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A Laplacian-energy-like invariant of a graph*

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Abstract: Let G be a simple graph with n vertices and m edges. Let λ_1, λ_2,... λ_n be the eigenvalues of the adjacency matrix of G, and let μ_1, μ_2,... μ_n be the eigenvalues of Laplacian matrix of G. The energy of G is defined as $E(G) = \sum\limits_{i=1}^{n} |\lambda_i|$. We now define and investigate a Laplacian-energy-like graph invariant $LEL(G) = \sum\limits_{i=1}^{n} \sqrt{\mu_i}$. There is a great deal of analogy between the properties of $E(G)$ and $LEL(G)$. We also establish a few sharp lower and upper bounds of $LEL(G)$.

1. Introduction

Let G be a simple graph with n vertices and m edges. In what follows we write $G(n,m)$ for it. Let A be the symmetric $(0,1)-$adjacency matrix of G and $D = diag(d_1, d_2, \ldots d_n)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $C = D - A$. Let λ_1, λ_2,... λ_n be the adjacency spectrum of G, and let μ_1, μ_2,... μ_n be the Laplacian spectrum of G. The adjacency and Laplacian spectrum obey the following relations

$$\sum_{i=1}^{n} \lambda_i = 0; \qquad \sum_{i=1}^{n} \lambda_i^2 = 2m, \tag{1.1}$$

$$\sum_{i=1}^{n} \mu_i = 2m; \qquad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2. \tag{1.2}$$

Furthermore, if the graph G has p components $(p \geq 1)$, and if the Laplacian eigenvalues are labelled so that $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$, then[18]

$$\mu_{n-i} = 0 \quad for \quad i = 0, \ldots, p-1 \quad and \quad \mu_{n-p} > 0. \tag{1.3}$$

Eichinger[20] has shown how the spectrum of C may be used to calculate the radius of gyration of a Gaussion molecule. Mohar[24] argues that, because of

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its importance in various physical and chemical theories, the spectrum of C is more natural and important than the more widely studied adjacency spectrum.

The energy of the graph G is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1.4}$$

This quantity, introduced by I. Gutman in 1978 ([4]), has a long known chemical application (see surveys [5-7]). There is currently a great interest of mathematical chemists towards $E(G)$. For some of the most recent works along these lines see [11-17].

$E(G)$ has the following basic properties

(a) $E(G) \geq 0$; equality is attained if and only if $m = 0$.

(b) If the graph G consists of (disconnected) components G_1 and G_2, then $E(G) = E(G_1) + E(G_2)$.

(c) If one component of the graph G is G_1 and all other components are isolated vertices, then $E(G) = E(G_1)$.

The Laplacian energy of the graph G has recently been defined ([8]) as

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| . \tag{1.5}$$

The Laplacian energy $LE(G)$ and the ordinary energy $E(G)$ were found to have a number of analogous properties ([8, 10]), but $LE(G)$ does not possess the basic properties (b), (c) as above.

Our intention is to conceive a new graph-energy-like quantity, that instead of Eq. (1.5) would be defined in terms of Laplacian eigenvalues, and that – hopefully – would preserve properties (b), (c). We introduce the auxiliary 'eigenvalues' ρ_i, $i = 1, 2, \ldots, n$, defined via $\rho_i = \sqrt{\mu_i}$. Then we have,

$$\sum_{i=1}^{n} \rho_i^2 = 2m = \sum_{i=1}^{n} \lambda_i^2 . \tag{1.6}$$

We introduce the Laplacian-energy-like invariant of a graph as follows

Definition 1.1. If the Laplacian eigenvalues of $G(n,m)$ are $\mu_1, \mu_2, \ldots, \mu_n$, then the Laplacian-energy-like invariant of G, denoted by $LEL(G)$, is equal to $\sum_{i=1}^{n} \sqrt{\mu_i}$, i. e.

$$LEL(G) = \sum_{i=1}^{n} \rho_i \tag{1.7}$$

where $\rho_i = \sqrt{\mu_i}$, $i = 1, 2, \ldots, n$.

In this paper, we report some properties of $LEL(G)$ and show that the above definition is well chosen. Furthermore, a few sharp lower and upper bounds of $LEL(G)$ are established.

2. Properties of LEL(G)

In this section, we present some properties of $LEL(G)$ which have a great deal of analogy with the properties (a), (b), (c) of $E(G)$.

