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New Bounds on the Energy of Graphs with Self–Loops

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Abstract

Let G_σ be the graph obtained from a simple graph G of order n by adding σ self-loops, one self-loop at each vertex in $S \subseteq V(G)$. Let $\lambda_1(G_\sigma), \lambda_2(G_\sigma), \ldots, \lambda_n(G_\sigma)$ be the eigenvalues of G_σ. The energy of G_σ, denoted by $\mathscr{E}(G_\sigma)$, is defined as $\mathscr{E}(G_\sigma) = \sum\limits_{i=1}^{n} \left|\lambda_i(G_\sigma) - \frac{\sigma}{n}\right|$. In this paper, using various analytic inequalities and previously established results, we derive several new lower and upper bounds on $\mathscr{E}(G_\sigma)$.

1 Introduction

Let G_σ be the graph obtained from the simple graph G, which has n vertices and m edges, by attaching σ self-loops, one self-loop at each vertex in $S \subseteq V(G)$.

The *adjacency matrix* $A(G_\sigma) = (a_{ij})_{n\times n}$ of G_σ is a square and symmetric matrix of order n. The (i, j)-element is defined as:

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$$(a_{ij})_{n\times n} = \begin{cases} 1, & \text{if vertices } v_i \text{ and } v_j \text{ are adjacent;} \\ 0, & \text{if vertices } v_i \text{ and } v_j \text{ are not adjacent;} \\ 1, & \text{if } i = j \text{ and } v_i \text{ has a loop;} \\ 0, & \text{if } i = j \text{ and } v_i \text{ has no loop.} \end{cases}$$

Since $A(G_\sigma)$ is a real and symmetric matrix, all its eigenvalues are real. We denote the eigenvalues of $A(G_\sigma)$ as $\lambda_1, \lambda_2, \ldots, \lambda_n$, with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. All eigenvalues of a graph G_σ with each respective algebraic multiplicity give the *spectrum* of G_σ, denoted by $\mathrm{Spec}(G_\sigma)$. The largest absolute value of the graph eigenvalues is called the *spectral radius.* The *energy of* G_σ was recently defined [15] as:

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

In 1978, Gutman [12] introduced the concept of graph energy, denoted as $\mathscr{E}(G)$, for a graph G. Graph energy is a vital topological indicator used to approximate the total energy of π-electrons in conjugated hydrocarbons and plays a significant role in chemistry. Graph energy has been applied to various areas, including mathematics and mathematical chemistry [5, 6, 16, 17].

Self-loop graphs have been found to play a significant role in the mathematical study of heteroconjugated molecules [13–15]. In 2022, Gutman et al. introduced the concept of graph energy with self-loops, which carries distinct chemical significance [15]. Notably, several results regarding the energy of self-loop graphs have been obtained [2, 15, 18, 24].

The complete graph of order n is denoted by K_n and the complete bipartite graph with parts M and N with sizes m and n, is denoted as $K_{m,n}$. In [2], Akbari et al. established a necessary and sufficient condition for the bipartiteness of a connected graph G, involving the spectra $\mathrm{Spec}(G_\sigma)$ and $\mathrm{Spec}(G_{\bar{\sigma}})$, where $G_{\bar{\sigma}}$ is the the graph obtained from G, by attaching $\bar{\sigma}$ self-loops, one self-loop at each vertex in $V(G)\backslash S$. In [2], it was also proven that $\mathscr{E}(G_\sigma) \geq \mathscr{E}(G)$ when G is bipartite. Additionally, they derived an upper bound for $\lambda_1(G_\sigma)$ and determined the spectra of

Spec $((K_n)\sigma)$ and Spec$((Km,n)_\sigma)$ for all $n, m \geq 1$.

In [18], Jovanović et al. presented a set of graphs that disproves the conjecture that for all simple graphs G, $\mathscr{E}(G_\sigma) > \mathscr{E}(G)$, where $1 \leq \sigma \leq n-1$ [15]. In [24], the authors obtained graphs such that $\mathscr{E}(G_\sigma) = \mathscr{E}(G)$ and $1 \leq \sigma \leq n-1$. More on topological indices with self-loops refer to [3,4,25].

In this paper, we introduce novel lower and upper bounds for the energy of graphs with self-loops.

Before proceeding further, we introduce some necessary notation. The *maximum degree* of a graph G, denoted by $\Delta(G) = \Delta$, is the degree of the vertex with the greatest number of edges incident to it. The *minimum degree* of a graph G, denoted by $\delta(G) = \delta$, is the degree of the vertex with the least number of edges incident to it. The *graph spread of* G, denoted by $s(G)$, is the maximum absolute difference between any two eigenvalues of the adjacency matrix of G.

