum_{r=1}^{n} \mu_r = 0 \quad \Rightarrow \quad |\mu_1| = \left| -\sum_{r=2}^{n} \mu_r \right| \leq \sum_{r=2}^{n} |\mu_r|.$$

Then,

$$\begin{aligned}
2m + \sigma - \frac{\sigma^2}{n} = \sum_{r=1}^{n} \mu_r^2 = \mu_1^2 + \sum_{r=2}^{n} \mu_r^2 &\geq \mu_1^2 + \frac{1}{n-1}\left(\sum_{r=2}^{n} |\mu_r|\right)^2 \\
&\geq \mu_1^2 + \frac{\mu_1^2}{n-1}.
\end{aligned}$$

So,

$$\mu_1 \leq \sqrt{\frac{(2m + \sigma - \frac{\sigma^2}{n})(n-1)}{n}} = \sqrt{\frac{2M_\sigma(n-1)}{n}}.$$

■

Now we put forward the following theorem.

Theorem 1. *Consider a connected (n,m)-graph G, and let G_S be the one that is derived by joining a self-loop at σ $(1 \leq \sigma < n)$ number of distinct vertices to the graph G. If the adjacency matrix of G_S is $A(G_S)$, then –*

(i) all the rational eigenvalues of $A(G_S)$ are integers, and

(ii) $B = A(G_S) - \frac{\sigma}{n} I_n$ is non-singular.

Proof. Let us consider that the eigenvalues of $A(G_S)$ and B are, respectively, λ_i and μ_i for $i = 1,2,\ldots,n$ with decreasing order. Clearly, $\mu_i = \lambda_i - \frac{\sigma}{n}$ for all $i \in \{1,2,\ldots,n\}$.

(i) Consider the characteristic polynomial of $A(G_S)$ denoted as $p(x) = \det(xI_n - A(G_s))$. Given that all elements of $A(G_S)$ are integers, and the coefficients of $p(x)$ are also integers. Additionally, as it is a monic polynomial, any rational root of $p(x)$ must be an integer.

(ii) Since $1 \leq \sigma < n$, we have $0 < \frac{\sigma}{n} < 1$. If $\lambda_i \in \mathbb{Q}$, then by case (i) above, $\lambda_i \notin (0,1)$ and so $\mu_i \neq 0$. If $\lambda_i \notin \mathbb{Q}$, then $\frac{\sigma}{n}$ being a rational number cannot be equal to λ_i and hence $\mu_i \neq 0$. Thus, in any case, $\det(B) = \Pi_{i=1}^{n}\mu_i \neq 0$. ■

A simple graph G without edges has zero energy, which is a trivial property. But, if the graph G_S derived by joining a self-loop at σ ($1 \leq \sigma < n$) number of distinct vertices to the graph G, then the energy of G_S is non-zero. In fact, we pose the subsequent theorem.

Theorem 2. *Assume that graph G has n isolated vertices, i.e., G has no edges. If the graph G_S is the one that is derived by joining a self-loop at σ ($1 \leq \sigma < n$) number of distinct vertices to the graph G then*

$$\varepsilon(G_S) = 2\sigma\left(1 - \frac{\sigma}{n}\right).$$

Proof. Assume, without losing generality, that the self-loops are connected to the vertices $v_1, v_2, \ldots, v_\sigma$. So,

$$A(G_S) = \begin{pmatrix} X_1 & X_2 \\ X_3 & X_4 \end{pmatrix}$$

where X_1 is $\sigma \times \sigma$ identity matrix and X_2, X_3, X_4 are zero matrix with order $\sigma \times (n-\sigma)$, $(n-\sigma) \times \sigma$ and $(n-\sigma) \times (n-\sigma)$ respectively. So the eigenvalues of $A(G_S) - \frac{\sigma}{n}I_n$ are $\{\underbrace{1 - \frac{\sigma}{n}, \ldots, 1 - \frac{\sigma}{n}}_{\sigma \text{ times}}, -\frac{\sigma}{n}, \ldots, -\frac{\sigma}{n}\}$. So, the energy of the graph G_S is

$$\varepsilon(G_S) = \sigma\left(1 - \frac{\sigma}{n}\right) + (n-\sigma)\frac{\sigma}{n} = 2\sigma\left(1 - \frac{\sigma}{n}\right).$$

■

2 Upper bound of energy of a graph with self-loops

An upper bound of energy of a graph with self-loops provided by Gutman et al. is as follows.

Lemma 7. *[7] Let G_S be a connected (n,m)-graph with σ self-loops. If $\varepsilon(G_S)$ be the energy of G_S, then*

$$\varepsilon(G_S) \leq \sqrt{2M_\sigma n}.$$

where $2M_\sigma = \left(2m + \sigma - \frac{\sigma^2}{n}\right)$.

Very recently, Liu et al. [11] have found the following upper bounds of energy of a graph with self-loops.

