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A Note on the Bounds of Laplacian–Energy–Like Invariant

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ABSTRACT

The Laplacian-energy-like of a simple connected graph G is defined as $\mathrm{LEL} = \mathrm{LEL}(G) = \sum_{i=1}^{n} \sqrt{\mu_i}$, where $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ are the Laplacian eigenvalues of the graph G. In this paper, some upper and lower bounds for LEL, as well as, some lower bounds for the spectral radius of graph are obtained.

1 INTRODUCTION

The graph energy is a graph-spectrum-based quantity, initiated in the 1970s. After a latent period of 20-30 years, it became a well-liked topic of research both in mathematical chemistry and in "pure" spectral graph theory, resulting in over 600 published papers. Considering the applications of graph energies, one can see them in entropy [5, 15], modeling the properties of proteins (especially those of biological relevance) in [6, 24, 28], applying them in the search for the genetic causes of Alzheimer disease [3] and also for modeling of the spread of epidemics [26].

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Suppose $G = (V, E)$ is a simple graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \cdots, n$. The maximum and minimum degree of G are denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively. Let $A(G)$ and $D(G) = \mathrm{diag}(d_1, d_2, \cdots, d_n)$ be the (0,1)-adjacency matrix of G and the diagonal matrix of vertex degrees, respectively. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. This matrix has nonnegative eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. Assume that $\mathrm{Spec}(G) = \{\mu_1, \mu_2, \cdots, \mu_n\}$ stands for the spectrum of $L(G)$, i.e., the Laplacian spectrum of G. As well-known [20], the Laplacian spectrum obeys the relations $\sum_{i=1}^{n} \mu_i = 2m$ and $\sum_{i=1}^{n} {\mu_i}^2 = 2m + \sum_{i=1}^{n} {d_i}^2$.

In 2008, Liu and Liu [18] considered a new Laplacian-spectrum-based graph invariant $LEL = LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$, and named it *Laplacian-energy-like invariant* (LEL for short). The motivation for initiating LEL is in its analogy [12] to the earlier much studied graph energy [10, 11, 16]. We refer to [17,18] for more details on LEL and encourage the interested readers to consult papers [4, 9, 12, 14, 25, 27, 29, 31] for mathematical properties of this graph invariant.

2. AN UPPER BOUND FOR LAPLACIAN–ENERGY–LIKE INVARIANT

In order to arrive at one of our main results, we begin by recalling a crucial lemma as follows.

Lemma 1 ([20]). Let G be a graph on n vertices with at least one edge. Then $\mu_1 \geq \Delta + 1$. Moreover, if G is connected, then the equality holds if and only if $\Delta = n - 1$.

We are now in a position to formulate the lower and upper bounds on LEL in terms of n, m and d_i, $i = 1, 2, \cdots, n$.

Theorem 1. Suppose that G is a simple connected graph on $n > 1$ vertices and m edges. Then the inequality

$$LEL \leq \sqrt{\Delta + 1} + (n-2)^{3/4} \sqrt[4]{2m - (\Delta + 1)^2 + \sum_{i=1}^{n} {d_i}^2} \qquad (1)$$

holds.

Proof. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be the eigenvalues of the Laplacian matrix with respect to the graph G. Then, as is well-known, we have $\mu_1 \geq \Delta + 1$ (see also Lemma 1). Moreover, since

$$\sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2 \tag{2}$$

must hold, we get $\sum_{i=2}^{n-1} \mu_i^2 = 2m - \mu_1^2 + \sum_{i=1}^{n} d_i^2$. Using this together with the Cauchy-Schwarz inequality for twice, applied to the vectors $(\sqrt{\mu_2}, \sqrt{\mu_3}, \cdots, \sqrt{\mu_{n-1}})$ and $(1, 1, \cdots, 1)$ with $n-2$ entries, we derive the inequality

$$\begin{aligned}\sum_{i=2}^{n-1} \sqrt{\mu_i} &\leq \sqrt{(n-2)\sum_{i=2}^{n-1} \mu_i} \leq (n-2)^{3/4} \sqrt[4]{\sum_{i=2}^{n-1} \mu_i^2} \\ &= (n-2)^{3/4} \sqrt[4]{2m - \mu_1^2 + \sum_{i=1}^{n} d_i^2}. \end{aligned} \tag{3}$$