2 Lower bounds for the energy of graphs with self-loops

In this section, we establish lower bounds for $\mathscr{E}(G_\sigma)$ based on the k-th spectral moment. Additionally, we derive lower bounds for $\mathscr{E}(G_\sigma)$ that are dependent on the parameters n, m, σ, δ, and Δ. Finally, by employing analytic inequalities and previously established results, we will provide lower bounds for $\mathscr{E}(G_\sigma)$ linked to the graph spread ($s(G)$) and the spectral radius (λ_1) of the graph.

There are known lower bounds of graph energy $\mathscr{E}(G)$ associated with the k-th spectral moment $M_k(G)$ [8,19,27]. In a similar manner to $M_k(G)$, we define the k-th spectral moment of a self-loop graph G_σ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ as

$$M_k(G_\sigma) = \sum_{i=1}^{n} \lambda_i^k \ .$$

Specifically, for $k = 1, 2$, according to [15], we have the following lemma:

Lemma 1. *[15] Let G_σ be a graph of order n with m edges and σ self-loops,* *and let* $\lambda_1, \lambda_2, \ldots, \lambda_n$ *be its eigenvalues. Then,*

$$M_1(G_\sigma) = \sum_{i=1}^{n} \lambda_i = \sigma\,; \;\; M_2(G_\sigma) = \sum_{i=1}^{n} \lambda_i^2 = 2m + \sigma \ .$$

Lemma 2. *[10] Let* $a_i, b_i, p_i,$ *and* q_i *be sequences of nonnegative real numbers, and* $\alpha, \beta > 1$ *with* $\frac{1}{\alpha} + \frac{1}{\beta} = 1$*. Then, the following inequality holds:*

$$\alpha \sum_{i=1}^{n} q_i \sum_{i=1}^{n} p_i b_i^\beta + \beta \sum_{i=1}^{n} p_i \sum_{i=1}^{n} q_i a_i^\alpha \geq \alpha\beta \sum_{i=1}^{n} p_i b_i \sum_{i=1}^{n} q_i a_i \ .$$

Lemma 3. *[10] Let* a_i, b_i, c_i *and* d_i *are sequences of real numbers and* p_i, q_i *are nonnegative for* $i = 1, 2, \ldots, n$*. Then, the following inequality is valid*

$$\sum_{i=1}^{n} p_i a_i^2 \sum_{i=1}^{n} q_i b_i^2 + \sum_{i=1}^{n} p_i c_i^2 \sum_{i=1}^{n} q_i d_i^2 \geq 2 \sum_{i=1}^{n} p_i a_i c_i \sum_{i=1}^{n} q_i b_i d_i \ .$$

Theorem 1. *Let* G_σ *be a self-loop graph with* m *edges,* n *vertices and* σ *self-loops. Let* $\lambda_1, \lambda_2 \ldots, \lambda_n$ *be the eigenvalues of* G_σ*. Then,*

$$M_k(G_\sigma) \geq \frac{k}{2}(2m+\sigma) - (\frac{k}{2} - 1)n\,,$$

where $k \in \mathbb{Z}^+$ *and* $k \geq 3$*.*

Proof. Using Lemma 2, for $i = 1, 2, \ldots, n$, let $\alpha = \frac{k}{2}, \beta = \frac{k}{k-2}, a_i = \lambda_i^2, b_i = p_i = q_i = 1$. Then,

$$\begin{aligned} \frac{k}{2} \sum_{i=1}^{n} 1 \cdot \sum_{i=1}^{n} 1 + \frac{k}{k-2} \sum_{i=1}^{n} 1 \cdot \sum_{i=1}^{n} \lambda_i^k &\geq \frac{k^2}{2(k-2)} \sum_{i=1}^{n} 1 \cdot \sum_{i=1}^{n} \lambda_i^2 \\ \frac{k}{2} n^2 + \frac{k}{k-2} n \sum_{i=1}^{n} \lambda_i^k &\geq \frac{k^2}{2(k-2)} n(2m+\sigma) \\ \sum_{i=1}^{n} \lambda_i^k &\geq \frac{k}{2}(2m+\sigma) - (\frac{k}{2} - 1)n \ . \end{aligned}$$

■

By setting $\sigma = 0$, it can be extended to simple graphs, leading to the following corollary.

Corollary 1. *Let G be a simple graph with n vertices and m edges. Let $\lambda_1, \lambda_2 \dots, \lambda_n$ be the eigenvalues of G. Then*

$$M_k(G) \geq km - \frac{k-2}{2}n\,,$$

where $k \in \mathbb{Z}^+$ and $k \geq 3$.