Lemma 8. *[11] Let G be a connected (n,m)-graph with maximum degree Δ. Let G_S be the graph derived from G by joining σ self-loops. If $\varepsilon(G_S)$ be the energy of G_S, then*

$$\varepsilon(G_S) \leq \sqrt{(n-1)\left(2m + \sigma - \frac{4m^2 + 4m\sigma + 2\sigma^2}{n^2} + \frac{2\sigma}{n}(\Delta + 1 - \frac{\sigma}{2})\right)} + \Delta + \frac{n-\sigma}{n}.$$

Lemma 9. *[11] With the same notation as in Lemma 8,*

$$\varepsilon(G_S) \leq \Delta + 1 + \frac{(n-2)\sigma}{n} + \sqrt{(n-1)\left(2m + \sigma - \frac{(2m+\sigma)^2}{n^2}\right)}.$$

Lemma 10. *[11] Let G_S be a connected (n,m)-graph with σ self-loops. Then,*

$$\varepsilon(G_S) \leq \sqrt{\frac{n^2 + (2m + \sigma - \frac{\sigma^2}{n})^2}{2}}.$$

Lemma 11. *[11] Let G_S be a connected (n,m)-graph with σ self-loops. Then,*

$$\varepsilon(G_S) \leq \frac{n + 2m + \sigma - \frac{\sigma^2}{n}}{2}.$$

Remarks: The upper bounds given in Lemma 10 and Lemma 11 are weaker than the upper bound given by Gutman et al. in Lemma 7. That can be easily verified, as shown below.

If the upper bound given in Lemma 10 is not weaker than that in Lemma 7, then

$$\begin{aligned} \sqrt{2M_\sigma n} &> \sqrt{\frac{n^2+(2M_\sigma)^2}{2}} \text{ where } 2M_\sigma = \left(2m+\sigma-\frac{\sigma^2}{n}\right) \\ \Rightarrow 0 &> (2M_\sigma - n)^2, \end{aligned}$$

which is impossible. So $\sqrt{2M_\sigma n} \leq \sqrt{\frac{n^2+(2M_\sigma)^2}{2}}$.

Similarly, if the upper bound given in Lemma 11 is not weaker than that in Lemma 7, then

$$\begin{aligned} \sqrt{2M_\sigma n} &> \frac{n+2M_\sigma}{2} \\ \Rightarrow 0 &> (2M_\sigma - n)^2, \end{aligned}$$

which is impossible. So $\sqrt{2M_\sigma n} \leq \frac{n+2m+\sigma-\frac{\sigma^2}{n}}{2}$.

In the following subsection, we provide a new upper bound of $\varepsilon(G_S)$ and we show that the new upper bound given in Theorem 4 is better than the upper bound given by Gutman et al. in Lemma 7, and hence also better than those given in Lemma 10 and Lemma 11.

2.1 Energy of a vertex of a graph with self-loops and its bounds

For a square matrix X, we represent its trace as $Tr(X)$. Additionally, we use $|X|$ to denote $(XX^T)^{\frac{1}{2}}$. Nikiforov [13] established that the energy of a graph G can be obtained from Schatten 1-norm of A, i.e., $\varepsilon(G) = Tr(|A|)$. Considering this, the idea of a graph's vertex energy was presented in [3] by Arizmendi et al. as a new advancement in the theory of graph energy. The energy of the i-th vertex, denoted by $\varepsilon_i(G)$ or simply by ε_i, is given by

$$\varepsilon_i = |A|_{ii} \text{ for } i \in \{1, 2, \ldots, n\}$$

and as such

$$\varepsilon(G) = \varepsilon_1 + \varepsilon_2 + \cdots + \varepsilon_n.$$

Similarly, we introduce the notion of energy of a vertex of a graph with self-loops. We denote the energy of the i-th vertex of the graph G_S by $\varepsilon(G_S)$ and define as

$$\varepsilon_i(G_S) = |A(G_S) - \frac{\sigma}{n} I_n|_{ii} = |B|_{ii} \text{ for } i \in \{1, 2, \ldots, n\}$$

and so

$$\varepsilon(G_S) = \varepsilon_1(G_S) + \varepsilon_2(G_S) + \cdots + \varepsilon_n(G_S).$$

Definition 1. Let G_S be a graph with n vertices and σ self-loops. $A(G_S)$ denotes the adjacency matrix of the graph G_S. For each $i \in \{1, 2, \ldots, n\}$, the energy of the i-th vertex of G_S, denoted by $\varepsilon_i(G_S)$ is given by

$$\varepsilon_i(G_S) = |A(G_S) - \frac{\sigma}{n} I_n|_{ii} = |B|_{ii}$$

where $|B| = \left(BB^T\right)^{\frac{1}{2}} = \left(B^2\right)^{\frac{1}{2}}$.

Theorem 3. *Let G_S be a graph with σ self-loops and n vertices which are labelled as $1, 2, \ldots, n$. If d_i be the degree of the i-th vertex, then*

$$\varepsilon_i(G_S) \leq \begin{cases} \sqrt{\left(1 - \frac{\sigma}{n}\right)^2 + d_i} & \textit{if there is a self-loop on the vertex } v_i \\ \sqrt{\frac{\sigma^2}{n^2} + d_i} & \textit{if there is no self-loop on the vertex } v_i. \end{cases}$$

Proof. Let us define a positive linear functional $\phi_i : M_n(\mathbb{R}) \to \mathbb{R}$ by

$$\phi_i(Y) \mapsto (Y)_{ii}.$$

Then

$$Tr(Y) = \phi_1(Y) + \phi_2(Y) + \cdots + \phi_n(Y).$$

If $B = A(G_S) - \frac{\sigma}{n} I_n$, then

$$
\begin{aligned}
\varepsilon(G_S) &= Tr\left(\left|A(G_S) - \frac{\sigma}{n} I_n\right|\right) \\
&= Tr(|B|) \\
&= \phi_1(|B|) + \phi_2(|B|) + \cdots + \phi_n(|B|). \qquad (5)
\end{aligned}
$$

