

ON ENERGY AND LAPLACIAN ENERGY OF GRAPHS*

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Abstract. Let $G = (V, E)$ be a simple graph of order n with m edges. The energy of a graph G , denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of all eigenvalues of G . The Laplacian energy of the graph G is defined as

$$LE = LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|,$$

where $\mu_1, \mu_2, \dots, \mu_{n-1}, \mu_n = 0$ are the Laplacian eigenvalues of graph G . In this paper, some lower and upper bounds for $\mathcal{E}(G)$ are presented in terms of number of vertices, number of edges, maximum degree and the first Zagreb index, etc. Moreover, a relation between energy and Laplacian energy of graphs is given.

Key words. Graph, Spectral radius, Energy, Laplacian energy, First Zagreb index, Determinant.

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1. Introduction. The energy $\mathcal{E}(G)$ of a graph G , defined as the sum of the absolute values of its eigenvalues, belongs to the most popular graph invariants in chemical graph theory. It originates from the π -electron energy in the Hückel molecular orbital model, but has also gained purely mathematical interest. Gutman introduced this definition of the energy of a simple graph in his paper “The energy of a graph” [12]. He notes that at first, very few mathematicians seemed to be attracted to the definition. In the past decade, interest in graph energy has increased and many different versions have been introduced. In 2006, Gutman and Zhou defined the Laplacian energy of a graph as the sum of the absolute deviations (i.e., distance from the mean) of the eigenvalues of its Laplacian matrix [15]. Similar variants of graph energy were developed for the signless Laplacian matrix, the distance matrix, the incidence matrix, and even for a general matrix not associated with a graph [23]. In 2010, Cavers, Fallat, and Kirkland first studied the Normalized Laplacian energy of a graph, also known as the Randić energy for its connection to the Randić index [3].

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and

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edge set $E(G)$, $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \dots, n$. The maximum and minimum vertex degrees are denoted by Δ and δ , respectively. Let N_i be the neighbor set of the vertex $v_i \in V(G)$. Denote by, ω , the clique number of graph G . If vertices v_i and v_j are adjacent, we denote that by $v_i v_j \in E(G)$. The adjacency matrix $A(G)$ of G is defined by its entries $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} \geq \lambda_n$ denote the eigenvalues of $A(G)$. The largest eigenvalue λ_1 is called the spectral radius of graph G . When more than one graph is under consideration, we write $\lambda_i(G)$ instead of λ_i . Some well known results are the following:

$$(1.1) \quad \sum_{i=1}^n \lambda_i = 0,$$

$$(1.2) \quad \sum_{i=1}^n \lambda_i^2 = 2m$$

$$\text{and } \det A = \prod_{i=1}^n \lambda_i.$$

Moreover, the spectral radius λ_1 is at least the average vertex degree in the graph, that is,

$$(1.3) \quad \lambda_1 \geq \frac{2m}{n}$$

with equality holding if and only if G is isomorphic to a regular graph.

The energy of the graph G is defined as

$$(1.4) \quad \mathcal{E}(G) = \sum_{i=1}^n |\lambda_i|,$$

where λ_i , $i = 1, 2, \dots, n$, are the eigenvalues of graph G . For its basic properties, applications including various lower and upper bounds, see [7, 9, 14, 17, 19, 20, 21, 29]. Maximum and minimum values of the energy are known for various classes of graphs, and in some cases also the second-largest/second-smallest and further values as well as the corresponding extremal graphs; see the book [20] for recent results and the references cited therein.

The Laplacian matrix of G is $L(G) = D(G) - A(G)$. The Laplacian matrix has nonnegative eigenvalues $n \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_n = 0$. Denote by $\text{Spec}(G) = \{\mu_1, \mu_2, \dots, \mu_n\}$ the spectrum of $L(G)$, i.e., the Laplacian spectrum of G . When more than one graph is under consideration, we write $\mu_i(G)$ instead of μ_i .

As well known [22],

$$(1.5) \quad \sum_{i=1}^n \mu_i = 2m.$$

The Laplacian energy of the graph G is defined as [15]

$$(1.6) \quad LE = LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|.$$

For its basic properties, including various lower and upper bounds, see [5, 6, 8, 10, 24, 28]. As usual, K_n and $K_{1,n-1}$, denote, respectively, the complete graph and the star on n vertices. For other undefined notations and terminology from graph theory, the readers are referred to [1].

The paper is organized as follows. In Section 2, we list some previously known results. In Section 3, we present a lower bound on energy $\mathcal{E}(G)$ of graph G . In Section 4, we obtain an upper bound on energy $\mathcal{E}(G)$ of graph G . In Section 5, we give a relation between energy and Laplacian energy of graphs.

2. Preliminaries. In this section, we list some previously known results that will be needed in the next three sections.

LEMMA 2.1. [25] *Let B be a $p \times p$ symmetric matrix and let B_k be its leading $k \times k$ submatrix; that is, B_k is matrix obtained from B by deleting its last $p - k$ rows and columns. Then for $i = 1, 2, \dots, k$*

$$(2.1) \quad \rho_{p-i+1}(B) \leq \rho_{k-i+1}(B_k) \leq \rho_{k-i+1}(B),$$

where $\rho_i(B)$ is the i -th largest eigenvalue of B .