Remark 1. If $k = 2$, by the above two results, we have $M_2(G_\sigma) \geq 2m+\sigma$, and $M_2(G) \geq 2m$. Noting that in this case our bounds in Theorem 1 and Corollary 1 are sharp.

Theorem 2. *Let G_σ be a self-loop graph with m edges, n vertices and σ self-loops. Let $\lambda_1, \lambda_2 \dots, \lambda_n$ be the eigenvalues of G_σ. Let k be even and $k \geq 2$. Then,*

(1) $M_k(G_\sigma) \geq \sqrt{\frac{(k+2)^2-8}{8}(2m+\sigma)^2 + \frac{(k-2)^2}{8}n^2 - \frac{k^2-4}{4}(2m+\sigma)n}\,;$

(2) $M_k(G_\sigma) \geq \sqrt{\frac{k^2}{8}(2m+\sigma)^2 + \frac{k^2-8k+8}{8}n^2 - \frac{k^2-4k}{4}(2m+\sigma)n}\ .$

Proof. By applying Lemma 3 and Theorem 1.

(1) For $i = 1, 2, \dots, n$, let $p_i = q_i = \lambda_i^2$, $a_i = b_i = \lambda_i^{\frac{k-2}{2}}$, $c_i = d_i = 1$. Then $\left(\sum\limits_{i=1}^{n} \lambda_i^k\right)^2 + \left(\sum\limits_{i=1}^{n} \lambda_i^2\right)^2 \geq 2\left(\sum\limits_{i=1}^{n} \lambda_i^{\frac{k+2}{2}}\right)^2$. That is

$$\left(\sum_{i=1}^{n} \lambda_i^k\right)^2 + (2m+\sigma)^2 \geq 2\left(\frac{k+2}{4}(2m+\sigma) - \frac{k-2}{4}n\right)^2$$

Thus, we get

$$\sum_{i=1}^{n} \lambda_i^k \geq \sqrt{\frac{(k^2+4k-4)}{8}(2m+\sigma)^2 + \frac{(k-2)^2}{8}n^2 - \frac{k^2-4}{4}(2m+\sigma)n}\ .$$

(2) For $i = 1, 2, \dots, n$, let $p_i = q_i = c_i = d_i = 1$, $a_i = b_i = \lambda_i^{\frac{k}{2}}$. Then

$\left(\sum\limits_{i=1}^{n}\lambda_i^k\right)^2+\sum\limits_{i=1}^{n}1\cdot\sum\limits_{i=1}^{n}1\geq 2\left(\sum\limits_{i=1}^{n}\lambda_i^{\frac{k}{2}}\right)^2$. That is

$$\left(\sum_{i=1}^{n}\lambda_i^k\right)^2+n^2\geq 2\left(\frac{k}{4}(2m+\sigma)-\frac{k-4}{4}n\right)^2.$$

Then, we get

$$\sum_{i=1}^{n}\lambda_i^k\geq\sqrt{\frac{k^2}{8}(2m+\sigma)^2+\frac{k^2-8k+8}{8}n^2-\frac{k^2-4k}{4}(2m+\sigma)n}\ .$$

■

Setting $\sigma=0$, it can be extended to simple graphs.

Corollary 2. *For a simple graph G with m edges and n vertices, where $\lambda_1,\lambda_2\ldots,\lambda_n$ are the eigenvalues of G, and assuming that k is even and $k\geq 2$. Then,*

$$(1)\ M_k(G)\geq\sqrt{\frac{k^2+4k-4}{2}m^2+\frac{(k-2)^2}{8}n^2-\frac{k^2-4}{2}mn}\,;$$

$$(2)\ M_k(G)\geq\sqrt{\frac{k^2}{2}m^2+\frac{k^2-8k+8}{8}n^2-\frac{k^2-4k}{2}mn}\ .$$

Remark 2. If $k=2$, then (1) in Theorem 2 and Corollary 2 simplifies to $M_2(G_\sigma)\geq 2m+\sigma$ and $M_2(G)\geq 2m$, indicating that our bounds are sharp in this scenario.

Lemma 4. *[27] Let $a_1,a_2,...,a_h$ be positive real numbers, where $h>1$. And let r,s,t be the non-negative real numbers, such that $4r=s+t+2$. Then*

$$\left[\sum_{i=1}^{h}(a_i)^r\right]^4\leq\left(\sum_{i=1}^{h}a_i\right)^2\cdot\sum_{i=1}^{h}(a_i)^s\cdot\sum_{i=1}^{h}(a_i)^t\,.$$

If $(s,t)\neq(1,1)$, then equality holds if and only if $a_1=a_2=\cdots=a_h$.