The Hölder's inequality is satisfied by all $\phi_i, i \in \{1, 2, \ldots, n\}$, since they are positive linear functionals on $M_n(\mathbb{R})$. Thus for $P, Q \in M_n(\mathbb{R})$ and for positive real numbers p, q satisfying $\frac{1}{p} + \frac{1}{q} = 1$, we have

$$
\phi_i(|PQ|) \leq \phi_i(|P|^p)^{\frac{1}{p}} \phi_i(|Q|^q)^{\frac{1}{q}}. \qquad (6)
$$

Choosing $P = B, Q = I_n, p = 2, q = 2$ and then squaring both sides, we get

$$
\phi_i(|B|)^2 \leq \phi_i(|B|^2) = \phi_i(B^2). \qquad (7)
$$

Now,

$$
\phi_i(B^2) = \begin{cases} \left(1 - \frac{\sigma}{n}\right)^2 + d_i & \text{if there is a self-loop on vertex } v_i \\ \frac{\sigma^2}{n^2} + d_i & \text{if there is no self-loop on vertex } v_i. \end{cases}
$$

So,

$$
\begin{aligned}
\varepsilon_i(G_S) &= \phi_i(|B|) \leq \sqrt{\phi_i(B^2)} \\
&= \begin{cases} \sqrt{\left(1 - \frac{\sigma}{n}\right)^2 + d_i} & \text{if there is a self-loop on vertex } v_i \\ \sqrt{\frac{\sigma^2}{n^2} + d_i} & \text{if there is no self-loop on vertex } v_i. \end{cases} \qquad (8)
\end{aligned}
$$

■

Theorem 4. *Let G be a graph with n vertices, m edges and G_S be the one obtained from G by attaching σ self-loops. If Δ be the maximum vertex* *degree in G and $\varepsilon(G_S)$ be the energy of the graph G_S then*

$$\varepsilon(G_S) \leq \begin{cases} \sqrt{(n-1)\left(2M_\sigma - \Delta - \left(1-\frac{\sigma}{n}\right)^2\right)} \\ +\sqrt{\left(1-\frac{\sigma}{n}\right)^2 + \Delta}, \ \textit{if } v_1 \textit{ has a self-loop} \\ \\ \sqrt{(n-1)\left(2M_\sigma - \Delta - \frac{\sigma^2}{n^2}\right)} + \sqrt{\frac{\sigma^2}{n^2} + \Delta} \\ \textit{if } v_1 \textit{ has no self-loop} \end{cases}$$

where $2M_\sigma = 2m + \sigma - \frac{\sigma^2}{n}\cdot$

Proof. From Theorem 3 we have

$$\varepsilon_i(G_S) \leq \begin{cases} \sqrt{\left(1-\frac{\sigma}{n}\right)^2 + d_i} & \text{if there is a self-loop on the vertex } v_i \\ \sqrt{\frac{\sigma^2}{n^2} + d_i} & \text{if there is no self-loop on the vertex } v_i. \end{cases}$$

We know that,

$$\begin{aligned} \varepsilon(G_S) &= \sum_{i=1}^{n} \varepsilon_i(G_S) = \varepsilon_1(G_S) + \sum_{i=2}^{n} \varepsilon_i(G_S) \\ &\leq \varepsilon_1(G_S) + \sqrt{(n-1)\sum_{i=2}^{n} \varepsilon_i^2(G_S)}. \end{aligned} \tag{9}$$

From (7) and (8), we have

$$\sum_{i=1}^{n} \varepsilon_i^2(G_S) = \sum_{i=1}^{n} \phi_i(|B|)^2 \leq \sum_{i=1}^{n} \phi_i(B^2) = 2m + \sigma - \frac{\sigma^2}{n} = 2M_\sigma \quad \text{and}$$

$$\sum_{i=2}^{n} \varepsilon_i^2(G_S) = \sum_{i=2}^{n} \phi_i(|B|)^2 \leq \sum_{i=1}^{n} \phi_i(B^2) - \phi_1(B^2) = 2M_\sigma - \phi_1(B^2). \tag{10}$$

Case - I: Let there be a self-loop on the vertex v_1. Then $\phi_1(B^2) =$

$\left(1-\frac{\sigma}{n}\right)^2+d_1$. So, from (10) and (8) we have

$$\sum_{i=2}^{n}\varepsilon_i^2(G_S)\le 2M_\sigma-\left(1-\frac{\sigma}{n}\right)^2-d_1 \quad \text{and} \quad \varepsilon_1(G_S)\le\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_1}.$$

So, the theorem follows from the relation (9).

