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Open Problem on σ-invariant

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Abstract. Let G be a graph of order n with m edges. Also let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ be the Laplacian eigenvalues of graph G and let $\sigma = \sigma(G)$ $(1 \leq \sigma \leq n)$ be the largest positive integer such that $\mu_\sigma \geq 2m/n$. In this paper, we prove that $\mu_2(G) \geq 2m/n$ for almost all graphs. Moreover, we characterize the extremal graphs for any graphs. Finally, we provide the answer to Problem 3 in [8], that is, the characterization of all graphs with $\sigma = 1$.

1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$, $|E(G)| = m$. Let d_i be the degree of the vertex v_i $(i = 1, 2, \ldots, n)$. The maximum vertex degree is denoted by Δ_1 $(= d_1)$ and the second maximum by Δ_2 $(= d_2)$. Let $N(v_i)$ be the neighbor set of vertex v_i, $i = 1, 2, \ldots, n$. We denote by $\overline{G}$, the complement of the graph G. Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal matrix of vertex degrees of G, respectively. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. This matrix has nonnegative eigenvalues $n \geq \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. To know more information about Laplacian eigenvalues of graphs, see [2, 4, 10, 16]. When more than one graph is under consideration, then we write $\mu_i(G)$ instead of μ_i.

For a graph G, consider the positive number $\sigma = \sigma(G)$ $(1 \leq \sigma \leq n)$ of the Laplacian eigenvalues greater than or equal to the average degree $2m/n$. More precisely σ is the largest positive integer for which $\mu_\sigma \geq 2m/n$. This number as a spectral graph invariant with several open problems and conjectures are introduced in [8].

Let I be an interval of the real line. Denote by $m_G(I)$ the number of Laplacian eigenvalues, multiplicities included, that belong to I. Notice that $m_G(I)$ is a natural extension of multiplicity $m_G(\mu)$ of a Laplacian eigenvalue μ. Merris in [16] presented several results on $m_G(I)$ and gave some references for its applications. This research topic

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was extensively investigated in many papers (see, [10,12,15–17]). Indeed, by the definition of σ, we have

$$\sigma(G) = m_G\left(\left[\frac{2m}{n}, n\right]\right).$$

It is worth noticing that the value of $\sigma(G)$ sheds light on the distribution of the Laplacian eigenvalues of a graph G. Actually it determines how many Laplacian eigenvalues of graph G are greater than or equal to the average of the Laplacian eigenvalues of graph.

A further Laplacian-spectrum-based graph invariant was put forward by Gutman and Zhou [11] as

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

For its basic properties, including various lower and upper bounds, see [5, 6, 20]. It is not difficult to see that

$$\mathrm{LE}(G) = 2\sum_{i=1}^{\sigma}\mu_i - \frac{4m\sigma}{n}. \tag{1.1}$$

This is another motivation to study this graph invariant for the Laplacian energy of a graph G.

Therefore, the spectral parameter σ is reasonable relevant in spectral graph theory. To know more information about this spectral graph invariant and its applications, see [7,8,19]. In [7], all graphs with $\sigma(G) = n-1$ were characterized and the result was applied for Laplacian energy of graphs. It is interesting to characterize all graphs for some specific value of $\sigma = \sigma(G)$ between 1 and $n-2$. In particular, the following problem is given in [8].

Problem 1.1. [8] Characterize the graphs with $\sigma = 1$.

Li and Pan [14] showed that

$$\mu_2(G) \geq \Delta_2 \tag{1.2}$$

with equality if G is an $r \times s$ complete bipartite graph $K_{r,s}$ $(r + s = n)$ or a tree T with degree sequence $\pi(T) = (n/2, n/2, \underbrace{1, \ldots, 1}_{n-2})$, where $n \geq 4$ is even. This result was improved by one of the present authors in [2] as follows:

$$\mu_2(G) \geq \begin{cases} (\Delta_2 + 2 + \sqrt{(\Delta_2 - 2)^2 + 4c_{12}})/2 & \text{if } v_1v_2 \in E(G), \\ (\Delta_2 + 1 + \sqrt{(\Delta_2 + 1)^2 - 4c_{12}})/2 & \text{if } v_1v_2 \notin E(G), \end{cases}$$

where v_1 and v_2 are the maximum and the second maximum degree vertices of graph G, respectively, and $c_{12} = |N(v_1) \cap N(v_2)|$. We refer to [2, 14, 22] for more background on the second largest Laplacian eigenvalues of graphs.