Theorem 3. *Let G_σ be a self-loop graph, and let r, s, and t be even, such that $4r=s+t+2$. Then, we have the inequality:*

$$\mathscr{E}(G_\sigma) \geq \frac{M_r(G_\sigma)^2}{\sqrt{M_t(G_\sigma)\cdot M_s(G_\sigma)}} + \sigma - \frac{2h\sigma}{n}\,,$$

where h is the number of nonzero eigenvalues in G_σ.

Before proceeding to the proof, we recall the following useful absolute value inequalities. For any real numbers a and b, it holds: $|a| - |b| \leq |a - b| \leq |a| + |b|$. Applying these inequalities to $\mathscr{E}(G_\sigma)$, we get:

$$\begin{aligned}\sum_{i=1}^{n}|\lambda_i| - \sigma = \sum_{i=1}^{n}\left(|\lambda_i| - \frac{\sigma}{n}\right) \leq \sum_{i=1}^{n}\left|\lambda_i - \frac{\sigma}{n}\right| &= \mathscr{E}(G_\sigma)\\ \leq \sum_{i=1}^{n}\left(|\lambda_i| + \frac{\sigma}{n}\right) &= \sum_{i=1}^{n}|\lambda_i| + \sigma\ .\end{aligned}$$

Proof. Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of G_σ, and suppose that $\lambda_{j1} \geq \lambda_{j2} \geq \cdots \lambda_{jh}$ are the nonzero eigenvalues of G_σ. Since G_σ has at least one edge, we have $\lambda_{j1} = \lambda_1 > 0$ and $\lambda_{jh} = \lambda_n < 0$. Using Lemma 4 for the positive numbers $a_i = |\lambda_{ji}|,\ i = 1, 2, \cdots, h$, and noting that r is even, we have, $\sum_{i=1}^{h}(a_i)^r = \sum_{i=1}^{h}|\lambda_{ji}|^r = \sum_{i=1}^{h}\lambda_{ji}^r = M_r(G_\sigma)$, and then

$$M_r(G_\sigma)^4 \leq \left(\sum_{i=1}^{h}|\lambda_{ji}|\right)^2 \cdot M_s(G_\sigma)\cdot M_t(G_\sigma)\ .$$

Furthermore,

$$\begin{aligned}\sum_{i=1}^{h}\left|\lambda_{ji} - \frac{\sigma}{n}\right| + \frac{(n-h)\sigma}{n} &\geq \sum_{i=1}^{h}|\lambda_{ji}| - \frac{h\sigma}{n} + \frac{(n-h)\sigma}{n}\\ &\geq \frac{M_r(G_\sigma)^2}{\sqrt{M_s(G_\sigma)\cdot M_t(G_\sigma)}} - \frac{h\sigma}{n} + \frac{(n-h)\sigma}{n}\ .\end{aligned}$$

That is

$$\mathscr{E}(G_\sigma) \geq \frac{M_r(G_\sigma)^2}{\sqrt{M_t(G_\sigma)\cdot M_s(G_\sigma)}} + \sigma - \frac{2h\sigma}{n}\ .$$

■

Apply Theorem 3 to $(s, t) = (2, 4)$, we have the following corollary.

Corollary 3. *Let G_σ be a graph of order n with m edges and σ self-loops. Let h be the number of nonzero eigenvalues of G_σ. Then*

$$\mathscr{E}(G_\sigma) \geq (2m+\sigma)\sqrt{\frac{2m+\sigma}{M_4(G_\sigma)}} + \sigma - \frac{2h\sigma}{n} \ .$$

By the following lemma, we will obtain a (n, m, σ)-type lower bound for $\mathscr{E}(G_\sigma)$.

Lemma 5. *[15] Let G_σ be a graph of order n with m edges and σ self-loops. Let $\lambda_1, \lambda_2 \cdots \lambda_n$ be its eigenvalues. Then,*

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

Theorem 4. *Let G_σ be a graph of order n with m edges and σ self-loops. Then,*

$$\mathscr{E}(G_\sigma) \geq \sqrt{2m + \sigma - \frac{\sigma^2}{n}} \ .$$

Proof. Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of G_σ.

$$\mathscr{E}(G_\sigma)^2 = \left(\sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|\right)^2 \geq \sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|^2 = 2m + \sigma - \frac{\sigma^2}{n} \ .$$

Hence, $\mathscr{E}(G_\sigma) \geq \sqrt{2m + \sigma - \frac{\sigma^2}{n}}$. ■

In order to prove Lemma 7, we need the following lemma.