Case - II: Let there be no self-loop on the vertex v_1. Then $\phi_1(B^2)=\frac{\sigma^2}{n^2}+d_1$. So, from (10) and (8) we have

$$\sum_{i=2}^{n}\varepsilon_i^2(G_S)\le 2M_\sigma-\frac{\sigma^2}{n^2}-d_1 \quad \text{and} \quad \varepsilon_1(G_S)\le\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_1}.$$

So, the theorem follows from the relation (9). ■

Remarks: The upper bounds of energy of a graph with self-loops given in Theorem 4 are better than the upper bound given by Gutman et al. in Lemma 7. We know that $\varepsilon(G_S)=\sum_{i=1}^{n}\varepsilon_i(G_S)$. Using the relation Arithmetic mean-Quadratic mean on n positive real numbers $\varepsilon_1(G_S),\ldots,\varepsilon_n(G_S)$ we have

$$\varepsilon(G_S)=\sum_{i=1}^{n}\varepsilon_i(G_S)\le\sqrt{n\left(\sum_{i=1}^{n}\varepsilon_i^2(G_S)\right)}\le\sqrt{n\left(2m+\sigma+\frac{\sigma}{n}\right)}.$$

Let $A=\sqrt{n\left(2m+\sigma+\frac{\sigma}{n}\right)}$ and $B=\sqrt{(n-1)\left(2M_\sigma-\Delta-\left(1-\frac{\sigma}{n}\right)^2\right)}+\sqrt{\left(1-\frac{\sigma}{n}\right)^2+\Delta}$ or $\sqrt{(n-1)\left(2M_\sigma-\Delta-\frac{\sigma^2}{n^2}\right)}+\sqrt{\frac{\sigma^2}{n^2}+\Delta}$ according as $v_1=v_\Delta$ has a self-loop or not. Then by Lemma 1 we can write $B\le A$. Also if $d_1=\Delta>d_n$, then $B<A$. So, the upper bounds of energy of a graph with self-loops given in the Theorem 4 is better than the upper bound given by Gutman et al. in Lemma 7.

Theorem 5. *Let G be a connected $(n.m)$-graph, and G_S be the one obtained from G by attaching σ self-loops. If Δ and δ be the maximum and* *minimum vertex degrees in G and $\varepsilon(G_S)$ be the energy of the graph G_S then*

$$\varepsilon(G_S) \leq \begin{cases} \sqrt{(n-2)\left(2M_\sigma - \Delta - \delta - 2\left(1-\frac{\sigma}{n}\right)^2\right)} + \sqrt{\left(1-\frac{\sigma}{n}\right)^2 + \Delta} \\ +\sqrt{\left(1-\frac{\sigma}{n}\right)^2 + \delta} \quad \text{if both } v_1 \text{ and } v_n \text{ has a self-loop} \\ \sqrt{(n-2)\left(2M_\sigma - \Delta - \delta - \frac{\sigma^2}{n^2} - \left(1-\frac{\sigma}{n}\right)^2\right)} + \sqrt{\frac{\sigma^2}{n^2} + \Delta} \\ +\sqrt{\left(1-\frac{\sigma}{n}\right)^2 + \delta} \quad \text{if } v_1 \text{ has no self-loop but } v_n \text{ has a self-loop} \\ \sqrt{(n-2)\left(2M_\sigma - \Delta - \delta - \frac{\sigma^2}{n^2} - \left(1-\frac{\sigma}{n}\right)^2\right)} + \sqrt{\frac{\sigma^2}{n^2} + \delta} \\ +\sqrt{\left(1-\frac{\sigma}{n}\right)^2 + \Delta} \quad \text{if } v_1 \text{ has a self-loop but } v_n \text{ has no self-loop} \\ \sqrt{(n-2)\left(2M_\sigma - \Delta - \delta - 2\frac{\sigma^2}{n^2}\right)} + \sqrt{\frac{\sigma^2}{n^2} + \delta} + \sqrt{\frac{\sigma^2}{n^2} + \Delta} \\ \quad \text{if both } v_1 \text{ and } v_n \text{ has no self-loop} \end{cases}$$

where $2M_\sigma = 2m + \sigma - \frac{\sigma^2}{n}\cdot$

Proof. From Theorem 3 we have

$$\varepsilon_i(G_S) \leq \begin{cases} \sqrt{\left(1-\frac{\sigma}{n}\right)^2 + d_i} & \text{if there is a self-loop on the vertex } v_i \\ \sqrt{\frac{\sigma^2}{n^2} + d_i} & \text{if there is no self-loop on the vertex } v_i. \end{cases}$$

We know that,

$$\begin{aligned} \varepsilon(G_S) &= \sum_{i=1}^{n} \varepsilon_i(G_S) = \varepsilon_1(G_S) + \sum_{i=2}^{n-1} \varepsilon_i(G_S) + \varepsilon_n(G_S) \\ &\leq \varepsilon_1(G_S) + \varepsilon_n(G_S) + \sqrt{(n-2)\sum_{i=2}^{n-1} \varepsilon_i^2(G_S)}. \end{aligned} \tag{11}$$

From (7) and (8), we have

$$\sum_{i=1}^{n} \varepsilon_i^2(G_S) = \sum_{i=1}^{n} \phi_i(|B|)^2 \leq \sum_{i=1}^{n} \psi_i(B^2) = 2m + \sigma - \frac{\sigma^2}{n} = 2M_\sigma \quad \text{and}$$

$$\begin{aligned}\sum_{i=2}^{n-1}\varepsilon_i^2(G_S) &\leq \sum_{i=1}^{n}\phi_i(B^2)-\phi_1(B^2)-\phi_n(B^2)\\ &= 2M_\sigma-\phi_1(B^2)-\phi_n(B^2). \qquad (12)\end{aligned}$$