Proposition 2.1.

(a) $LEL(G) \geq 0$; equality is attained if and only if $m = 0$.

(b) If the graph G consists of (disconnected) components G_1 and G_2 , then $LEL(G) = LEL(G_1) + LEL(G_2)$.

(c) If one component of the graph G is G_1 and all other components are isolated vertices, then $LEL(G) = LEL(G_1)$.

Proposition 2.2.

$LEL(G) \leq \sqrt{2m(n-p)}$, p is the number of components of $G(n, m)$. Equality is attained if and only if G is regular of degree 0 or G consists of n_1 copies of complete graphs of order k and $n - kn_1$ isolated vertices.

Proof. Let

$$S = \sum_{i=1}^{n-p} \sum_{j=1}^{n-p} (\sqrt{\mu_i} - \sqrt{\mu_j})^2$$

.

$$= 2\sum_{i=1}^{n-p} 2m - 2\left(\sum_{i=1}^{n-p} \sqrt{\mu_i}\right)\left(\sum_{j=1}^{n-p} \sqrt{\mu_j}\right)$$

$$= 4m(n-p) - 2LEL(G)^2$$

Since $S \geq 0$,we have $LEL(G) \leq \sqrt{2m(n-p)}$.

The equality is attained if and only if $\sqrt{\mu_i} = \sqrt{\mu_j}$, for all $i, j = 1, 2, \ldots, n-p$, and then from above we conclude that G has at most two distinct Laplacian eigenvalues

(1) $\mu_1 = \ldots = \mu_{n-p} = \frac{2m}{n-p} \quad (n \neq p)$;

(2) $\mu_{n-p+1} = \ldots = \mu_n = 0$.

If $m \neq 0$, then G has exactly two distinct Laplacian eigenvalues. A connected graph has exactly two distinct Laplacian eigenvalues if and only if its diameter is equal to unity, i. e., if it is a complete graph.

If $n = p$ or $m = 0$, then G is regular of degree 0. ■

The following lemma will be used in next proposition

Lemma 2.1. [9]

If G has at least one edge, then $\mu_1 \geq \Delta + 1$ (Δ is the greatest vertex degree in G). For G being a connected graph on $n > 1$ vertices, equality is attained if and only if $\Delta = n - 1$.

Proposition 2.3.

If G has at least one edge, then $LEL(G) \leq \sqrt{\Delta + 1} + \sqrt{(n - p - 1)(2m - \Delta - 1)}$.

Proof. Using the Cauchy-Schwarz inequality

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right), \tag{2.1}$$

which holds for arbitrary real-valued numbers $a_i, b_i, i = 1, 2, \ldots n$, we have

$$\left(\sum_{i=2}^{n-p} \sqrt{\mu_i}\right)^2 \leq (n - p - 1)\left(\sum_{i=2}^{n-p} \mu_i\right)$$

(choosing in (2.1) $a_i = \sqrt{\mu_i}$, and $b_i = 1$).

$$(LEL(G) - \sqrt{\mu_1})^2 \leq (n - p - 1)(2m - \mu_1).$$

Thus $\quad LEL(G) \leq \sqrt{\mu_1} + \sqrt{(n - p - 1)(2m - \mu_1)}$.

Since $\mu_1 \geq \Delta + 1$ ($m \neq 0$), where Δ is the greatest vertex degree of G.

By direct analysis we verify that the function $f(x) = x + \sqrt{(n - 1)(2m - x^2)}$ monotonically decreases in the interval $(\sqrt{\frac{2m}{n}}, \sqrt{2m})$, for both $\sqrt{\Delta + 1}$ and $\sqrt{\mu_1}$

belong to this interval, and therefore, we have

$$LEL(G) \leq \sqrt{\Delta+1} + \sqrt{(n-p-1)(2m-\Delta-1)}\ . \tag{2.2}$$

■

Remark 1. The equality (2.1) is attained if and only if $\frac{a_i}{b_i} = c$, c is a constant, for all $i = 1, 2, \ldots n$. By direct analysis we conclude that equality in (2.2) holds if and only if $\mu_1 = \Delta+1$ and $\mu_2 = \mu_3 = \ldots = \mu_{n-p}$. If $\mu_1 = \mu_2$, since a connected graph has exactly two distinct Laplacian eigenvalues if and only if its diameter is equal to unity, we obtain that for $p = 1$, $G = K_n$ (K_r is the complete graph of order r), for other p, $G = \alpha K_k \cup (n-k\alpha)K_1$, $\alpha \geq 1$, $k \geq 2$, provided $(k-1)\alpha = n-p$. If $\mu_1 \neq \mu_2$, then the graph G has three distinct Laplacian eigenvalues, for instance $G = K_{1,n-1}$ and also for other graphs.