Lemma 6. *[7] Let $y = (y_1, y_2, \ldots, y_n)^t$ in $\mathbb{C}^n$ then*

$$\sum_{i=1}^{n} |y_i| \leq \sqrt{n \sum_{i=1}^{n} |y_i|^2} \ .$$

Equality holds if and only if $|y_1| = \cdots = |y_n| = \sqrt{\frac{1}{n} \sum_{i=1}^{n} |y_i^2|}$.

The inequality of next Lemma will be used in the proof of Theorem 5.

Lemma 7. *Let G_σ be a self-loop graph with m edges, n vertices and σ self-loops. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G_σ. Then,*

$$\sum_{i=1}^{n} |\lambda_i| \leq \sqrt{n(2m+\sigma)}\ .$$

Proof. By applying Lemma 6, we have

$$\sum_{i=1}^{n} |\lambda_i| \leq \sqrt{n \sum_{i=1}^{n} |\lambda_i|^2} = \sqrt{n(2m+\sigma)}\ .$$

■

Lemma 8. *[22] Let $y = (y_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, n$, be real number sequences such that $\sum\limits_{i=1}^{n} |y_i| = 1$, and $\sum\limits_{i=1}^{n} y_i = 0$. Then,*

$$\left| \sum_{i=1}^{n} b_i y_i \right| \leq \frac{1}{2} \left(\max_{1\leq i\leq n} (b_i) - \min_{1\leq i\leq n} (b_i) \right).$$

Theorem 5. *Let G_σ be a self-loop graph with m edges, n vertices and σ self-loops. Let $d_1, d_2, \ldots, d_n$ be the degree of vertices in G_σ and $\delta = \min\limits_{1\leq i\leq n} d_i$, $\Delta = \max\limits_{1\leq i\leq n} d_i$. Then,*

$$\mathscr{E}(G_\sigma) \geq \frac{4\frac{\sigma}{n}(m+\sigma) - 2\Delta\sqrt{n(2m+\sigma)}}{\Delta - \delta}\ .$$

Proof. Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of G_σ. Set $b_i = d_i$ and $y_i = \frac{\lambda_i - \frac{\sigma}{n}}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|}$ for each $i = 1, 2, \ldots, n$. Using the fact $\sum\limits_{i=1}^{n} \lambda_i = \sigma$, we obtain $\sum\limits_{i=1}^{n} y_i = \frac{\sum\limits_{i=1}^{n} \lambda_i - \sigma}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} = 0$, $\sum\limits_{i=1}^{n} |y_i| = \frac{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} = 1$, and $\sum\limits_{i=1}^{n} d_i = 2(m+\sigma)$. By using Lemma 8, we have

$$\left| \sum_{i=1}^{n} b_i y_i \right| = \left| \frac{\frac{\sigma}{n} \sum\limits_{i=1}^{n} d_i}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} - \frac{\sum\limits_{i=1}^{n} d_i \lambda_i}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} \right| \leq \frac{1}{2}(\Delta - \delta)\ .$$

Since $\left|\sum_{i=1}^{n} d_i\lambda_i\right| \leq \sum_{i=1}^{n} |d_i\lambda_i| \leq \Delta \sum_{i=1}^{n} |\lambda_i|$ and applying Lemma 7, we have

$$\left|\frac{\frac{\sigma}{n}\sum_{i=1}^{n} d_i}{\sum_{i=1}^{n}|\lambda_i - \frac{\sigma}{n}|} - \frac{\sum_{i=1}^{n} d_i\lambda_i}{\sum_{i=1}^{n}|\lambda_i - \frac{\sigma}{n}|}\right| \geq \frac{\frac{\sigma}{n}\sum_{i=1}^{n} d_i}{\sum_{i=1}^{n}|\lambda_i - \frac{\sigma}{n}|} - \left|\frac{\sum_{i=1}^{n} d_i\lambda_i}{\sum_{i=1}^{n}|\lambda_i - \frac{\sigma}{n}|}\right|$$
$$\geq \frac{\frac{\sigma}{n}2(m+\sigma)}{\mathscr{E}(G_\sigma)} - \frac{\Delta\sqrt{n(2m+\sigma)}}{\mathscr{E}(G_\sigma)} .$$

Combining two inequalities above, we have

$$\mathscr{E}(G_\sigma) \geq \frac{4\frac{\sigma}{n}(m+\sigma) - 2\Delta\sqrt{n(2m+\sigma)}}{\Delta - \delta} .$$

■

The spread of a complex matrix A is defined as the diameter of its spectrum: $s(A) = \max_{i,j} |\lambda_i - \lambda_j| = \lambda_1 - \lambda_n$. If A is the adjacency matrix of G_σ, then $s(A) = s(G_\sigma)$.