Case - I: Let there be a self-loop on the both vertices v_1 and v_n. Then $\phi_1(B^2)=\left(1-\frac{\sigma}{n}\right)^2+d_1$ and $\phi_n(B^2)=\left(1-\frac{\sigma}{n}\right)^2+d_n$. So, from (12) and (8) we have

$$\sum_{i=2}^{n}\varepsilon_i^2(G_S)\leq 2M_\sigma-\left(1-\frac{\sigma}{n}\right)^2-d_1-\left(1-\frac{\sigma}{n}\right)^2-d_n \quad \text{and}$$

$$\varepsilon_1(G_S)\leq\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_1} \quad \text{and} \quad \varepsilon_1(G_S)\leq\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_n}.$$

So, the theorem follows from the relation (11).

Case - II: Let there be a self-loop on the vertex v_n and no self-loop on the vertex v_1. Then $\phi_1(B^2)=\frac{\sigma^2}{n^2}+d_1$ and $\phi_n(B^2)=\left(1-\frac{\sigma}{n}\right)^2+d_n$. So, from (12) and (8) we have

$$\sum_{i=2}^{n}\varepsilon_i^2(G_S)\leq 2M_\sigma-\frac{\sigma^2}{n^2}-d_1-\left(1-\frac{\sigma}{n}\right)^2-d_n \quad \text{and}$$

$$\varepsilon_1(G_S)\leq\sqrt{\frac{\sigma^2}{n^2}+d_1} \quad \text{and} \quad \varepsilon_1(G_S)\leq\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_n}.$$

So, the theorem follows from the relation (11).

Case - III: Let there be a self-loop on the vertex v_1 and no self-loop on the vertex v_n. Then $\phi_1(B^2)=\left(1-\frac{\sigma}{n}\right)^2+d_1$ and $\phi_n(B^2)=\frac{\sigma^2}{n^2}+d_n$. So, from (12) and (8) we have

$$\sum_{i=2}^{n}\varepsilon_i^2(G_S)\leq 2M_\sigma-\left(1-\frac{\sigma}{n}\right)^2-d_1-\frac{\sigma^2}{n^2}-d_n \quad \text{and}$$

$$\varepsilon_1(G_S)\leq\sqrt{\left(1-\frac{\sigma}{n}\right)^2+d_1} \quad \text{and} \quad \varepsilon_1(G_S)\leq\sqrt{\frac{\sigma^2}{n^2}+d_n}.$$

So, the theorem follows from the relation (11).

Case - IV: Let there be no self-loop on both the vertices v_1 and v_n. Then

$\phi_1(B^2) = \frac{\sigma^2}{n^2} + d_1$ and $\phi_n(B^2) = \frac{\sigma^2}{n^2} + d_n$. So, from (12) and (8) we have

$$\sum_{i=2}^{n} \varepsilon_i^2(G_S) \leq 2M_\sigma - \frac{\sigma^2}{n^2} - d_1 - \frac{\sigma^2}{n^2} - d_n \quad \text{and}$$

$$\varepsilon_1(G_S) \leq \sqrt{\frac{\sigma^2}{n^2} + d_1} \quad \text{and} \quad \varepsilon_1(G_S) \leq \sqrt{\frac{\sigma^2}{n^2} + d_n}.$$

So, the theorem follows from the relation (11). ■

Remarks: The upper bounds of energy of a graph with self-loops given in the Theorem 5 is a little bit more complicated than the bounds given in in the Theorem 4. By the above way, it is easy to verify that the bounds given in the Theorem 5 are better than the bounds given in the Theorem 4 and hence also better than the upper bound given by Gutman et al. in Lemma 7.

In the following theorem, we give another upper bound of the energy of a graph with self-loops.

Theorem 6. *Suppose that G is a connected graph of size m and order n $(n \geq 3)$. If G_S is the graph derived from G by attaching σ number of self-loops and $\varepsilon_S(G)$ is the energy of G_S, then*

$$\varepsilon(G_S) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2M_\sigma - \left(\frac{2m}{n}\right)^2\right)}$$

where $2M_\sigma = 2m + \sigma - \frac{\sigma^2}{n}$·

Proof. Let us consider the matrix $B = A(G_S) - \frac{\sigma}{n} I_n$. Furthermore, consider that the eigenvalues of $A(G_S)$ and B are, respectively, λ_i and μ_i for $i = 1, 2, \ldots, n$ with decreasing order. Therefore, the energy $\varepsilon(G_S)$ of the graph G_S is given by

$$\varepsilon(G_S) = \sum_{r=1}^{n} \left|\lambda_r - \frac{\sigma}{n}\right| = \sum_{r=1}^{n} |\mu_r|.$$

Now,

$$
\begin{aligned}
\varepsilon(G_S) &= \sum_{r=1}^{n} |\mu_r| = \mu_1 + \sum_{r=2}^{n} |\mu_r| \\
&\leq \mu_1 + \sqrt{(n-1)\sum_{r=2}^{n} \mu_r^2} \\
&= \mu_1 + \sqrt{(n-1)\left(\sum_{r=1}^{n} \mu_r^2 - \mu_1^2\right)} \qquad (13) \\
&\leq \mu_1 + \sqrt{(n-1)\left(2m + \sigma - \frac{\sigma^2}{n} - \mu_1^2\right)} \quad \text{(using Lemma 3)} \\
&= \mu_1 + \sqrt{(n-1)(K - \mu_1^2)} \text{ where } K = 2m + \sigma - \frac{\sigma^2}{n}\cdot \qquad (14)
\end{aligned}
$$

It is easy to show that the function $f(x) = x + \sqrt{(n-1)(K-x^2)}$ is decreasing on the interval $\left[\sqrt{\frac{K}{n}}, \sqrt{K}\right]$.