Hence, we must have

$$LEL \leq \sqrt{\mu_1} + (n-2)^{3/4} \sqrt[4]{2m - \mu_1^2 + \sum_{i=1}^{n} d_i^2}. \tag{4}$$

Now, consider the real function $f(x) = \sqrt{x} + A\sqrt[4]{B - x^2}$, where $A = (n-2)^{3/4}$ and $B = 2m + \sum_{i=1}^{n} d_i^2$. It is obvious that f is decreasing on the interval

$$I = \left[\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}, \sqrt{B}\right).$$

On the other hand, we claim $\sqrt{\frac{B}{A^{\frac{4}{3}}+1}} \leq \Delta + 1$. Since $\Delta \leq n-1$,

$$\begin{aligned} B = 2m + \sum_{i=1}^{n} d_i^2 &= \sum_{i=1}^{n} d_i(d_i + 1) \leq n\Delta(\Delta + 1) \\ &\leq (n-1)(\Delta+1)^2 = (A^{\frac{4}{3}} + 1)(\Delta + 1)^2 \end{aligned}$$

which proves our claim. Moreover, in view of Lemma 1 and Equations (2) and (4), we see that $\Delta + 1 \leq \mu_1 \leq \sqrt{B}$, and hence

$$LEL \leq f(\mu_1) \leq f(\Delta + 1) \leq f\left(\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}\right). \tag{5}$$

Remark 1. In virtue of the proof of Theorem 1, we can analyze the growth of the obtained bounds, i.e., (5), which can be fruitful for the investigation on the energy of hyperstructures, that is, the models with large size.

$$\begin{aligned} LEL \leq f\left(\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}\right) &= \frac{\sqrt[4]{B}}{\sqrt{n-1}} + \frac{\sqrt[4]{B}\cdot(n-2)}{\sqrt[4]{n-1}} \\ &\leq \frac{\sqrt[4]{n\Delta(\Delta+1)}}{\sqrt{n-1}} + \frac{\sqrt[4]{n\Delta(\Delta+1)}\cdot(n-2)}{\sqrt[4]{n-1}} \sim \sqrt[4]{n\Delta(\Delta + 1)}.\, O(n) \end{aligned}$$

which yields an upper bound for LEL related to the graphs with high order and Δ as a fixed parameter. We note that a same fashion with using (1) implies the same result:

$$LEL \leq f(\Delta+1) \leq \sqrt{\Delta+1} + (n-2)^{3/4}\sqrt[4]{n\Delta(\Delta+1)-(\Delta+1)^2} \sim \sqrt[4]{\Delta(\Delta+1)}.O(n).$$

3. BOUNDS OF SPECTRAL RADIUS OF GRAPHS IN TERMS OF THE NUMBER OF TRIANGLES

For a given graph G, let us suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the corresponding eigenvalues of the adjacency matrix A which are called A-eigenvalues and also let Δ_G be the number of triangles in G. Throughout this section, we give upper and lower bounds for λ_1 such that each edge of G belongs to at least Δ_G triangles. The goal is to utilize the upper bound obtained in order to result a lower bound for Laplacian-energy-like invariant.

Theorem 2. Assume G is a simple graph with n vertices and m edges. If each edge of G belongs to at least Δ_G triangles, $\Delta_G \geq 1$, then

$$|\lambda_1| \leq \sqrt{2m-\delta-\Delta_G(\delta-1)}. \tag{6}$$

Proof. Suppose that A_i stands for the i-th row of A. Clearly, d_i is its row sum. Without loss of generality, let $\boldsymbol{u} = (u_1, u_2, \cdots, u_n)^T$ be a unit eigenvector of $A(G)$ corresponding to $\lambda_1 = \lambda_1(G)$. Assume $\boldsymbol{u}(i)$ indicates the vector obtained from $\boldsymbol{u}$ by replacing u_j with 0 if v_i is not adjacent to v_j where $1 \leq j \leq n$. Since $A(G)\boldsymbol{u} = \lambda_1\boldsymbol{u}$, considering the i −th component of the vectors in both sides of recent equality, we derive $\lambda_1 u_i = A_i\boldsymbol{u} = A_i\boldsymbol{u}(i)$. Therefore, by taking the $|\cdot|^2$, applying the well-known Lagrange identity and simplifying the right hand side we see for each i that