Theorem 6. *Let G be a simple connected graph with m edges, n vertices. Let G_σ be a graph obtained from G by attaching σ self-loops. Then,*

$$\mathscr{E}(G_\sigma) \geq \frac{4m + 2\sigma - 2\frac{\sigma^2}{n}}{s(G_\sigma)} .$$

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G_σ. Using Lemma 8, we set $b_i = \lambda_i$ and $y_i = \frac{\lambda_i - \frac{\sigma}{n}}{\sum|\lambda_i - \frac{\sigma}{n}|}$ for each $i = 1, 2, \ldots, n$. Since $\sum_{i=1}^{n} \lambda_i^2 = 2m + \sigma$, we get

$$\left|\sum_{i=1}^{n} b_i y_i\right| = \left|\sum_{i=1}^{n} \frac{\lambda_i^2 - \frac{\sigma}{n}\lambda_i}{\sum_{i=1}^{n}|\lambda_i - \frac{\sigma}{n}|}\right| \leq \frac{1}{2}\left(\max_{1\leq i\leq n}(b_i) - \min_{1\leq i\leq n}(b_i)\right) = \frac{1}{2}s(G_\sigma) .$$

Furthermore,

$$\left| \frac{\sum\limits_{i=1}^{n} \lambda_i^2 - \frac{\sigma}{n} \sum\limits_{i=1}^{n} \lambda_i}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} \right| \geq \frac{\sum\limits_{i=1}^{n} \lambda_i^2}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} - \frac{\left| \frac{\sigma}{n} \sum\limits_{i=1}^{n} \lambda_i \right|}{\sum\limits_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|} = \frac{2m + \sigma - \frac{\sigma^2}{n}}{\mathscr{E}(G_\sigma)} .$$

Combining two inequalities above, we have $\mathscr{E}(G_\sigma) \geq \dfrac{4m + 2\sigma - 2\frac{\sigma^2}{n}}{s(G_\sigma)}$. ■

Lemma 9. *Let G_σ be a graph of order n with m edges and σ self-loops. Then,*

$$s(G_\sigma) \leq \lambda_1 + \sqrt{2m + \sigma - \lambda_1^2} \leq \sqrt{2(2m + \sigma)} .$$

Proof. Since $\sum\limits_{i=1}^{n} \lambda_i^2 = 2m + \sigma$, we have $\lambda_1^2 + \lambda_n^2 \leq 2m + \sigma$. That is $-\sqrt{2m + \sigma - \lambda_1^2} \leq \lambda_n \leq \sqrt{2m + \sigma - \lambda_1^2}$. Then,

$$s(G_\sigma) = \lambda_1 - \lambda_n \leq \lambda_1 + \sqrt{2m + \sigma - \lambda_1^2} .$$

Now we consider the function $F(x) = x + \sqrt{2m + \sigma - x^2}$, where $x < \sqrt{2m + \sigma}$. By taking its first derivation, we can find that $F(x)$ takes the maximum value $\sqrt{2(2m + \sigma)}$, when x is equal to $\sqrt{\frac{2m+\sigma}{2}}$. Thus $s(G_\sigma) \leq \sqrt{2(2m + \sigma)}$. ■

Combining Theorem 6 and Lemma 9, we immediately obtain the following consequence.

Corollary 4. *For any connected self-loop graph G_σ with m edges and σ self-loops, we have*

$$\mathscr{E}(G_\sigma) \geq \frac{4m + 2\sigma - 2\frac{\sigma^2}{n}}{\lambda_1 + \sqrt{2m + \sigma - \lambda_1^2}} ;$$

$$\mathscr{E}(G_\sigma) \geq \frac{\sqrt{2}(2m + \sigma - \frac{\sigma^2}{n})}{\sqrt{2m + \sigma}} .$$

Lemma 10. *[9] Let a_i and b_i be the real numbers satisfy $ra_i \leq b_i \leq Ra_i$,* *for all* $i = 1, 2, \ldots, n$. *Then,*

$$\sum_{i=1}^{n} b_i^2 + rR \sum_{i=1}^{n} a_i^2 \leq (r+R) \sum_{i=1}^{n} a_i b_i \ .$$

Equality holds if and only if either $b_i = r a_i$ *or* $b_i = R a_i$, *for all* $i = 1, 2, \ldots, n$.