LEMMA 2.2. [11] *Let B and C be two real symmetric matrices of size n . Then for any $1 \leq k \leq n$,*

$$\sum_{i=1}^k \lambda_i(B + C) \leq \sum_{i=1}^k \lambda_i(B) + \sum_{i=1}^k \lambda_i(C),$$

where $\lambda_i(M)$ is the i -th largest eigenvalue of M .

The following upper bound on λ_1 has been given in [18]:

LEMMA 2.3. [18] *Let G be a connected graph of order n with m edges. Then*

$$(2.2) \quad \lambda_1 \leq \sqrt{2m - n + 1}$$

with equality holding if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

A d -regular graph G on n vertices is strongly d -regular (denote by $\text{srg}(n, d, \lambda, \mu)$) if there exist positive integers d, λ and μ such that every vertex has d neighbors, every adjacent pair of vertices has λ common neighbors, and every nonadjacent pair has μ common neighbors.

The following result is well known [2]:

LEMMA 2.4. *Let G be isomorphic to $\text{srg}(n, d, \lambda, \mu)$. Then the eigenvalues of G are*

(i) d of multiplicity 1,

(ii) $\frac{\lambda - \mu + \sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}{2}$ of multiplicity $\frac{1}{2} \left[n - 1 - \frac{2d + (n-1)(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}} \right]$,

(iii) $\frac{\lambda - \mu - \sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}{2}$ of multiplicity $\frac{1}{2} \left[n - 1 + \frac{2d + (n-1)(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}} \right]$.

COROLLARY 2.5. *Let G be isomorphic to $\text{srg}(n, d, \lambda, \mu)$. Then*

$$\mathcal{E}(\text{srg}(n, d, \lambda, \mu)) = d + \frac{2(n-1)(d - \mu) - d(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}.$$

Proof. By (1.4),

$$\begin{aligned} \mathcal{E}(G) &= d + \frac{1}{2} \left[n - 1 - \frac{2d + (n-1)(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}} \right] \times \frac{\lambda - \mu + \sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}{2} \\ &\quad + \frac{1}{2} \left[n - 1 + \frac{2d + (n-1)(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}} \right] \times \frac{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)} - (\lambda - \mu)}{2} \\ &= d + \frac{(n-1)\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}{2} - \frac{(\lambda - \mu)[2d + (n-1)(\lambda - \mu)]}{2\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}} \\ &= d + \frac{2(n-1)(d - \mu) - d(\lambda - \mu)}{\sqrt{(\lambda - \mu)^2 + 4(d - \mu)}}. \quad \square \end{aligned}$$

COROLLARY 2.6. *Let G be isomorphic to $\text{srg}(n, d, \lambda, \lambda)$. Then*

$$\mathcal{E}(\text{srg}(n, d, \lambda, \lambda)) = d + (n-1)\sqrt{d - \lambda}.$$

LEMMA 2.7. [4] *Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. Then*

$$(2.3) \quad \sum_{v_j \in V(G), j \neq i} |N_i \cap N_j| = \sum_{v_j: v_i v_j \in E(G)} (d_j - 1), \quad v_i \in V(G),$$

where d_i is the degree of the vertex v_i and $|N_i \cap N_j|$ is the cardinality of the common neighbors of v_i and v_j .

3. Lower bound for the energy of graphs. In this section, we give a lower bound on energy $\mathcal{E}(G)$ in terms of n , m and the determinant of the adjacency matrix of graph G . First we mention three popular lower bounds on energy $\mathcal{E}(G)$ of graphs.

Li et al. [20] gave the following lower bound in terms of m :

$$(3.1) \quad \mathcal{E}(G) \geq 2\sqrt{m}$$

with equality holding if and only if G consists of a complete bipartite graph $K_{a,b}$ such that $ab = m$ and arbitrarily many isolated vertices. McClelland [21] obtained the following lower bound in terms of n , m and the determinant of the adjacency matrix of graph G :

$$(3.2) \quad \mathcal{E}(G) \geq \sqrt{2m + n(n-1)|\det A|^{2/n}}.$$

Recently, Das et al. [9] presented a lower bound for nonsingular graph (i.e., a graph for which 0 is not an eigenvalue, and hence $|\det A| > 0$) and the bound is as follows:

$$(3.3) \quad \mathcal{E}(G) \geq \frac{2m}{n} + n - 1 + \ln \left(\frac{n|\det A|}{2m} \right).$$

We now give a lower bound on $\mathcal{E}(G)$ of graph G in terms of n , m and $\det A$.

THEOREM 3.1. *Let G be a connected graph of order n and m edges. Then*

$$(3.4) \quad \mathcal{E}(G) \geq \min \left\{ \frac{2m}{n} + \sqrt{2m - \frac{4m^2}{n^2} + Z}, \sqrt{2m - n + 1} + \sqrt{n - 1 + Z} \right\},$$

where

$$Z = (n-1)(n-2) \left(\frac{(\det A)^2}{2m - n + 1} \right)^{\frac{1}{n-1}}$$

and $\det A$ is the determinant of the adjacency matrix of graph G . Moreover, equality holds in (3.4) if and only if $G \cong K_n$.