For two vertex-disjoint graphs G_1 and G_2, we use $G_1 \cup G_2$ to denote their union. The join $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph obtained from the disjoint union of G_1 and G_2 by adding all edges between $V(G_1)$ and $V(G_2)$. For any two sets $A, B \subseteq V(G)$ $(E(G))$, let $A \setminus B$ be the set of vertices (edges) belongs to A, but not B. Denote by $|A|$ the cardinality of the set A. As usual, K_n, $K_{1,n-1}$ and $DS_{p,q}$ ($p \geq q \geq 2$, $p+q=n$), denote, respectively, the complete graph, the star graph, and the double star graph on n vertices.

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we give a lower bound on the second largest Laplacian eigenvalue of graph G and characterize the extremal graphs. We present an upper bound for the third smallest Laplacian eigenvalue of G. In Section 4, we obtain the solution for Problem 1.1. Finally we apply this result for Laplacian energy of graphs.

2. Preliminaries

In this section, we shall list some previously known results that will be needed in the next two sections. We begin with first two results on symmetric matrices of order n.

Lemma 2.1. [9] *Let A and B be two real symmetric matrices of size n. Then for any $1 \leq k \leq n$,*

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

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

Lemma 2.2. [21] *Let B be an $n \times n$ symmetric matrix and let B_k be its leading $k \times k$ submatrix. Then, for $i = 1, 2, \ldots, k$,*

$$\lambda_{n-i+1}(B) \leq \lambda_{k-i+1}(B_k) \leq \lambda_{k-i+1}(B),$$

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

The following result is well-known as interlacing theorem on Laplacian eigenvalues.

Lemma 2.3. [13] *Let G be a graph of n vertices and let H be a subgraph of G obtained by deleting an edge in G. Then*

$$\begin{aligned}\mu_1(G) \geq \mu_1(H) \geq \mu_2(G) \geq \mu_2(H) \geq \mu_3(G) \geq \cdots \\ \geq \mu_{n-1}(G) \geq \mu_{n-1}(H) \geq \mu_n(G) \geq \mu_n(H) \geq 0,\end{aligned}$$

where $\mu_i(F)$ is the i-th largest Laplacian eigenvalue of the graph F.

Merris in [16] gave a lower bound on Laplacian spectral radius of a graph G as follows:

Lemma 2.4. [16] *Let G be a graph on n vertices which has at least one edge. Then*

$$\mu_1 \geq \Delta_1 + 1. \tag{2.1}$$

Moreover, if G is connected, then the equality holds in (2.1) if and only if $\Delta_1 = n - 1$.

We now mention an upper bound on the Laplacian spectral radius of graph G:

Lemma 2.5. [1] *Let G be a graph. Then*

$$\mu_1(G) \leq \max\{d_i + d_j \mid v_i v_j \in E(G)\} \leq \Delta_1 + \Delta_2,$$

where d_i is the degree of vertex $v_i \in V(G)$.

The following result is obtained in [3].

Lemma 2.6. [3] *Let G be a connected graph with $n \geq 3$ vertices. Then $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$ if and only if $G \cong K_n$, $G \cong K_{1,n-1}$ or $G \cong K_{n/2,n/2}$ (n is even).*

Pan and Hou [18] obtained the necessary condition for a graph to have an equality of the second largest Laplacian eigenvalue μ_2 and its lower bound Δ_2:

Lemma 2.7. [18] *Let $G \ncong K_{1,n-1}$ be a connected graph of order $n \geq 3$ with maximum degree vertex v_1 and the second maximum degree vertex v_2, where $v_1 v_2 \in E(G)$. If $\mu_2(G) = \Delta_2$, then*

(1) $N(v_1) \cap N(v_2) = \emptyset$;

(2) $\Delta_1 = \Delta_2$;

(3) $\Delta_1 + \Delta_2 = n$.

The nice relation between Laplacian spectrum of graph G and the Laplacian spectrum of graph $\overline{G}$ is the following:

Lemma 2.8. [16] *Let G be a graph with Laplacian spectrum $\{0 = \mu_n, \mu_{n-1}, \ldots, \mu_2, \mu_1\}$. Then the Laplacian spectrum of $\overline{G}$ is $\{0, n - \mu_1, n - \mu_2, \ldots, n - \mu_{n-2}, n - \mu_{n-1}\}$, where $\overline{G}$ is the complement of the graph G.*

3. Lower bound for the second largest Laplacian eigenvalue of graphs

In this section we give some lower bounds on the second largest Laplacian eigenvalue of graph G and characterize the extremal graphs. Moreover, we give an upper bound for the third smallest Laplacian eigenvalue of graph G. From now we always assume that $\Delta_1 = d_1 \geq \Delta_2 = d_2 \geq \cdots \geq d_n$. Let k ($2 \leq k \leq n$) be the largest positive integer such that