Theorem 7. *Let* G *be a simple graph with* n *vertices and* m *edges. Let* G_σ *be a self-loop graph obtained from* G *by attaching* σ *self-loops. Then,*

$$\mathscr{E}(G_\sigma) \geq \frac{2m + \sigma - n\lambda_1 \sqrt{2m + \sigma - \lambda_1^2} - \frac{2\sigma^2}{n}}{\lambda_1 + \sqrt{2m + \sigma - \lambda_1^2}} - \sigma.$$

Proof. Applying Lemma 10, setting $r = \lambda_n - \frac{\sigma}{n}$, $R = \lambda_1 + \frac{\sigma}{n}$, $b_i = \left|\lambda_i - \frac{\sigma}{n}\right|$, $a_i = 1$, for $i = 1, 2, \ldots, n$, we have

$$\sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|^2 + (\lambda_n - \frac{\sigma}{n})(\lambda_1 + \frac{\sigma}{n}) \sum_{i=1}^{n} 1 \leq (\lambda_n + \lambda_1) \sum_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|.$$

Recall that $\sum\limits_{i=1}^{n} \left|\lambda_i - \frac{\sigma}{n}\right|^2 = 2m + \sigma - \frac{\sigma^2}{n}$. Then,

$$2m + \sigma - \frac{2\sigma^2}{n} + n\lambda_1\lambda_n + \sigma(\lambda_n - \lambda_1) \leq (\lambda_1 + \lambda_n)\mathscr{E}(G_\sigma).$$

Since $-\sqrt{2m + \sigma - \lambda_1^2} \leq \lambda_n \leq \sqrt{2m + \sigma - \lambda_1^2}$, we get

$$\mathscr{E}(G_\sigma) \geq \frac{2m + \sigma - \frac{2\sigma^2}{n} - n\lambda_1 \sqrt{2m + \sigma - \lambda_1^2}}{\lambda_1 + \sqrt{2m + \sigma - \lambda_1^2}} - \sigma.$$

■

3 Upper bounds for the energy of graphs with self-loops

In this section, we present new upper bounds for $\mathscr{E}(G_\sigma)$ that are dependent on the parameters n, m, σ, and Δ.

For simple graphs G, there are numerous known results regarding the spectral radius $\lambda_1(G)$. In the case of $\lambda_1(G_\sigma)$, several new bounds for $\lambda_1(G_\sigma)$ have been provided as follows [2].

Lemma 11. *[2] Let G be a connected graph of order n and size m. Then,*

$$\lambda_1(G_\sigma) \geq \frac{2m}{n} + \frac{\sigma}{n} \ .$$

Lemma 12. *[2] Let G_σ be a self-loop graph of order n. Then,*

$$\lambda_1(G_\sigma) \leq \triangle(G) + 1 \leq n \ .$$

Moreover, $\lambda_1(G_\sigma) = n$ if and only if $G_\sigma = (K_n)_n$, the complete graph with n self-loops.

By the above two lemmas and the Cauchy-Schwarz inequality, we will obtain some upper bounds of $\mathscr{E}(G_\sigma)$.

Theorem 8. *Let G be a connected graph of order n and size m with maximum degree Δ. Let G_σ be the graph obtained from G by attaching σ self-loops. Then,*

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

Proof. Suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G_σ. By the Cauchy-Schwarz inequality, we get

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

By Lemma 5, we have

$$\sum_{i=2}^{n}\left|\lambda_i - \frac{\sigma}{n}\right|^2 = 2m+\sigma-\frac{\sigma^2}{n}-\left|\lambda_1 - \frac{\sigma}{n}\right|^2 = 2m+\sigma-\lambda_1^2+2\frac{\sigma}{n}\lambda_1-\frac{(1+n)\sigma^2}{n^2}.$$

Applying Lemmas 11, 12, we have

$$\begin{aligned}\mathscr{E}(G_\sigma) &= \sum_{i=1}^{n}\left|\lambda_i - \frac{\sigma}{n}\right| \\ &\le \sqrt{(n-1)\left(2m+\sigma-\lambda_1^2+2\frac{\sigma}{n}\lambda_1-\frac{(1+n)\sigma^2}{n^2}\right)}+\left|\lambda_1-\frac{\sigma}{n}\right| \\ &\le \sqrt{(n-1)\left(2m+\sigma-\frac{4m^2+4m\sigma+2\sigma^2}{n^2}+2\frac{\sigma}{n}(\Delta+1-\frac{\sigma}{2})\right)} \\ &\quad +\Delta+\frac{n-\sigma}{n}\ . \end{aligned}$$

■

Theorem 9. *Let G be a connected graph of order n with m edges and maximum degree Δ. Let G_σ be the graph obtained from G by attaching σ self-loops. Then,*

$$\mathscr{E}(G_\sigma) \le \Delta+1+\frac{(n-2)\sigma}{n}+\sqrt{(n-1)\left(2m+\sigma-\frac{(2m+\sigma)^2}{n^2}\right)}\ .$$