Proof. From (1.2) and (1.4), we get

$$\begin{aligned} \mathcal{E}^2(G) &= \sum_{i=1}^n \lambda_i^2 + 2 \sum_{1 \leq i < j \leq n} |\lambda_i \lambda_j| \\ &= 2m + 2\lambda_1 \sum_{i=2}^n |\lambda_i| + 2 \sum_{2 \leq i < j \leq n} |\lambda_i \lambda_j| \\ (3.5) \quad &= 2m + 2\lambda_1(\mathcal{E}(G) - \lambda_1) + 2 \sum_{2 \leq i < j \leq n} |\lambda_i \lambda_j|. \end{aligned}$$

By the Arithmetic-Geometric mean inequality, we get

$$(3.6) \quad \sum_{2 \leq i < j \leq n} |\lambda_i \lambda_j| \geq \frac{(n-1)(n-2)}{2} \left(\prod_{i=2}^n |\lambda_i| \right)^{2/(n-1)}$$

$$(3.7) \quad = \frac{(n-1)(n-2)}{2} \left(\frac{|\det A|}{\lambda_1} \right)^{2/(n-1)}.$$

Using inequality (3.7) in (3.5), we get

$$\mathcal{E}^2(G) \geq 2m + 2\lambda_1(\mathcal{E}(G) - \lambda_1) + (n-1)(n-2) \left(\frac{(\det A)^2}{\lambda_1^2} \right)^{1/(n-1)},$$

that is,

$$\mathcal{E}^2(G) - 2\lambda_1\mathcal{E}(G) - \left[2m - 2\lambda_1^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{\lambda_1^2} \right)^{\frac{1}{n-1}} \right] \geq 0.$$

By solving the above inequality with $\mathcal{E}(G) > \lambda_1$, we get

$$\mathcal{E}(G) \geq \lambda_1 + \sqrt{2m - \lambda_1^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{\lambda_1^2} \right)^{\frac{1}{n-1}}}.$$

Using (2.2), we have

$$(3.8) \quad \mathcal{E}(G) \geq \lambda_1 + \sqrt{2m - \lambda_1^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{2m - n + 1} \right)^{\frac{1}{n-1}}}.$$

Let

$$f(x) = x + \sqrt{2m - x^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{2m - n + 1} \right)^{\frac{1}{n-1}}}.$$

Then

$$f'(x) = 1 - \frac{x}{\sqrt{2m - x^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{2m - n + 1} \right)^{\frac{1}{n-1}}}}.$$

Thus, $f(x)$ is an increasing function on

$$x \leq \sqrt{m + \frac{1}{2}(n-1)(n-2) \left(\frac{(\det A)^2}{2m - n + 1} \right)^{\frac{1}{n-1}}}$$

and decreasing function on

$$x \geq \sqrt{m + \frac{1}{2}(n-1)(n-2) \left(\frac{(\det A)^2}{2m-n+1} \right)^{\frac{1}{n-1}}}.$$

From (1.3) and Lemma 2.3, we get

$$\frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m-n+1}.$$

From (3.8), we get

$$\mathcal{E}(G) \geq \min \left\{ f \left(\frac{2m}{n} \right), f \left(\sqrt{2m-n+1} \right) \right\},$$

which gives the required result in (3.4). This completes the first part of the proof.

Suppose that equality holds in (3.4). Then all the inequalities in the above must be equalities. In particular, from equality in (3.6), we get

$$|\lambda_2| = |\lambda_3| = \cdots = |\lambda_n|.$$

From equality in (3.8), we get $G \cong K_n$ or $G \cong K_{1,n-1}$, by Lemma 2.3. The above result holds for complete graph K_n . Moreover, all other inequalities in the above must be equalities for complete graph K_n .

Conversely, let $G \cong K_n$. Since the adjacency spectrum of K_n is

$$(n-1, \underbrace{-1, -1, \dots, -1}_{n-1}),$$

we have

$$Z = (n-1)(n-2) \left(\frac{(\det A)^2}{2m-n+1} \right)^{\frac{1}{n-1}} = (n-1)(n-2).$$

Now, we have

$$\frac{2m}{n} + \sqrt{2m - \frac{4m^2}{n^2} + M} = 2(n-1) \quad \text{and} \quad \sqrt{2m-n+1} + \sqrt{n-1+M} = 2(n-1).$$

Hence, the equality holds in (3.4) for complete graph K_n . $\square$

COROLLARY 3.2. *Let G be a connected graph of order n and m edges. Then*

$$(3.9) \quad \mathcal{E}(G) \geq \frac{2m}{n} + \sqrt{(n-1) \left[1 + (n-2) \left(\frac{(\det A)^2}{2m-n+1} \right)^{\frac{1}{n-1}} \right]},$$

where $\det A$ is the determinant of the adjacency matrix of graph G . Moreover, equality holds in (3.9) if and only if $G \cong K_n$.