$d_2 = \cdots = d_k = \Delta_2$. For $G \cong DS_{p,q}$ $(p \geq q \geq 2,\ p+q = n)$, we have $\Delta_2 = d_2 = q > 1 = d_3$ and hence $k = 2$. For $G \cong K_{1,n-1}$, we have $d_2 = d_3 = \cdots = d_n = \Delta_2$ and $k = n$. For any graph G we have

$$\frac{2m}{n} = \frac{\Delta_1 + \Delta_2 + \sum_{i=3}^{n} d_i}{n} \leq \Delta_2 + \frac{\Delta_1 - \Delta_2}{n} < \Delta_2 + 1. \tag{3.1}$$

Now we have the following result:

Lemma 3.1. *Let G be a graph of order $n > 2$ with m edges. If $\Delta_2 < 2m/n$, then*

(i) $\Delta_1 - \Delta_2 > \sum_{i=3}^{n}(\Delta_2 - d_i)$,

(ii) $\Delta_2 = d_3$,

(iii) $\Delta_1 > \Delta_2 + n - k$,

(iv) $k \geq \Delta_2 + n + 1 - \Delta_1 \geq \Delta_2 + 2$.

Proof. (i) Since $\Delta_2 < 2m/n$, we have

$$\sum_{i=1}^{n} d_i = 2m > n\Delta_2, \quad \text{that is,} \quad \Delta_1 - \Delta_2 > \sum_{i=3}^{n}(\Delta_2 - d_i).$$

(ii) We have $\Delta_2 \geq d_3$. If $\Delta_2 > d_3$, then

$$\Delta_1 > \Delta_2 + \sum_{i=3}^{n}(\Delta_2 - d_i) \geq \Delta_2 + n - 2 \geq n - 1,$$

a contradiction. Hence $\Delta_2 = d_3$.

(iii) From (i), we have

$$\Delta_1 \geq \Delta_2 + 1 + \sum_{i=k+1}^{n}(\Delta_2 - d_i) \geq \Delta_2 + 1 + n - k > \Delta_2 + n - k.$$

(iv) From (iii), we have

$$k \geq \Delta_2 + n + 1 - \Delta_1 \geq \Delta_2 + 2.$$

This completes the proof of the result. $\square$

Let S be the set of vertices $v_j \in V(G) \setminus \{v_1\}$ such that $d_j = \Delta_2$, that is,

$$S = \{v_j \in V(G) \setminus \{v_1\} \mid d_j = \Delta_2\}.$$

Since $\Delta_2 = d_2$, we have $|S| \geq 1$. Denote by $T = V(G) \setminus (S \cup \{v_1\})$ (see Figure 3.1). Then we have $d_i \leq \Delta_2 - 1$ for any vertex $v_i \in T$. Since $d_2 = \cdots = d_k = \Delta_2$, we have $|S| = k - 1$ and hence $|T| = n - k$. Let S_1 and S_2 be two sets of vertices such that

$$S_1 = \{v_j \in S \mid v_1 v_j \in E(G)\}, \quad S_2 = S \setminus S_1.$$

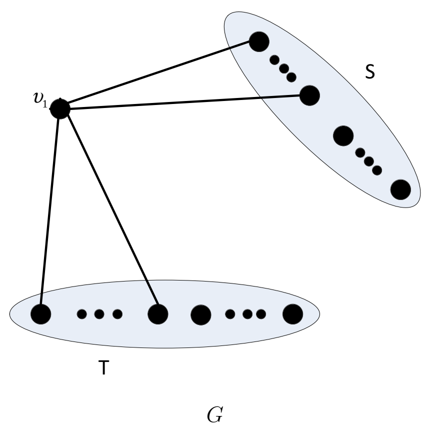


Figure 3.1: The graph G with the vertex set $V(G) = \{v_1\} \cup S \cup T$.

We need the following two results for our main result on the lower bound of μ_2.

Lemma 3.2. *Let G be a graph of order $n > 2$ with m edges. If there is an edge in the subgraph induced by S in G and $\Delta_2 < 2m/n$, then $\mu_2(G) > 2m/n$.*

Proof. Let v_i and v_j be two vertices in the subgraph induced by S in G such that $v_i v_j \in E(G)$. Here we consider the following two cases:

Case 1*: $v_i, v_j \in S_1$ or $v_i, v_j \in S_2$.* In this case the 3×3 leading principal submatrix M^* (two possibilities) corresponding to vertices v_1, v_i, v_j is of the form

$$M^* = \begin{pmatrix} \Delta_1 & a & a \\ a & \Delta_2 & -1 \\ a & -1 & \Delta_2 \end{pmatrix}, \quad \text{where } a \in \{0, -1\}.$$

One can easily see that the eigenvalues of M^* are Δ_1, $\Delta_2 + 1$, $\Delta_2 - 1$ for $a = 0$, and

$$\frac{\Delta_1 + \Delta_2 - 1}{2} \pm \frac{1}{2}\sqrt{(\Delta_1 - \Delta_2)(\Delta_1 - \Delta_2 + 2) + 9}, \quad \Delta_2 + 1 \quad \text{for } a = -1.$$