Proposition 2.4.

$\sqrt{2m} \leq LEL(G) \leq \sqrt{2}m$, the right equality is attained if and only if $G = rK_2 \bigcup (n-2r)K_1$, where $0 \leq r \leq [\frac{n}{2}]$, $[x]$ is the integral part of x, while $LEL(G) = \sqrt{2m} = \sqrt{2}m$ if and only if $G = rK_2 \bigcup (n-2r)K_1$, $r = 0, 1$.

Proof. (1) Let p be the number of components of $G(n,m)$, then

$$LEL(G) = \sum_{i=1}^{n-p} \sqrt{\mu_i}.$$

Therefore

$$(LEL(G))^2 = \sum_{i=1}^{n-p} (\sqrt{\mu_i})^2 + 2\sum_{i \neq j} \sqrt{\mu_i}\sqrt{\mu_j} \geq \sum_{i=1}^{n-p} \mu_i = 2m\ .$$

The left equality is attained if and only if $\mu_1 = \ldots = \mu_{n-p} = 0$ or $\mu_1 > 0$ and $\mu_2 = \ldots = \mu_{n-p} = 0$, i.e ., if G is regular of degree 0 or $G = K_2 \cup (n-2)K_1$.

(2) Since $LEL(G) \leq \sqrt{2m(n-p)}$ (Proposition 2.2), and $n-p \leq m$, where $p \geq 1$, we obtain $LEL(G) \leq \sqrt{2}m$. Note that Proposition 2.2 and $n-p = m$ if and only if G is a forest. We obtain that $LEL(G) = \sqrt{2}m$ if and only if $G = rK_2 \bigcup (n-2r)K_1$, where $0 \leq r \leq [\frac{n}{2}]$

Combining (1) and (2), we complete the proof of Proposition 2.4. ■

Now, we study the relation among the iterated line graphs of G.

The line graph of G will be denoted by $L(G)$. The iterated line graphs of G are then defined recursively as $L^2(G) = L(L(G))$,$L^3(G) = L(L^2(G))\ldots$, $L^k(G) = L(L^{k-1}(G)),\ldots$ It is consistent to set $L(G) \equiv L^1(G)$ and $G \equiv L^0(G)$.

The line graph $L(G)$ of a regular graph G is a regular graph. Let n_t and r_t denote the order and degree of $L^t(G)$ respectively, $t = 1, 2, \ldots, k$. Then (see [1,2])

$$n_k = \frac{1}{2} r_{k-1} n_{k-1} \quad and \quad r_k = 2r_{k-1} - 2 \ \ldots\ldots$$

Therefore,

$$r_k = 2^k r_0 - 2^{k+1} + 2 \tag{2.3}$$

and

$$n_k = \frac{n_0}{2^k} \prod_{i=0}^{k-1} r_i = \frac{n_0}{2^k} \prod_{i=0}^{k-1} (2^i r_0 - 2^{i+1} + 2)\ . \tag{2.4}$$

We have

Proposition 2.5. Let G be a regular graph of order n_0 and of degree r_0, then $LEL(L^k(G)) = LEL(L^{k-1}(G)) + \sqrt{2r_{k-1}}(n_k - n_{k-1})$.

Proof. Let $C_G(\mu)$ (or $C_{L(G)}(\mu)$) be the Laplacian characteristic polynomial of G (or $L(G)$), and let $P_G(\lambda)$ (or $P_{L(G)}(\lambda)$) be the characteristic polynomial of the adjacency matrix of G (or $L(G)$).

It is well known that

$$P_{L(G)}(\lambda) = (\lambda + 2)^{n_1 - n_0} P_G(\lambda + 2 - r_0) \tag{2.5}$$

and

$$C_G(\mu) = (-1)^{n_0} P_G(-\mu + r_0)\ . \tag{2.6}$$

Then by equation (2.6) we have

$$C_{L(G)}(\mu) = (-1)^{n_1} P_{L(G)}(-\mu + (2r_0 - 2))\ . \tag{2.7}$$

Combining (2.5) and (2.7), we get $C_{L(G)}(\mu) = (\mu - 2r_0)^{n_1 - n_0} C_G(\mu)$.