We shall now show that for $n \geq 3$, $\frac{2m}{n} \geq \sqrt{\frac{K}{n}}$.

Let us consider a real-valued function $g(x) = x - x^2$ where $0 \leq x \leq 1$. Then $g(x)$ has a maximum at $x = \frac{1}{2}$. As $0 \leq \frac{\sigma}{n} < 1$, the function $g\left(\frac{\sigma}{n}\right) = \frac{\sigma}{n} - \frac{\sigma^2}{n^2}$ has a maximum at $\frac{\sigma}{n} = \frac{1}{2}$. Thus,

$$
\sqrt{\frac{K}{n}} = \sqrt{\frac{2m}{n} + \frac{\sigma}{n} - \frac{\sigma^2}{n^2}} \leq \sqrt{\frac{2m}{n} + \frac{1}{2} - \frac{1}{4}} = \sqrt{\frac{2m}{n} + \frac{1}{4}}\cdot \qquad (15)
$$

Let us consider another real-valued function $h(x) = (3x-4)^2 - 2x^2$. Proving that the function $h(x) \geq 0$ for $x \geq 3$ is straightforward. So, for $n \geq 3$, we have

$$
(3n-4)^2 \geq 2n^2 \quad \Rightarrow \quad \frac{1}{2} \leq \left(\frac{4(n-1)-n}{2n}\right)^2\cdot \qquad (16)
$$

Since G is a connected graph with at least one edge, then $m \geq n-1$. Again since $n \geq 3$,

$$
\left(\frac{2m}{n} - \frac{1}{2}\right)^2 = \left(\frac{4m-n}{2n}\right)^2 \geq \left(\frac{4(n-1)-n}{2n}\right)^2 \geq \frac{1}{2}
$$

$$\Rightarrow \qquad \left(\frac{2m}{n}\right)^2 \geq \frac{1}{4} + \frac{2m}{n}.$$

With the positive square root applied to both sides, we get

$$\sqrt{\frac{1}{4} + \frac{2m}{n}} \leq \frac{2m}{n}. \tag{17}$$

Using the inequalities (15) and (17), for $n \geq 3$

$$\frac{2m}{n} \geq \sqrt{\frac{1}{4} + \frac{2m}{n}} \geq \sqrt{\frac{2m}{n} + \frac{\sigma}{n} - \frac{\sigma^2}{n^2}} = \sqrt{\frac{K}{n}}. \tag{18}$$

Thus, $f(x)$ is decreasing in $\left[\frac{2m}{n}, \sqrt{K}\right]$ also.
From Lemma 6, we have $\frac{2m}{n} \leq \mu_1 < \sqrt{K}$.
Hence,

$$\begin{aligned} f\left(\frac{2m}{n}\right) &\geq f(\mu_1) \\ \Rightarrow \frac{2m}{n} + \sqrt{(n-1)\left(K - \left(\frac{2m}{n}\right)^2\right)} &\geq \mu_1 + \sqrt{(n-1)(K-\mu_1^2)}. \end{aligned}$$

Thus, from (14), we have

$$\begin{aligned} \varepsilon(G_S) &\leq \mu_1 + \sqrt{(n-1)(K-\mu_1^2)} \\ &\leq \frac{2m}{n} + \sqrt{\left(K - \left(\frac{2m}{n}\right)^2\right)(n-1)} \\ &\leq \frac{2m}{n} + \sqrt{(n-1)\left(2m + \sigma - \frac{\sigma^2}{n} - \left(\frac{2m}{n}\right)^2\right)} \\ &= \frac{2m}{n} + \sqrt{(n-1)\left(2M_\sigma - \left(\frac{2m}{n}\right)^2\right)}. \end{aligned}$$

■

3 Lower bounds of energy of a graph with self-loops

Here are a few lower bounds of $\varepsilon(G_S)$, provided by Liu et al. [11].

Lemma 12. *[11] Let G be an (n, m) graph and G_S is the graph derived from G by attaching σ self-loops. If Δ and δ are the minimum and maximum degree in G_S respectively, then*

$$\varepsilon(G_S) \geq \frac{4\frac{\sigma}{n}(m+\sigma) - 2\Delta\sqrt{n(2m+\sigma)}}{\Delta - \delta}.$$

Lemma 13. *[11] With the same notations as in Lemma 7,*

$$\varepsilon(G_S) \geq \sqrt{2m + \sigma - \frac{\sigma^2}{n}}.$$

Lemma 14. *[11] With the same notations as in Lemma 7,*

$$\varepsilon(G_S) \geq \frac{4m + 2\sigma - 2\frac{\sigma^2}{n}}{s(G_S)}$$

where $s(G_S)$ is the diameter of spectrum of $A(G_S)$.