Proof. Again from (1.3) and Lemma 2.3, we get

$$\frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m - n + 1}$$

with left (right) equality holding if and only if G is a regular graph ($G \cong K_n$ or $G \cong K_{1,n-1}$). Bearing this in mind, from Theorem 3.1, we get

$$\begin{aligned} \mathcal{E}(G) &\geq \lambda_1 + \sqrt{2m - \lambda_1^2 + (n-1)(n-2) \left(\frac{(\det A)^2}{\lambda_1^2} \right)^{\frac{1}{n-1}}} \\ &\geq \frac{2m}{n} + \sqrt{n-1 + (n-1)(n-2) \left(\frac{(\det A)^2}{2m-n+1} \right)^{\frac{1}{n-1}}}, \end{aligned}$$

which gives the required result in (3.9). Moreover, equality holds in (3.9) if and only if $G \cong K_n$. $\square$

COROLLARY 3.3. *Let G be a connected graph of order n with m edges and maximum degree Δ . Then*

$$(3.10) \quad \mathcal{E}(G) \geq \frac{2m}{n} + \sqrt{(n-1) \left[1 + (n-2) \left(\frac{\det A}{\Delta} \right)^{\frac{2}{n-1}} \right]},$$

where $\det A$ is the determinant of the adjacency matrix of graph G . Moreover, equality holds in (3.10) if and only if $G \cong K_n$.

Proof. It is well known that for connected graph G , $\lambda_1 \leq \Delta$ with equality holding if and only if G is a regular graph. Using this result, from the proof of Corollary 3.2, we get the lower bound in (3.10). Moreover, equality holds in (3.10) if and only if $G \cong K_n$. $\square$

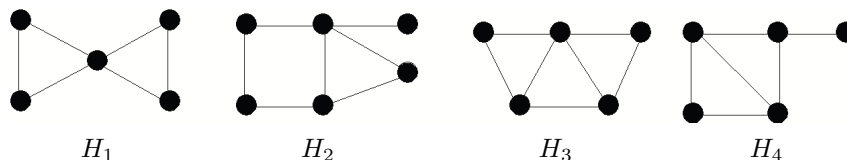


Figure 1. Graphs H_1 , H_2 , H_3 and H_4 .

EXAMPLE 3.4. Four graphs H_1 , H_2 , H_3 and H_4 have been shown in Figure 1. The numerical results related to $\mathcal{E}(G)$ and the bounds (that mentioned above) are

listed in the following. These show that our bound (3.4) is better than the other three bounds (3.1), (3.2) and (3.3) for the graphs H_1 , H_2 , H_3 and H_4 . We should note that these results are presenting as rounded to three decimal places.

G	$\mathcal{E}(G)$	(3.1)	(3.2)	(3.3)	(3.4)
H_1	7.123	4.899	6.843	6.911	6.929
H_2	7.664	5.292	6.633	6.486	6.964
H_3	7.107	5.292	6.355	6.464	6.763
H_4	6.73	4.899	6.196	6.218	6.441

Table 1. The energy and the values of the lower bounds (3.1), (3.2), (3.3), and (3.4) for the graphs depicted in Figure 1.

4. Upper bound for the energy of graphs. In this section, we give an upper bound on energy $\mathcal{E}(G)$. The rank of a matrix B is the maximal number of linearly independent rows or columns of B . Let r be the rank of adjacency matrix $A(G)$ of graph G . The first Zagreb index $M_1 = M_1(G)$ is equal to the sum of squares of the vertex degrees of the graph G [13]. First we mention four upper bounds on energy $\mathcal{E}(G)$ of graphs. Koolen et al. [19] gave the following upper bound in terms of n and m :

$$(4.1) \quad \mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1) \left[2m - \left(\frac{2m}{n} \right)^2 \right]}.$$

Bo Zhou [29] obtained the following upper bound in terms of n , m and the first Zagreb index $M_1(G)$:

$$(4.2) \quad \mathcal{E}(G) \leq \sqrt{\frac{M_1(G)}{n}} + \sqrt{(n-1) \left[2m - \left(\sqrt{\frac{M_1(G)}{n}} \right)^2 \right]}.$$

Das et al. [7] gave the two following upper bounds:

$$(4.3) \quad \mathcal{E}(G) \leq \sqrt{2m(n-\delta) + 4\sqrt{m^3(1-1/\omega)}}$$

and

$$(4.4) \quad \mathcal{E}(G) \leq \frac{2(m-\delta)}{n-1} + \sqrt{(n-1) \left[2m - \frac{4(m-\delta)^2}{(n-1)^2} \right]}.$$

We are now ready to give an upper bound on energy $\mathcal{E}(G)$ of graphs G in terms of n, m, r, Δ and $M_1(G)$.