Therefore, the Laplacian spectrum of $L(G)$ is

$$\begin{pmatrix} 2r_0 & \mu_1 & \mu_2 & \ldots & \mu_{n_0} \\ n_1 - n_0 & 1 & 1 & \ldots & 1 \end{pmatrix}$$

where $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n_0}$ is the Laplacian spectrum of G.

In an analogous manner as above, we have the Laplacian spectrum of $L^2(G)$

$$\begin{pmatrix} 2r_1 & 2r_0 & \mu_1 & \mu_2 & \dots & \mu_{n_0} \\ n_2-n_1 & n_1-n_0 & 1 & 1 & \dots & 1 \end{pmatrix}$$

then for the Laplacian spectrum of $L^k(G)$

$$\begin{pmatrix} 2r_{k-1} & 2r_{k-2} & \dots & 2r_0 & \mu_1 & \mu_2 & \dots & \mu_{n_0} \\ n_k-n_{k-1} & n_{k-1}-n_{k-2} & \dots & n_1-n_0 & 1 & 1 & \dots & 1 \end{pmatrix}$$

for all $k = 1, 2, \dots$.

Therefore $\quad LEL(L^k(G)) = LEL(L^{k-1}(G)) + \sqrt{2r_{k-1}}(n_k - n_{k-1})$.

The proof is complete. ■

Now, we would like to give a pair of non-cospectral graphs of the same order, having equal LEL-energies. Let $G_1 = K_{1,7}$ be a star of order 8. Then the Laplacian eigenvalues of G_1 are $\mu_{11} = 8$, $\mu_{12} = \mu_{13} = \dots = \mu_{17} = 1$, $\mu_{18} = 0$. Let $G_2 = 2K_2 \bigcup K_4$ be another graph of order 8. Then the Laplacian eigenvalues of G_2 are $\mu_{21} = \mu_{22} = \mu_{23} = 4$, $\mu_{24} = \mu_{25} = 2$, $\mu_{26} = \mu_{27} = \mu_{28} = 0$. It is straightforward to check that $LEL(G_1) = LEL(G_2)$.

At the end of this section we point out the dissimilarities between $E(G)$, $LE(G)$, and $LEL(G)$.

Dissimilarity 2.A.

In Proposition 2.1, we can see that $LEL(G)$ and $E(G)$ preserve the three elementary properties (a), (b), (c), and also they have the same square sum by equality (1.6). This is the advantage of $LEL(G)$ over $LE(G)$. Since the ordinary energy $E(G)$ has a long known application in molecular-orbital theory of organic molecules (see [5-7]), we preconceive that $LEL(G)$ would also have some chemical application.

Dissimilarity 2.B.

If the graph G is regular of degree k, then $LE(G) = E(G)$, while $LEL(G) = \sum_{i=1}^{n} \sqrt{k - \lambda_{n-i+1}}$ differs from $E(G)$. This is an advantage of $LE(G)$ over $LEL(G)$. However, if $k = 0$ or $G = K_4$, then we have $E(G) = LE(G) = LEL(G)$. In addition, for a regular graph G, $LEL(G)$ satisfies Proposition 2.5 as above.

3. Further $(n, m)-$type bounds for $LEL(G)$

There are numerous known results (especially lower and upper bounds) that are obtained by using the relations (1.1) and that depend on the parameters n and m. Then one could expect analogous results for LEL, obtained by means of the relations (1.2), that would depend on the parameters n, m and d_i. Indeed, a number of such results could be deduced in section 2.

In this section we point out a few more $(n, m)-$type new bounds for $LEL(G)$. Furthermore, we prove that for all simple graphs with n vertices, the complete graph K_n has the maximum LEL(G).

In Proposition 2.2 we proved that,

$$LEL(G) \leq \sqrt{2m(n-p)}, \tag{3.1}$$

We now show that the right-hand side expression in (3.1) is a decreasing function of the parameter p, then we have,

Theorem 3.1.

For any graph G, $LEL(G) \leq \sqrt{2m(n-1)}$. Equality holds if and only if $G = K_n$.