The lower bound given in Lemma 12 is become meaningless if $\Delta = \delta$ in G_S. The following lower bound is given by Sehtty and Bhat [16].

Lemma 15. *[14, 16] With the same notations as in Lemma 7,*

$$\varepsilon(G_S) \geq \sqrt{4m + 2\left(\sigma - \frac{\sigma^2}{n}\right)}$$

with equality holds if and only if G_S is totally disconnected graph with $\sigma = 0$ or $\sigma = n$.

Remarks: The above lower bound of energy of a graph with self-loops, $\sqrt{4m + 2\left(\sigma - \frac{\sigma^2}{n}\right)}$, is better than the lower bound $\sqrt{2m + \left(\sigma - \frac{\sigma^2}{n}\right)}$ given in the Lemma 13.

Now, we provide a lower bound of $\varepsilon(G_S)$ in terms of the number of vertices n and the number of edges m.

Theorem 7. *With the same notations as in Theorem 1, if $\varepsilon(G_S)$ is the energy of G_S, then*

$$\varepsilon(G_S) \geq \frac{4m}{n}\cdot$$

Proof. Let the eigenvalues of $A(G_S) - \frac{\sigma}{n}I_n$ are $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. Then

$$\varepsilon(G_S) = \sum_{i=1}^{n} |\mu_i| \text{ and } \sum_{i=1}^{n} \mu_i = 0.$$

If μ_1 be the spectral radius of $A(G_S) - \frac{\sigma}{n}I_n$, then $\varepsilon(G_S) \geq 2\mu_1$. From Lemma 6, we can write $\mu_1 \geq \frac{2m}{n}$. So, $\varepsilon(G_S) \geq \frac{4m}{n}\cdot$ ■

Theorem 8. *Suppose G be an (n,m)-graph and let G_S be the one obtained from G by attaching a self-loop with σ $(1 \leq \sigma < n)$ number of vertices of G. If $A(G_S)$ is the adjacency matrix of G_S and $B = A(G_S) - \frac{\sigma}{n}I_n$, then $\varepsilon(G_S)$, the energy of G_S satisfies the following relation,*

$$\varepsilon(G_S) \geq \sqrt{2m + \sigma - \frac{\sigma^2}{n} + n(n-1)\,|\det(B)|^{\frac{2}{n}}}.$$

Proof.

$$\varepsilon^2(G_S) = \left(\sum_{i=1}^{n} |\mu_i|\right)^2 = \sum_{i=1}^{n} |\mu_i|^2 + \sum_{\substack{1\leq i,j\leq n \\ i\neq j}} |\mu_i||\mu_j|. \tag{19}$$

Using arithmetic mean-geometric mean inequality on $|\mu_i||\mu_j|$, we have

$$\frac{\sum\limits_{\substack{1\leq i,j\leq n \\ i\neq j}} |\mu_i||\mu_j|}{n(n-1)} \geq \left(\prod_{\substack{1\leq i,j\leq n \\ i\neq j}} |\mu_i||\mu_j|\right)^{\frac{1}{n(n-1)}} = \left(\prod_{1\leq i\leq n} |\mu_i|\right)^{\frac{2}{n}}.$$

Thus, From (19)

$$\varepsilon^2(G_S) \geq \sum_{i=1}^{n} |\mu_i|^2 + \left(\prod_{1\leq i\leq n} |\mu_i|\right)^{\frac{2}{n}} n(n-1)$$

$$= \quad 2m + \sigma - \frac{\sigma^2}{n} + n(n-1)\,|\det(B)|^{\frac{2}{n}} \cdot$$

Therefore, the result follows. ■

Next, we obtain a lower bound of $\varepsilon(G_S)$ and show that in some cases, that lower bound is better than all other existing lower bounds as observed from the comparison table provided in Section 4.

Theorem 9. *With the same notation as in Theorem 8,*

$$\varepsilon(G_S) \geq \frac{2m}{n} + n - 1 + \ln|\det(B)| - \ln\frac{2m}{n}\cdot$$

Proof. Let the eigenvalues of B be $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. From Theorem 1, we know that B is non-singular, i.e., $|\mu_i| > 0$ for $i = 1, 2, \ldots, n$.

Consider a real-valued function g such that $g : \mathbb{R}^+ \to \mathbb{R}$ and

$$g(x) = x - 1 - \ln(x).$$

It is trivial to verify that the function $g(x)$ is decreasing on the interval $0 < x \leq 1$ and increasing on the interval $[1, \infty)$. So, for all $x > 0$

$$g(x) \geq g(1) \qquad \Rightarrow \qquad x \geq 1 + \ln(x).$$

Thus,

$$\begin{aligned}
\varepsilon(G_S) &= \mu_1 + \sum_{i=2}^{n} |\mu_i| \\
&\geq \mu_1 + n - 1 + \sum_{i=2}^{n} \ln|\mu_i| \\
&= \mu_1 + n - 1 + \ln\prod_{i=2}^{n} |\mu_i| \\
&= \mu_1 + n - 1 + \ln|\det(B)| - \ln\mu_1. \qquad (20)
\end{aligned}$$

Again, consider the function $h : \mathbb{R}^+ \to \mathbb{R}$ such that

$$h(x) = x + n - 1 + \ln|\det(B)| - \ln x.$$

Clearly, in the interval $1 \leq x \leq n$, the function $h(x)$ is increasing. From (3), we have $\mu_1 \geq \frac{2m}{n}\cdot$ Since $1 \leq \frac{2m}{n} \leq \mu_1 \leq n$, it follows that

$$h(\mu_1) \geq h\left(\frac{2m}{n}\right)$$
$$\Rightarrow \quad h(\mu_1) \geq \frac{2m}{n} + n - 1 + \ln|\det(B)| - \ln\frac{2m}{n}\cdot$$

Hence, the theorem follows from (20). ■

Remarks: Applying Theorem 9 to the Figure 3, the resultant lower bound is 4.0364, which is better than all other existing lower bounds.