THEOREM 4.1. *Let G be a connected graph of order n with m edges, Δ maximum degree and the first Zagreb index $M_1(G)$. Then*

$$(4.5) \quad \mathcal{E}(G) \leq \Delta + \sqrt{\frac{2m(n^2 - 2m)}{n^2}} + P,$$

where

$$P = \sqrt{\binom{r-1}{2} \left[\frac{8m^2(n^2 - 2m)^2}{n^4} - 2M_1(G) - \frac{2(M_1(G) - 2m)^2}{n(n-1)} + 2\Delta^4 \right]}$$

and r is the rank of the adjacency matrix of graph G . Moreover, equality holds in (4.5) if and only if $G \cong K_n$ or $G \cong K_{n/2, n/2}$ or $G \cong \text{srg}\left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1}\right)$.

Proof. Since r is the rank of the adjacency matrix of graph G , there are exactly r non-zero eigenvalues and hence $r \leq n$. We can assume that

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_r| > 0.$$

Let us consider the matrix $A^2(G)$. Since the (i, j) entry of $A^2(G)$ is

$$\begin{cases} d_i & \text{if } i = j, \\ |N_i \cap N_j| & \text{otherwise,} \end{cases}$$

we have

$$(4.6) \quad \sum_{i=1}^n \lambda_i^4 = \text{tr}(A^4) = \sum_{i=1}^n d_i^2 + 2 \sum_{1 \leq i < j \leq n} |N_i \cap N_j|^2.$$

By the Cauchy-Schwarz inequality, we have

$$(4.7) \quad \left(\sum_{1 \leq i < j \leq n} |N_i \cap N_j| \right)^2 \leq \frac{n(n-1)}{2} \sum_{1 \leq i < j \leq n} |N_i \cap N_j|^2$$

with equality holding if and only if $|N_i \cap N_j| = |N_k \cap N_\ell|$ for any $(v_i, v_j) \neq (v_k, v_\ell)$, $i \neq j, k \neq \ell$. From (2.3), we get

$$\sum_{v_i \in V(G)} \sum_{v_j \in V(G), j \neq i} |N_i \cap N_j| = \sum_{v_i \in V(G)} \sum_{v_j: v_i v_j \in E(G)} (d_j - 1).$$

We denote the average degree of the adjacent vertices of vertex v_i of graph G by m_i . From the above, we get

$$2 \sum_{1 \leq i < j \leq n} |N_i \cap N_j| = \sum_{v_i \in V(G)} d_i m_i - \sum_{v_i \in V(G)} d_i.$$

Since

$$M_1(G) = \sum_{i=1}^n d_i^2 = \sum_{v_i \in V(G)} d_i m_i \quad \text{and} \quad \sum_{i=1}^n d_i = 2m,$$

we get

$$(4.8) \quad \sum_{1 \leq i < j \leq n} |N_i \cap N_j| = \frac{1}{2} M_1(G) - m.$$

From (4.6), (4.7) and (4.8), we get

$$(4.9) \quad \sum_{i=1}^r \lambda_i^4 = \sum_{i=1}^n \lambda_i^4 \geq M_1(G) + \frac{1}{n(n-1)} (M_1(G) - 2m)^2$$

with equality holding in (4.9) if and only if $|N_i \cap N_j| = |N_k \cap N_\ell|$ for any $(v_i, v_j) \neq (v_k, v_\ell)$, $i \neq j$, $k \neq \ell$.

Since

$$(4.10) \quad \sum_{i=1}^r \lambda_i^2 = 2m,$$

and by the Cauchy-Schwarz inequality, we have

$$\begin{aligned} \mathcal{E}(G) &= \sum_{i=1}^r |\lambda_i| = \lambda_1 + \sqrt{\sum_{i=2}^r \lambda_i^2 + 2 \sum_{2 \leq i < j \leq r} |\lambda_i \lambda_j|} \\ &= \lambda_1 + \sqrt{2m - \lambda_1^2 + 2 \sum_{2 \leq i < j \leq r} |\lambda_i \lambda_j|} \\ (4.11) \quad &\leq \lambda_1 + \sqrt{2m - \lambda_1^2 + \sqrt{2(r-1)(r-2) \sum_{2 \leq i < j \leq r} \lambda_i^2 \lambda_j^2}} \\ &= \lambda_1 + \sqrt{2m - \lambda_1^2 + \sqrt{(r-1)(r-2) \left[\left(\sum_{i=2}^r \lambda_i^2 \right)^2 - \sum_{i=2}^r \lambda_i^4 \right]}}. \end{aligned}$$

Since

$$\frac{2m}{n} \leq \lambda_1 \leq \Delta$$

with (4.9) and (4.10), we get

$$\begin{aligned} \mathcal{E}(G) &\leq \lambda_1 + \sqrt{2m - \lambda_1^2} + \sqrt{(r-1)(r-2) \left[(2m - \lambda_1^2)^2 - M_1(G) - \frac{(M_1(G) - 2m)^2}{n(n-1)} + \lambda_1^4 \right]} \\ &\leq \Delta \\ &\quad + \sqrt{\frac{2m(n^2 - 2m)}{n^2}} + \sqrt{\binom{r-1}{2} \left[\frac{8m^2(n^2 - 2m)^2}{n^4} - 2M_1(G) - \frac{2(M_1(G) - 2m)^2}{n(n-1)} + 2\Delta^4 \right]}. \end{aligned} \quad (4.12)$$

This completes the first part of the proof.