Proof. We consider the function

$$f(x) = \sqrt{2m(n-x)} \quad 1 \leq x \leq n.$$

Then

$$f'(x) = \frac{-m}{\sqrt{2m(n-x)}} \leq 0 \quad 1 \leq x \leq n.$$

Because the upper bound (3.1) increases with decreasing p, by setting $p = 1$ we obtain the estimate

$$LEL(G) \leq \sqrt{2m(n-1)}, \tag{3.2}$$

which holds for all graphs G. And combining with the Proposition 2.2, we have that the equality holds if and only if $G = K_n$.

■

Let $f(m)=\sqrt{2m(n-1)}\quad 0\leq 2m\leq n(n-1)$. Obviously, $f(m)$ is a increasing function of the parameter m, then we have proved,

Theorem 3.2.

Let G be a simple graph of order n, then $LEL(G)\leq (n-1)\sqrt{n}$. Equality holds if and only if $G=K_n$, i.e., the graph of order n with maximum LEL is K_n.

In Proposition 2.3 we proved,

$$LEL(G)\leq \sqrt{d_1+1}+\sqrt{(n-p-1)(2m-d_1-1)}. \tag{3.3}$$

Similar to the proof of inequality (3.2), we now show that the right-hand side expression in (3.3) is a decreasing function of the parameter p. Then the following result holds immediately,

Theorem 3.3.

If G has at least one edge, then $LEL(G)\leq \sqrt{d_1+1}+\sqrt{(n-2)(2m-d_1-1)}$. Equality holds if and only if $G=K_n$.

Proof. We consider the function

$$f(x)=\sqrt{d_1+1}+\sqrt{(n-x-1)(2m-d_1-1)}\quad 1\leq x\leq n.$$

Then

$$f'(x)=\frac{1}{2}\frac{d_1+1-2m}{\sqrt{(n-x-1)(2m-d_1-1)}}\quad 1\leq x\leq n.$$

The derived function $f'(x)\leq 0$ if and only if $d_1+1\leq 2m$, which holds for any graph G has at least one edge.

Because the upper bound (3.3) increases with decreasing p, by setting $p=1$ we obtain the estimate

$$LEL(G)\leq \sqrt{d_1+1}+\sqrt{(n-2)(2m-d_1-1)}. \tag{3.4}$$

The inequality (3.4) is sharp. Equality holds if and only if $G=K_n$. ■

We now show that the bound (3.4) is better than (3.2).

Indeed,

$$\sqrt{d_1+1}+\sqrt{(n-2)(2m-d_1-1)}\leq \sqrt{2m(n-1)}$$

holds if and only if

$$(n-2)(2m-d_1-1) \leq (\sqrt{2m(n-1)} - \sqrt{d_1+1})^2,$$

i.e.,

$$2m+(n-1)(d_1+1) \leq 2\sqrt{2m(n-1)(d_1+1)},$$

which is directly transformed into

$$(\sqrt{2m} - \sqrt{(n-1)(d_1+1)})^2 \geq 0,$$

and holds for any m, n, d_1. The equality holds if and only if $2m = (n-1)(d_1+1) = (n-1)d_1 + (n-1)$. Since $2m = \sum_{i=1}^{n} d_i \leq (n-1)d_1 + (n-1)$, hence $G = K_n$, i.e., the equality holds if and only if $G = K_n$.

4. The degree of vertex and the bounds for $LEL(G)$

In this section we present some bounds for $LEL(G)$ which depend on the vertex degrees, and we show that for all connected graphs with n vertices, the star $K_{1,n-1}$ has the minimal LEL(G).

Lemma 4.1. [23]

If G is a connected graph on $n > 2$ vertices, then $\mu_2 \geq d_2$.

Theorem 4.1.

If G is a connected graph on $n > 2$ vertices, then $LEL(G) \geq \sqrt{d_1+1} + \sqrt{d_2}$. Equality is attained if and only if $G = P_3$ (P_n is the path of order n).