4 Comparison of bounds

In this section, we compare the numerical values of the upper bounds and lower bounds of the energy of some graphs with self-loops (Figures 1 – 8).

It is found from Table 1 that the upper bounds given in Theorem 4 and Theorem 5 are always better than that given in Lemma 7 and hence from those given in Lemma 10 and Lemma 11, as already discussed in Section 2. It is also found that the bound given in Theorem 6 is better than all other bounds for the considered graphs. Although the goodness of this bound could not be established analytically, it is assured that at least in some cases it outperforms.

It is found from Table 2 that the Lemma 12 for Figure 2 and Figure 6 gives no lower bounds as $\Delta = \delta$ for these graphs and yields negative values for the other graphs. As already mentioned in Section 3, the lower bounds obtained from Lemma 15 are always better than those obtained from Lemma 13. Although we could not establish analytically, Lemma 14 yields better lower bounds than those obtained from Lemma 15 and from Lemma 13. Again, the lower bounds obtained from Theorem 7, Theorem 8 and Theorem 9 are incomparable with those obtained from Lemma 14 and Lemma 15.

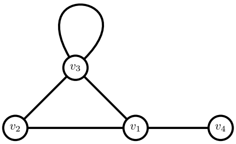

Figure 1

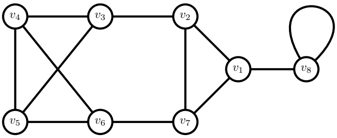

Figure 2

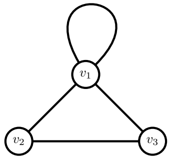

Figure 3

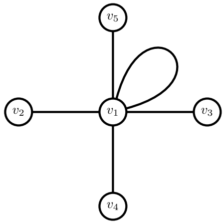

Figure 4

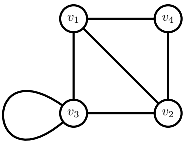

Figure 5

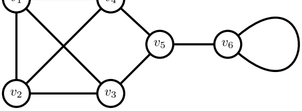

Figure 6

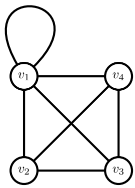

Figure 7

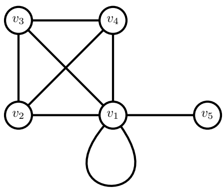

Figure 8

Figure	Lemma 7	Lemma 8	Lemma 9	Lemma 10	Lemma 11
1	5.9161	7.8579	7.9369	6.8030	6.3750
2	13.5277	14.3228	14.9058	17.1357	15.4375
3	4.4721	5.1611	5.0972	5.1694	4.8333
4	6.6332	10.2845	10.4000	7.1568	6.9000
5	6.5574	7.6711	7.7113	8.1106	7.3750
6	10.0499	10.9436	11.3645	12.6364	11.4167
7	7.1414	7.2678	7.2042	9.4489	8.3750
8	8.6023	10.3714	10.4990	11.0463	9.9000

Figure	Theorem 4	Theorem 5	Theorem 6	Energy
1	5.8807	5.8222	5.7749	5.0164
2	13.5270	13.4846	13.1031	12.3012
3	4.4694	4.4694	4.3094	4.1617
4	6.2333	6.2333	6.5960	4.7232
5	6.5523	6.5402	6.1742	5.6858
6	10.0483	10.0020	9.6389	8.2400
7	7.1374	7.1374	6.3541	6.1056
8	8.5290	8.4045	8.0763	7.2000

Table 1. Comparison of different upper bounds.

Figure	Lemma 12	Lemma 13	Lemma 15	Lemma 14
1	−14.333	2.9580	4.1833	4.4143
2		4.7828	6.7639	9.3528
3	−15.664	2.5820	3.6515	3.9053
4	−15.299	2.9665	4.1952	4.2685
5	−23.533	3.2787	4.6368	5.1726
6		4.1028	5.8023	6.5069
7	−32.555	3.5707	5.0498	5.9264
8	−20.051	3.8471	5.4406	6.7056

Figure	Theorem 7	Theorem 8	Theorem 9	Energy
1	4.000	4.3659	4.0034	5.0164
2	5.500	11.2494	11.2020	12.3012
3	4.000	4.0528	4.0364	4.1617
4	3.200	3.7321	1.7278	4.7232
5	5.000	5.0078	4.9384	5.6858
6	5.333	6.5402	6.2496	8.2400
7	6.000	5.6776	5.8709	6.1056
8	5.600	6.4752	6.5324	7.2000

Table 2. Comparison of different lower bounds.

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