$$\begin{aligned}
{\lambda_1}^2{u_i}^2 = |A_i\boldsymbol{u}(i)|^2 = |A_i|^2 \cdot |\boldsymbol{u}(i)|^2 - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2 \\
= d_i \sum_{\substack{1\leq j\leq n \\ a_{ij}\neq 0}} {u_j}^2 - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2 \\
= d_i\left(1-\sum_{\substack{1\leq j\leq n \\ a_{ij}=0}} {u_j}^2\right) - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2.
\end{aligned}$$

Summing over $1 \leq i \leq n$ in both sides we obtain,

$$\lambda_1{}^2 = 2m - \sum_{i=1}^{n} d_i \left(\sum_{\substack{1 \le j \le n \\ a_{ij}=0}} u_j{}^2 \right) - \sum_{i=1}^{n} \sum_{\substack{1 \le j < k \le n \\ a_{ij}=a_{ik}=1}} \left(u_j - u_k\right)^2. \qquad (7)$$

On the other hand, one can notice that

$$\sum_{i=1}^{n} d_i \left(\sum_{\substack{1 \le j \le n \\ a_{ij}=0}} u_j{}^2 \right) \ge \sum_{i=1}^{n} d_i\, u_i{}^2 \ge \delta.$$

Moving forward, since each edge belongs to at least Δ_G triangles, then applying Cauchy-Schwarz inequality we derive the following

$$\begin{aligned} \sum_{i=1}^{n} \sum_{\substack{1 \le j < k \le n \\ a_{ij}=a_{ik}=1}} \left(u_j - u_k\right)^2 &\ge \Delta_G \sum_{\substack{1 \le j < k \le n \\ a_{jk}=1}} \left(u_j - u_k\right)^2 \\ &= \Delta_G \sum_{i=1}^{n} d_i\, u_i{}^2 - 2\Delta_G \sum_{\substack{1 \le j < k \le n \\ a_{jk}=1}} u_j u_k \\ &\ge \Delta_G \delta - \Delta_G \sum_{j \ne k} \left|u_j u_k\right| \\ &\ge \Delta_G (\delta - 1). \end{aligned}$$

Now, viewing the equality (7) yields the following

$$|\lambda_1| \le \sqrt{2m - \delta - \Delta_G(\delta - 1)}.$$

3.1. CLOSED WALKS IN GRAPH

Throughout this subsection, we aim to derive some results related to lower bound of spectral radius of graph by using the term of Δ_G which may be useful in further investigations. Before present the next result, we need some preliminaries. We recall that a *closed walk* in G is a walk that ends where it begins. The number of closed walks in G of length ℓ starting at v_i is thus given by $(A(G)^{\ell})_{ii}$, so the total number $f_G(\ell)$ of closed walks of length ℓ is given by

$$f_G(\ell) = \sum_{i=1}^{n} (A(G)^{\ell})_{ii} = \mathrm{tr}(A(G)^{\ell})$$

where tr denotes the trace (sum of the main diagonal entries). From the theory of matrices, we know that if the matrix A has eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ then A^{ℓ} has eigenvalues $\lambda_1^{\ell}, \lambda_2^{\ell}, \cdots, \lambda_n^{\ell}$. Therefore,

$$f_G(\ell) = \sum_{i=1}^{n} \lambda_i^{\ell}. \qquad (8)$$

Some immediate consequences of (8) are as follows:

i. For $\ell = 1, \sum_{i=1}^{n} \lambda_i = 0$ which is deduced by noting that the sum of the eigenvalues is the trace of the adjacency matrix which is 0 since A is 0 on the diagonal.

ii. For $\ell = 2$, $\sum_{i=1}^{n} \lambda_i^2 = 2m$ which is followed by the fact that the sum of the squares of the eigenvalues is the same as the trace of A^2. The diagonal entries of A^2 count the number of closed walks of length 2 (a closed walk is a walk that starts and ends at the same vertex; since we are on the diagonal the starting and ending vertices are the same), for which each edge is counted exactly twice.

iii. For $\ell = 3$, $\sum_{i=1}^{n} \lambda_i^3 = 6\Delta_G$. This is obeyed by the fact that the sum of the cubes of the eigenvalues is the same as the trace of A^3, i.e., the same as the number of closed walks of length 3. Each triangle will be counted exactly six times (i.e., a choice of 3 initial vertices and 2 directions for each triangle).