Proof. It is easy to see from the Lemma 2.1 and Lemma 4.1 that $LEL(G) \geq \sqrt{d_1+1} + \sqrt{d_2}$, equality is attained if and only if $\mu_1 = d_1 + 1$, $\mu_2 = d_2$, $\mu_3 = \ldots = \mu_n = 0$. Since G is a connected graph, so we have $p = 1$, this implies $n = 3$. From Lemma 2.1, we have $d_1 = 2$, $\mu_1 = 3$. Since $\sum_{i=1}^{3} \mu_i = \sum_{i=1}^{3} d_i$, we have $(d_1+1) + d_2 + 0 = d_1 + d_2 + d_3$, thus $d_3 = 1$ and then $d_2 = 1$. Therefore $G = P_3$. ■

Now, we will give another lower bound of $LEL(G)$ for the connected graphs.

Let $a = (a_1, a_2, \ldots, a_n)$, $a_k \geq 0$, $1 \leq k \leq n$, then $A_n(a) = \frac{1}{n}\sum_{k=1}^{n} a_k$ is called the algebraic average value of $a_1, a_2, \ldots, a_n$, $G_n(a) = \sqrt[n]{a_1 a_2 \ldots a_n}$ is called the geometry average value of $a_1, a_2, \ldots, a_n$. It is well known that,

Lemma 4.2. [22]

$$G_n(a) \leq A_n(a). \tag{4.1}$$

Equality holds if and only if $a_1 = a_2 = \ldots = a_n$.

Let G be a connected graph and let $t(G)$ denote the number of spanning trees contained in G.

Lemma 4.3. [3]

Let G be a connected multigraph on n vertices, then $t(G) = \frac{1}{n}\prod_{i=1}^{n-1} \mu_i$.

It is easy to see that if G is connected then $t(G) \geq 1$. Thus we prove the following result.

Theorem 4.2.

Let G be a connected simple graph on n vertices, then $LEL(G) \geq \sqrt{n} + (n-2)$. Equality holds if and only if $G = K_{1,n-1}$, i.e., the connected simple graph of order n with minimal LEL is $K_{1,n-1}$.

Proof. Using inequality (4.1), we have

$$\frac{\sqrt{\mu_2} + \sqrt{\mu_3} + \ldots + \sqrt{\mu_{n-1}}}{n-2} \geq \sqrt[2(n-2)]{\mu_2 \mu_3 \cdots \mu_{n-1}},$$

equality holds if and only if $\mu_2 = \mu_3 = \ldots = \mu_{n-1}$.

It is well known that $\mu_1 \leq n$. So

$$\prod_{i=2}^{n-1} \mu_i \geq t(G) \geq 1,$$

the first equality holds if and only if $\mu_1 = n$, the second equality holds if and only if G is a tree.

Hence, $\sqrt{\mu_2} + \sqrt{\mu_3} + \ldots + \sqrt{\mu_{n-1}} \geq n - 2$.

Therefore

$$LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i} = \sqrt{\mu_1} + (\sqrt{\mu_2} + \ldots + \sqrt{\mu_{n-1}}) \geq \sqrt{\mu_1} + (n-2),$$

equality holds if and only if $\mu_1 = n$ and $\mu_2 = \mu_3 = \ldots = \mu_{n-1}$ and G is a tree, which implies that $G = K_{1,n-1}$ and $LEL(G) \geq \sqrt{n} + (n-2)$. ■

Now, we will give upper bounds of $LEL(G)$ for the connected graphs.

Definition 4.1. [9] If vector $(a) = (a_1, a_2, \cdots a_r)$ and $(b) = (b_1, b_2, \cdots b_s)$ are nonincreasing sequences of real numbers, then (a) majorizes (b) if

$$\sum_{i=1}^{k} a_i \geq \sum_{i=1}^{k} b_i \quad k = 1, 2, \cdots, min\{r, s\},$$

and

$$\sum_{i=1}^{r} a_i = \sum_{i=1}^{s} b_i.$$

We denote it by $b \prec a$.

Definition 4.2. [25] The relation $x \prec\prec y$ means that $x \prec y$ and x is not the rearrangement of y.

Definition 4.3. [22] A real valued function $f(x)$ defined on a convex set D is said to be convex if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y),$$

for all $0 \leq \lambda \leq 1$ and all $x, y \in D$. If the above inequality is always strict for $0 < \lambda < 1$ and $x \neq y$, then f is called strictly convex. If $-f$ is a convex function, then f is called concave.