Suppose that equality holds in (4.5). Then all the inequalities in the above must be equalities. From equality in (4.12), we get

$$\lambda_1 = \Delta = \frac{2m}{n}.$$

Therefore, G is a regular graph. Suppose G is d -regular graph. Since r is the rank of the adjacency matrix of connected graph G , we have $r \geq 2$. We consider two cases: (i) $r = 2$, (ii) $r > 2$.

Case (i) : $r = 2$. In this case, G has two non-zero eigenvalues. Since

$$\sum_{i=1}^n \lambda_i = 0,$$

we must have $\lambda_1 = -\lambda_n$, $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = 0$. By (1.2), we get $\lambda_1^2 = m = \frac{4m^2}{n^2}$, that is, $m = \frac{n^2}{4}$ and $\lambda_1 = n/2 = -\lambda_n$. Hence, $G \cong K_{n/2, n/2}$.

Case (ii) : $r > 2$. From equality in (4.11), we get

$$(4.13) \quad |\lambda_2| = |\lambda_3| = \cdots = |\lambda_r|.$$

From equality in (4.9), we get

$$(4.14) \quad |N_i \cap N_j| = |N_k \cap N_\ell| \quad \text{for any } (v_i, v_j) \neq (v_k, v_\ell), \quad i \neq j, \quad k \neq \ell.$$

If any $(v_i, v_j) \in E(G)$ ($i \neq j$), then $G \cong K_n$ and also the equality holds in (4.13). Otherwise, there exists at least one $(v_i, v_j) \notin E(G)$ ($i \neq j$). Using (4.14), we get

$$\lambda = |N_i \cap N_j| = |N_k \cap N_\ell| = \mu \quad \text{for } (v_i, v_j) \in E(G), (v_k, v_\ell) \notin E(G).$$

By Lemma 2.7 with the above result, we get

$$\lambda = \mu = \frac{d(d-1)}{n-1}.$$

Since G is d -regular graph, from the above we must have

$$G \cong \text{srg} \left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1} \right).$$

Moreover, by Lemma 2.4, (4.13) holds for $\text{srg} \left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1} \right)$.

Conversely, we have to prove that the equality holds in (4.5) for K_n , $K_{n/2, n/2}$ and $\text{srg} \left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1} \right)$. First consider $G \cong K_n$.

$$\Delta = n-1, \quad r = n, \quad 2m = n(n-1) \quad \text{and} \quad M_1(K_n) = n(n-1)^2.$$

Thus, we have

$$\begin{aligned} P &= \sqrt{\binom{r-1}{2} \left[\frac{8m^2(n^2-2m)^2}{n^4} - 2M_1(G) - \frac{2(M_1(G)-2m)^2}{n(n-1)} + 2\Delta^4 \right]} \\ &= \sqrt{\frac{(n-1)(n-2)}{2} [2(n-1)^2 - 2n(n-1)^2 - 2n(n-1)(n-2)^2 + 2(n-1)^4]} \\ &= (n-1)(n-2), \end{aligned}$$

and hence,

$$\Delta + \sqrt{\frac{2m(n^2-2m)}{n^2}} + P = 2(n-1) = \mathcal{E}(K_n).$$

Next consider $G \cong K_{n/2, n/2}$. We have $r = 2$, $\Delta = n/2$ and $2m = n^2/2$. Then $P = 0$, and hence,

$$\Delta + \sqrt{\frac{2m(n^2-2m)}{n^2}} + P = n = \mathcal{E}(K_{n/2, n/2}).$$

Finally, consider the case that $G \cong \text{srg} \left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1} \right)$. Therefore, $r = n$ and $M_1(G) = nd^2$. By Corollary 2.5, we get

$$\mathcal{E}(G) = d + \sqrt{(n-1)d(n-d)}.$$

Now,

$$\begin{aligned} P &= \sqrt{\binom{r-1}{2} \left[\frac{8m^2(n^2-2m)^2}{n^4} - 2M_1(G) - \frac{2(M_1(G)-2m)^2}{n(n-1)} + 2\Delta^4 \right]} \\ &= \sqrt{\frac{(n-1)(n-2)}{2} \left[2d^2(n-d)^2 - 2nd^2 - \frac{2nd^2(d-1)^2}{n-1} + 2d^4 \right]} \\ &= \sqrt{(n-2)d^2[(n-1)(n-d)^2 - n(n-1) - n(d-1)^2 + d^2(n-1)]} \\ &= (n-2)d(n-d), \end{aligned}$$

and hence,

$$\Delta + \sqrt{\frac{2m(n^2-2m)}{n^2}} + P = d + \sqrt{(n-1)d(n-d)} = \mathcal{E}(G). \quad \square$$

COROLLARY 4.2. *Let G be a d -regular connected graph of order n . Then*

$$(4.15) \quad \mathcal{E}(G) \leq d + \sqrt{(n-1)d(n-d)}$$

with equality holding if and only if $G \cong K_n$ or $G \cong \text{srg}\left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1}\right)$.