One can continue this process but it becomes impractical to get some effective information about a graph. Next, using (iii) we study on bounds of Δ_G and then spectral radius of graph. Let the A-eigenvalues of G be in form of $\lambda_1 \geq \cdots \geq \lambda_k \geq 0 > \lambda_{k+1} \geq \cdots \geq \lambda_n$ and $\Lambda_+ = \sum_{i=1}^{k} \lambda_i^3 > 0$, $\Lambda_- = \sum_{i=k+1}^{n} \lambda_i^3 < 0$, $\Lambda = \sum_{i=1}^{n} |\lambda_i|^3$. This implies that $\Lambda_+ + \Lambda_- = 6\Delta_G$, $\Lambda_+ - \Lambda_- = \Lambda$, which yields that $36\Delta_G^2 = \Lambda^2 + 4\Lambda_+ \cdot \Lambda_-$. Therefore,

$$\Lambda = \sqrt{36\Delta_G^2 - 4\Lambda_+ \cdot \Lambda_-} \leq 6\Delta_G + 2\sqrt{-\Lambda_+ \cdot \Lambda_-} \leq 6\Delta_G + 2n|\lambda_1 \lambda_n|^{\frac{3}{2}}. \tag{9}$$

On the other hand, by Hölder inequality one can see that

$$\sum_{i=1}^{n} |\lambda_i|^2 \leq \Lambda^{\frac{2}{3}} \cdot \sqrt[3]{n}$$

which means that

$$\sqrt{\frac{8m^3}{n}} \leq \Lambda. \tag{10}$$

Equations (9) and (10) derive the following relation

$$\sqrt{\frac{2m^3}{n}} \leq \frac{\Lambda}{2} \leq 3\Delta_G + n|\lambda_1 \lambda_n|^{\frac{3}{2}}$$

which shows Δ_G is bounded below by

$$\frac{1}{3}\left(\sqrt{\frac{2m^3}{n}} - n|\lambda_1 \lambda_n|^{\frac{3}{2}}\right).$$

The recent bound seems good for the graph with big size, i.e., $m \to \infty$. Now, to obtain a lower bound for the spectral radius of G, inspired by (iii), we easily see that

$$\lambda_1 \geq \sqrt[3]{\frac{6\Delta_G}{n}}. \tag{11}$$

With the help of inequality (11), one can make some lower bounds only in terms of m, n following some well-known results.

$\Delta_G \geq *$(Results in previous)	Hypotheses	$\lambda_1 \geq *$
$\Delta_G \geq \frac{(4m-n^2)m}{3n}$(Nordhaus et al. [22])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{2(4m-n^2)m}{n^2}}$
$\Delta_G \geq \frac{9mn-2n^3-2(n^2-3m)^{\frac{3}{2}}}{27}$(Fisher [8])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{2(9mn-2n^3-2(n^2-3m)^{\frac{3}{2}})}{9n}}$
$\Delta_G = (m - \lfloor \frac{n^2}{4} \rfloor) \lfloor \frac{n}{2} \rfloor$(Nikiforov et al. [21], Lovász et al. [19])	$\lfloor \frac{n^2}{4} \rfloor \leq m \leq \lfloor \frac{n^2}{4} \rfloor + \lfloor \frac{n}{2} \rfloor$	$\lambda_1 \geq \sqrt[3]{\frac{6(m - \lfloor \frac{n^2}{4} \rfloor) \lfloor \frac{n}{2} \rfloor}{n}}$
$\Delta_G \geq \frac{(4m-n^2)n}{9}$(Bollobás [2])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{8m-2n^2}{3}}$

Table 1: A list of lower bounds of spectral radius

Remark 2. Concentrating on Table 1, we observe that since the lower bound of Δ_G obtained by Fisher [8] is the best bound in comparison with the others in the list above, hence the corresponding lower bound of spectral radius is the best in the list.