Lemma 4.4. [25] Let $(x) = (x_1, x_2, \cdots x_n)$ be majorized by $(y) = (y_1, y_2, \cdots y_n)$, i.e., $x \prec y$, then for any convex function φ, the following inequality holds,

$$\sum_{j=1}^{n} \varphi(x_j) \leq \sum_{j=1}^{n} \varphi(y_j).$$

Lemma 4.5. [25] Let $x \prec\prec y$, then for any strictly convex function φ, the following inequality holds,

$$\sum_{j=1}^{n} \varphi(x_j) < \sum_{j=1}^{n} \varphi(y_j).$$

For convenience, letting (d) denote the nonincreasing sequence $(d) = (d_1 + 1, d_2, \cdots, d_{n-1}, d_n - 1)$ of vertex degrees and letting (μ) denote the nonincreasing sequence $(\mu) = (\mu_1, \mu_2, \cdots, \mu_{n-1}, \mu_n)$ of nonnegative real Laplacian eigenvalues.

Lemma 4.6. [21] Let G be a connected graph on $n \geq 2$ vertices, then (d) is majorized by (μ).

Theorem 4.3.

Let G be a connected graph on $n \geq 2$ vertices, then $LEL(G) \leq \sqrt{d_1 + 1} + \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1}$, where the equality holds if and only if $(d) = (\mu)$.

Proof. Let $\varphi(x) = -\sqrt{x}$, $x \in [0, +\infty)$, then $\varphi(x)$ is a convex function. Since (d) is majorized by (μ), using Lemma 4.4 we have,

$(-\sqrt{d_1 + 1}) + (-\sqrt{d_2}) + \cdots + (-\sqrt{d_{n-1}}) + (-\sqrt{d_n - 1}) \leq (-\sqrt{\mu_1}) + (-\sqrt{\mu_2}) + \cdots + (-\sqrt{\mu_{n-1}}) + (-\sqrt{\mu_n})$,

which is directly transformed into

$(\sqrt{\mu_1}) + (\sqrt{\mu_2}) + \cdots + (\sqrt{\mu_{n-1}}) + (\sqrt{\mu_n}) \leq (\sqrt{d_1 + 1}) + (\sqrt{d_2}) + \cdots + (\sqrt{d_{n-1}}) + (\sqrt{d_n - 1})$,

i.e.,

$$LEL(G) \leq \sqrt{d_1 + 1} + \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1}. \tag{4.2}$$

And it is easy to see from Lemma 4.5 that the equality holds if and only if $(d) = (\mu)$. ■

Remark 2. We now show that the bounds (3.4) and (4.2) are incomparable. Firstly, we show the case when inequality (4.2) is better than (3.4). In fact, if $d_n = 1$, then by Cauchy-Schwarz inequality, $\sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1} = \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} \leq \sqrt{(n-2)(2m - d_1 - 1)}$. Equality holds if and only if $d_2 = \cdots = d_{n-1}$. Therefore, if $d_n = 1$, then the upper bound (4.2) is better than (3.4).

However, if $d_n \geq 2$, we can give some graphs to show that the upper bound (3.4) is better than (4.2). For example, it is easy to check that the upper bound

(3.4) is better than (4.2) when $G = C_3$ or $G = C_6$.

Remark 3. We show that the bounds (3.2) and (4.2) are also incomparable. Let H_1, H_2 be the graphs shown in Figure 1.

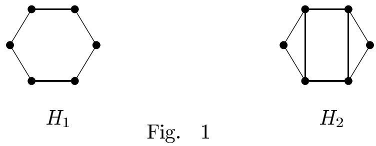

Fig. 1

Then for $G = H_1$ the upper bound (3.2) is better than (4.2). On the other hand, if $G = H_2$ then the upper bound (4.2) is better than (3.2).

We now discuss the case $LEL(G) = \sqrt{d_1 + 1} + \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1}$.

Lemma 4.7. [19] If an isolated vertex is connected by edges to all the vertices of a graph G of order n, then the Laplacian eigenvalues of the resultant graph are as follows: one of the eigenvalues is $n + 1$, the other eigenvalues can be obtained by incrementing the eigenvalues of the old graph G by 1 except the lowest one and 0 as another eigenvalue.

Example 4.1. Let G_1, G_2 be the graphs shown in Figure 2. The Laplacian spectrum of G_1 is $(3, 1, 0)$. We want to find out the spectrum of G_2.

Fig. 2

Applying Lemma 4.7, we can easily get the spectrum of G_2 is $(4, 4, 2, 0)$.