Proof. Since $r \leq n$ and $d_i = d$ in (4.5), we get the required result in (4.15). Moreover, equality holds in (4.15) if and only if $G \cong \text{srg}\left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1}\right)$ or $G \cong K_n$, by Theorem 4.1. $\square$

COROLLARY 4.3. *Let G be a connected graph of order n with m edges, maximum degree Δ and the first Zagreb index $M_1(G)$. Then*

$$(4.16) \quad \mathcal{E}(G) \leq \Delta + \sqrt{\frac{2m(n^2-2m)}{n^2}} + P,$$

where

$$P = \sqrt{\binom{n-1}{2} \left[\frac{8m^2(n^2-2m)^2}{n^4} - 2M_1(G) - \frac{2(M_1(G)-2m)^2}{n(n-1)} + 2\Delta^4 \right]}.$$

Moreover, equality holds in (4.16) if and only if $G \cong \text{srg}\left(n, d, \frac{d(d-1)}{n-1}, \frac{d(d-1)}{n-1}\right)$ or $G \cong K_n$.

Proof. Since $r \leq n$, the result follows from Theorem 4.1. $\square$

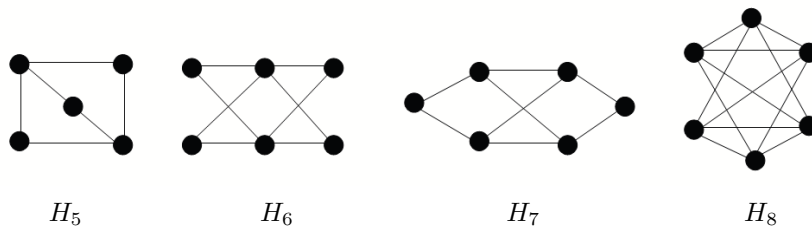


Figure 2. Graphs H_5 , H_6 , H_7 and H_8 .

G	$\mathcal{E}(G)$	(4.1)	(4.2)	(4.3)	(4.4)	(4.5)
H_5	4.899	7.396	7.348	8.807	7.657	5.498
H_6	5.657	9.333	9.153	11.314	9.555	6.981
H_7	6.928	9.333	9.291	11.314	9.555	8.667
H_8	8	10.324	10.324	13.556	11.494	8.257

Table 2. The energy and the values of the upper bounds (4.1), (4.2), (4.3), (4.4), and (4.5) for the graphs depicted in Fig. 2.

EXAMPLE 4.4. Four graphs H_5 , H_6 , H_7 and H_8 have been shown in Figure 2. The numerical results related to $\mathcal{E}(G)$ and the bounds (that mentioned above) are listed in Table 2 (these results are presenting as rounded to three decimal places). From the Table 2, we show that our bound (4.5) is better than the other four bounds (4.1), (4.2), (4.3), and (4.4) for the graphs H_5 , H_6 , H_7 and H_8 .

5. Relation between energy and Laplacian energy of graphs. In this section, we give a relation between energy and Laplacian energy of graphs. Let σ ($1 \leq \sigma \leq n - 1$) be the largest positive integer such that

$$(5.1) \quad \mu_\sigma \geq \frac{2m}{n}.$$

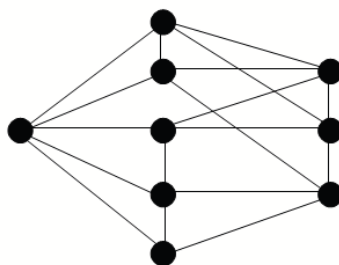
Then from [6], we have

$$(5.2) \quad LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right| = 2S_\sigma(G) - \frac{4m\sigma}{n}$$

$$(5.3) \quad = \max_{1 \leq i \leq n} \left\{ 2S_i(G) - \frac{4m i}{n} \right\},$$

where

$$S_{\sigma}(G) = \sum_{i=1}^{\sigma} \mu_i.$$



H_9

Figure 3. Graph H_9 .

For $G = K_{1, n-1}$ ($n > 2$),

$$LE(G) = 2n - 4 + \frac{4}{n} > 2\sqrt{n-1} = \mathcal{E}(G).$$

For $G = H_9$, (see, [27])

$$LE(G) \approx 14.9799 < 15.035 \approx \mathcal{E}(G).$$

From the above, it is easy to see that energy and Laplacian energy are incomparable. So it is interesting to find an upper bound on $LE(G) - \mathcal{E}(G)$. Recently, So et al. [26] presented the following relation between energy and Laplacian energy of graphs with using Ky Fan Theorem,

$$(5.4) \quad LE(G) \leq \mathcal{E}(G) + \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right|.$$

We now give another relation between energy and Laplacian energy of graphs.

THEOREM 5.1. *Let G be a graph of order n with m edges and vertex degrees $d_1, d_2, \dots, d_n$. Then*

$$(5.5) \quad LE(G) \leq \mathcal{E}(G) + 2 \sum_{i=1}^{\sigma} \left(d_i - \frac{2m}{n} \right),$$

where σ is the largest positive integer satisfying (5.1).