4. Lower Bound on Laplacian−Energy−Like Invariant

Throughout this section, applying a crucial lemma we derive a lower bound for Laplacian-energy-like invariant.

The following result which is known as Weyl's inequalities, is concerned with the eigenvalues of sum of Hermitian matrices (see Theorem III.2.1, [1]).

Lemma 2. Let $A, B \in M_n$ be Hermitian matrices and assume that A and $A + B$ are arranged in non-increasing order. Then

$$\lambda_k(A) + \lambda_n(B) \leq \lambda_k(A+B) \leq \lambda_k(A) + \lambda_1(B), \quad k = 1, 2, \cdots, n. \tag{12}$$

Let us recall that algebraic connectivity of G (called by Fiedler [7]) is denoted by μ_{n-1}. Obviously, since G is connected, $\mu_{n-1} \neq 0$. Using the terms of algebraic connectivity and edge connectivity of G, i.e., $\eta = \eta(G)$, we obtain a lower bound for Laplacian-energy-like invariant as follows:

Theorem 3. Assume G is a simple connected graph with n vertices and m edges. Then, the following inequality holds

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}} \tag{13}$$

where λ_1 is the spectral radius of G and

$$\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}.$$

Proof. Since $D(G) = A(G) + L(G)$ and A, B are Hermitian matrices, by Lemma 2 we get

$$\lambda_k(L) + \lambda_n(A) \leq \lambda_k(D) \leq \lambda_k(L) + \lambda_1(A), \quad k = 1, 2, \cdots, n$$

which is simplified as

$$\mu_k + \lambda_n \leq d_k \leq \mu_k + \lambda_1, \quad k = 1, 2, \cdots, n.$$

Let $\mu_k + \lambda_1 \leq \alpha\lambda_1\mu_k$ for a proper constant α large enough such that $\alpha \geq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$. Indeed, for $k = 1, 2, \cdots, n-1$ we see

$$\sqrt{\frac{n}{2m}} + \frac{1}{\mu_k} \leq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}} \leq \alpha \iff \frac{\mu_k + \sqrt{\frac{2m}{n}}}{\mu_k\sqrt{\frac{2m}{n}}} \leq \alpha \iff \frac{\mu_k}{\alpha\mu_k - 1} \leq \sqrt{\frac{2m}{n}} \leq \lambda_1.$$

Moving forward, $\sqrt{d_k} \leq \sqrt{\mu_k + \lambda_1} \leq \sqrt{\alpha\lambda_1\mu_k}$ which shows that

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}}$$

for any $\alpha \geq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$.

Thus we get the required result by the value $\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$ in recent inequality.

In the following we give some immediate consequences.

Corollary 1. Suppose that G is a simple connected graph with n vertices and m edges. Then, the following inequality holds

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}}$$

where

$$\alpha = \sqrt{\frac{n}{2m} + \frac{1}{2\eta(1-\cos\frac{\pi}{n})}}.$$

Following the formula mentioned in Theorem 2 and the bounds below we have the following immediate consequences:

a) $\lambda_1 \le \sqrt{2m-n+1}$, (see Hong [13])

b) $\lambda_1 \le \frac{\sqrt{1+8m}-1}{2}$, (see Stanley [23])

c) $\lambda_1 \le \sqrt{2m-\delta-\Delta_G(\delta-1)}$, (Equation (6)).

Theorem 4. Assume G is a simple connected graph with n vertices and m edges. Then, the following inequalities hold

i) $LEL \ge \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\sqrt{2m-n+1}}}$

ii) $LEL \ge \sum_{k=1}^{n} \sqrt{\frac{2d_k}{\alpha(\sqrt{1+8m}-1)}}$

iii) $LEL \ge \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\sqrt{2m-\delta-\Delta_G(\delta-1)}}}$

where

$$\alpha = \sqrt{\frac{n}{2m} + \frac{1}{2\eta(1-\cos\frac{\pi}{n})}}.$$

Proof. Viewing (a)−(c) and Corollary 1, the results (i)−(iii) are clear.

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