Theorem 4.4.

Let G be a connected graph on $n \geq 2$ vertices, then $(d) = (\mu)$ if and only if $G = K_{1,n-1}$.

Proof. If $G = K_{1,n-1}$ then $(d) = (\mu)$.

Conversely, let $(d) = (\mu)$, we are to show that G is a star. If $(d_1 + 1, d_2, \cdots, d_{n-1}, d_n - 1) = (\mu_1, \mu_2, \cdots, \mu_{n-1}, \mu_n)$, then we have $\mu_1 = d_1 + 1$.

Since G is a connected graph, using Lemma 2.1, we have $d_1 = n-1$.

Let $G' = (V', E')$ be a graph with vertex set $V' = \{v_1, v_2, \cdots, v_{n-1}\}$, and edge set $E' \neq \emptyset$, let $a_1 \geq a_2 \geq \cdots \geq a_{n-1} = 0$ be the Laplacian eigenvalues of G', and let $b_1 \geq b_2 \geq \cdots \geq b_{n-1}$ be the nonincreasing vertex degrees of G'. Let G be a graph obtained from G' by adding a new vertex v_n, which is connected by edges to all the vertices of G'.

Applying Lemma 4.7, the Laplacian spectrum of G is $(n, a_1+1, a_2+1, \cdots a_{n-2}+1, 0)$, which we denoted it by (μ). If $(\mu) = (d) = (d_1+1, d_2, \cdots, d_{n-1}, d_n - 1)$ then $d_1 = n-1$, $d_2 = b_1 + 1 = a_1 + 1$. Hence $b_1 = a_1$. Since $E' \neq \emptyset$, using Lemma 2.1, we have $a_1 \geq b_1 + 1$, a contradiction. Thus $E' = \emptyset$, which implies $G = K_{1,n-1}$. ■

According to Theorem 4.3 and Theorem 4.4 and noting $(d) \prec (\mu)$ we obtain the following theorem.

Theorem 4.5.

Let G be a connected graph on $n \geq 2$ vertices, then $LEL(G) = \sqrt{d_1+1} + \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1}$ if and only if $G = K_{1,n-1}$.

Now we give another upper bound depended on the vertex degrees.

Theorem 4.6.

Let G be a connected graph on $n \geq 2$ vertices, then

$$LEL(G) \leq \frac{1}{2}\left(\sqrt{n-1} + \sqrt{\frac{1}{n-1}}\right)\left(\sum_{i=1}^{n} \sqrt{d_i}\right).$$

Proof. Using Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^{n} \sqrt{\mu_i}\right)^2 \leq n\left(\sum_{i=1}^{n} \mu_i\right).$$

On the other hand, since G is a connected graph on $n \geq 2$ vertices, thus $1 \leq d_i \leq n-1$ for any integer $1 \leq i \leq n$. Then by Polya-Szegö inequality, we have

$$n\left(\sum_{i=1}^{n} d_i\right) \leq \frac{1}{4}\left(\sqrt{n-1} + \sqrt{\frac{1}{n-1}}\right)^2 \left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2,$$

Since $n\left(\sum_{i=1}^{n}\mu_i\right) = n\left(\sum_{i=1}^{n}d_i\right)$, hence

$$LEL(G) \leq \frac{1}{2}\left(\sqrt{n-1}+\sqrt{\frac{1}{n-1}}\right)(\sum_{i=1}^{n}\sqrt{d_i}). \tag{4.3}$$

This completes the proof of the theorem. ■

Remark 4. Using Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^{n}\sqrt{d_i}\right) \leq \sqrt{n\left(\sum_{i=1}^{n}d_i\right)} = \sqrt{2mn}.$$

Combining with inequality (4.3), we obtain

$$LEL(G) \leq \frac{1}{2}\left(\sqrt{n-1}+\sqrt{\frac{1}{n-1}}\right)\sqrt{2mn}. \tag{4.4}$$

Unfortunately, the bound (4.4) is not better than the bound (3.2). In fact, by direct calculation, $\sqrt{2m(n-1)} \leq \frac{1}{2}\left(\sqrt{n-1}+\sqrt{\frac{1}{n-1}}\right)\sqrt{2mn}$ if and only if $n^3-4n^2+8n-4 \geq 0$, where the inequality always holds for any integer number n.

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