Proof. For any k ($1 \leq k \leq n$),

$$\sum_{i=1}^k \lambda_i(-A(G)) = -\sum_{i=1}^k \lambda_{n-i+1},$$

where $\lambda_i(-A(G))$ is the i -th largest eigenvalue of $-A(G)$. Using this result with Lemma 2.2, we get

$$\sum_{i=1}^k \mu_i \leq \sum_{i=1}^k d_i - \sum_{i=1}^k \lambda_{n-i+1}.$$

From the definition of graph energy, we have

$$\begin{aligned} \mathcal{E}(G) &= \sum_{i=1}^n |\lambda_i| = 2 \sum_{\lambda_i \geq 0} \lambda_i = -2 \sum_{\lambda_i < 0} \lambda_i = 2 \max \left\{ -\sum_{i=1}^k \lambda_{n-i+1} : 1 \leq k \leq n-1 \right\} \\ &\geq -2 \sum_{i=1}^k \lambda_{n-i+1} \quad \text{for any } k, 1 \leq k \leq n-1. \end{aligned}$$

From the above two results, for any k , we get

$$2 \sum_{i=1}^k \mu_i \leq 2 \sum_{i=1}^k d_i + \mathcal{E}(G).$$

Since σ is the largest positive integer satisfying (5.1), from the above, we can write

$$2 \sum_{i=1}^{\sigma} \mu_i - \frac{4m\sigma}{n} \leq 2 \sum_{i=1}^{\sigma} d_i + \mathcal{E}(G) - \frac{4m\sigma}{n}.$$

Using (5.2), from the above, we get the required result in (5.5). $\square$

REMARK 5.2. Our result in (5.5) is always better than the result in (5.4).

Proof. Let ν be the largest positive integer such that $d_{\nu} \geq \frac{2m}{n}$ (assume that $d_1 \geq d_2 \geq \dots \geq d_n$). Thus, we have

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

Moreover,

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

From the above two relations, we get

$$(5.6) \quad \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right| = 2 \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right).$$

Now we have to show that

$$\sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) = \max \left\{ \sum_{i=1}^k \left(d_i - \frac{2m}{n} \right) : 1 \leq k \leq n \right\},$$

that is,

$$(5.7) \quad \sum_{i=1}^k \left(d_i - \frac{2m}{n} \right) \leq \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) \quad \text{for any } k, k = 1, 2, \dots, n.$$

If $k = \nu$, then the equality holds in (5.7). Otherwise, $k \neq \nu$. We now consider two following cases:

Case (i) : $k < \nu$. Since

$$\sum_{i=k+1}^{\nu} \left(d_i - \frac{2m}{n} \right) \geq 0 \quad \text{and} \quad \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) = \sum_{i=1}^k \left(d_i - \frac{2m}{n} \right) + \sum_{i=k+1}^{\nu} \left(d_i - \frac{2m}{n} \right),$$

we get the result in (5.7).

Case (ii) : $k > \nu$. Again, since

$$\sum_{i=\nu+1}^k \left(d_i - \frac{2m}{n} \right) < 0,$$

we have

$$\sum_{i=1}^k \left(d_i - \frac{2m}{n} \right) = \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) + \sum_{i=\nu+1}^k \left(d_i - \frac{2m}{n} \right) < \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right)$$

which gives the result in (5.7). Thus,

$$\begin{aligned} \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right| &= 2 \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) = 2 \max \left\{ \sum_{i=1}^k \left(d_i - \frac{2m}{n} \right) : 1 \leq k \leq n \right\} \\ &\geq 2 \sum_{i=1}^{\sigma} \left(d_i - \frac{2m}{n} \right). \quad \square \end{aligned}$$

So et al. [26] obtained a lower bound for bipartite graph as follows:

$$(5.8) \quad LE(G) \geq \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right|.$$

In [16], it has been proved the following result: For connected graph G with vertex degrees $d_1 \geq d_2 \geq \dots \geq d_n > 0$, we have

$$(5.9) \quad \sum_{i=1}^k \mu_i \geq \sum_{i=1}^k d_i + 1 \quad \text{for any } k, 1 \leq k \leq n-1.$$

Now we present a lower bound on LE of graph G that always is better than the lower bound in (5.8). Moreover, our result is true for all connected graphs.

THEOREM 5.3. *Let G be a connected graph of order n with m edges. Then*

$$(5.10) \quad LE(G) \geq 2 + \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right|.$$

Proof. Let ν be the largest positive integer such that $d_\nu \geq \frac{2m}{n}$. Using the result (5.9), from (5.3), we get

$$\begin{aligned} LE(G) &\geq 2S_\nu - \frac{4m\nu}{n} \\ &\geq 2 \left(\sum_{i=1}^{\nu} d_i + 1 \right) - \frac{4m\nu}{n} \\ &= 2 \sum_{i=1}^{\nu} \left(d_i - \frac{2m}{n} \right) + 2 \\ &= 2 + \sum_{i=1}^n \left| d_i - \frac{2m}{n} \right| \quad \text{by (5.6).} \quad \square \end{aligned}$$

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