Proof. Suppose that $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ are the eigenvalues of G_σ. By the Cauchy-Schwarz inequality and Lemma 1,

$$\left(\sum_{i=2}^{n}|\lambda_i|\right)^2 \le (n-1)\sum_{i=2}^{n}|\lambda_i|^2 = (n-1)(2m+\sigma-\lambda_1^2)\ .$$

Immediately, we have

$$\begin{aligned}\mathscr{E}(G_\sigma) &= |\lambda_1-\frac{\sigma}{n}|+\sum_{i=2}^{n}|\lambda_i-\frac{\sigma}{n}| \\ &\le \Delta+1-\frac{\sigma}{n}+\sqrt{(n-1)(2m+\sigma-\lambda_1^2)}+\frac{(n-1)\sigma}{n} \\ &\le \Delta+1+\frac{(n-2)\sigma}{n}+\sqrt{(n-1)\left(2m+\sigma-\frac{(2m+\sigma)^2}{n^2}\right)}\ .\end{aligned}$$

■

The inequality in the next lemma will be used in the proof of Theorem 10.

Lemma 13. *[26] Let $A=(a_{ij})$ be an $n\times n$ nonnegative symmetric matrix* *with positive row sums $d_1, d_2, \ldots, d_n$. Then,*

$$\lambda_1(A) \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}$$

with equality if and only if A is regular or semiregular.

Theorem 10. *Let G_σ be a self-loop graph with n vertices, m edges and σ self-loops. Let λ_1 be the maximum eigenvalue of G_σ. Then,*

$$\lambda_1 \geq \frac{2(m+\sigma)}{n} - 1.$$

Proof. Let A be the adjacency matrix of G_σ. Let $A^{'} = A + I_n$ with positive row sums $c_1, c_2, \ldots, c_n$. Let $d_1, d_2, \ldots, d_n$ be the degree of vertices in G_σ. By applying Lemma 6, we have $\sum_{i=1}^{n} |d_i| \leq \sqrt{n \sum_{i=1}^{n} d_i^2}$. That is $2(m+\sigma) \leq \sqrt{n \sum_{i=1}^{n} d_i^2}$. Thus, we get

$$\sum_{i=1}^{n} d_i^2 \geq \frac{4(m+\sigma)^2}{n}.$$

Then, using Lemma 13, we obtain

$$\lambda_1(A^{'}) \geq \sqrt{\frac{\sum_{i=1}^{n} c_i^2}{n}} \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} \geq \frac{2(m+\sigma)}{n}.$$

What's more, $\lambda_1(A^{'}) = \lambda_1(A) + 1$. Combining inequalities above, we get

$$\lambda_1(A) \geq \frac{2(m+\sigma)}{n} - 1 \ .$$

■

Now we will give two (n, m, σ)-type upper bounds for $\mathscr{E}(G_\sigma)$.

Theorem 11. *Let G_σ be a self-loop graph with n vertices, m edges and σ*

self-loops. Then,

$$\mathscr{E}(G_\sigma) \leq \sqrt{\frac{n^2 + (2m + \sigma - \frac{\sigma^2}{n})^2}{2}} \ .$$

Proof. Let $a_i = b_i = q_i = p_i = 1$ and $c_i = d_i = |\lambda_i - \frac{\sigma}{n}|, i = 1, 2, \ldots, n$. By Lemma 3, we have

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n} 1 + \left(\sum_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}|^2 \right)^2 \geq 2 \left(\sum_{i=1}^{n} |\lambda_i - \frac{\sigma}{n}| \right)^2$$

$$n^2 + \left(2m + \sigma - \frac{\sigma^2}{n} \right)^2 \geq 2\mathscr{E}(G_\sigma)^2$$

$$\mathscr{E}(G_\sigma) \leq \sqrt{\frac{n^2 + (2m + \sigma - \frac{\sigma^2}{n})^2}{2}} \ .$$

■

Theorem 12. *Let G_σ be a self-loop graph with n vertices, m edges and σ self-loops. Then,*

$$\mathscr{E}(G_\sigma) \leq \frac{2m + \sigma - \frac{\sigma^2}{n} + n}{2} \ .$$

Proof. Applying Lemma 3, for $i = 1, 2, \ldots, n$, let $a_i = \left| \lambda_i - \frac{\sigma}{n} \right|$, $b_i = p_i = q_i = c_i = d_i = 1$. Then,

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

$$\left(2m + \sigma - \frac{\sigma^2}{n} \right) n + n^2 \geq 2n\mathscr{E}(G_\sigma)$$

$$\mathscr{E}(G_\sigma) \leq \frac{2m + \sigma - \frac{\sigma^2}{n} + n}{2} \ .$$ ■

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