Hence by Lemma 2.2 with the above and (3.1), we obtain

$$\mu_2(G) \geq \mu_2(M^*) = \Delta_2 + 1 > \frac{2m}{n}.$$

Case 2: $v_i \in S_1$, $v_j \in S_2$. Since $\Delta_2 < 2m/n$, from Lemma 3.1(iii) with $|T| = n-k$, we get $\Delta_1 \geq \Delta_2 + 1 + |T|$. Since $N(v_1) \subseteq S_1 \cup T$, therefore there are at least $\Delta_2 + 1$ vertices in S_1, adjacent to v_1. Thus we have $|S_1| \geq \Delta_2 + 1 \geq 3$ (as $\Delta_2 = d_i \geq 2$) and $|S_2| \geq 0$. From this result, we can assume that a vertex set $W = \{w_1, \ldots, w_{\Delta_2}\} \subseteq S_1$, where $v_i \notin W$. If there exists an edge (say, $v_r v_\ell$) in the subgraph induced by $W \cup \{v_i\}$ in G, then by Case 1 (M^* corresponding to vertices v_1, v_r and v_ℓ), we get the required result. Otherwise, $W \cup \{v_i\}$ is an independent set in G. First we assume that $v_j w_i \notin E(G)$ for $1 \leq i \leq \Delta_2$. Then $K_{1,\Delta_2} \cup K_{1,\Delta_2}$ is a subgraph of G with one star K_{1,Δ_2} induced by $\{v_1, w_1, w_2, \ldots, w_{\Delta_2}\}$ and the other star K_{1,Δ_2} induced by $\{v_j\} \cup N(v_j)$, where $\{v_1, w_1, w_2, \ldots, w_{\Delta_2}\} \cap (\{v_j\} \cup N(v_j)) = \emptyset$ and $|N(v_j)| = \Delta_2$. By Lemma 2.3, we have

$$\mu_2(G) \geq \mu_2(K_{1,\Delta_2} \cup K_{1,\Delta_2}) = \Delta_2 + 1 > \frac{2m}{n}$$

by (3.1).

Next we assume that there exists at least one vertex in W, w_q (say), adjacent to v_j. In this case we consider 4×4 leading principal submatrix N^* corresponding to vertices v_1, v_i, w_q and v_j of Laplacian matrix $L(G)$, where

$$N^* = \begin{pmatrix} \Delta_1 & -1 & -1 & 0 \\ -1 & \Delta_2 & 0 & -1 \\ -1 & 0 & \Delta_2 & -1 \\ 0 & -1 & -1 & \Delta_2 \end{pmatrix}.$$

Let $g(x) = \det(xI - N^*)$ be the characteristic polynomial of N^*. For $b \in \{1,2,3\}$, we obtain

(3.2)

$$\begin{aligned} g(\Delta_2 + b/3) &= \det((\Delta_2 + b/3)I - N^*) \\ &= \begin{vmatrix} \Delta_2 - \Delta_1 + b/3 & 1 & 1 & 0 \\ 1 & b/3 & 0 & 1 \\ 1 & 0 & b/3 & 1 \\ 0 & 1 & 1 & b/3 \end{vmatrix} = \begin{vmatrix} \Delta_2 - \Delta_1 + b/3 & 0 & 0 & -b/3 \\ 1 & b/3 & 0 & 1 \\ 1 & 0 & b/3 & 1 \\ 0 & 1 & 1 & b/3 \end{vmatrix} \\ &= (\Delta_1 - \Delta_2 - b/3)\left(\frac{2}{3}b - \frac{1}{27}b^3\right) - \frac{2}{9}b^2. \end{aligned}$$

Similarly, we have

$$g(\Delta_1) = -2(\Delta_1 - \Delta_2)^2 < 0 \quad \text{as } \Delta_1 > \Delta_2. \tag{3.3}$$

From $\Delta_1 \geq \Delta_2 + 1$, we now consider the following two subcases:

Subcase 2.1*: $\Delta_1 = \Delta_2 + i$, where $i = 1$ or 2.* From (3.2), one can easily see that

$$g\left(\Delta_2 + \frac{i}{3}\right) = -\frac{2}{81}i^4 + \frac{2}{9}i^2 > 0.$$

From the above result with (3.3), we conclude that $\mu_2(N^*) > \Delta_2 + i/3$ as $\mu_1(N^*) > \Delta_1$. Since in this case $n \geq 4$, by Lemma 2.2 and (3.1), we get

$$\mu_2(G) \geq \mu_2(N^*) > \Delta_2 + \frac{i}{3} > \Delta_2 + \frac{i}{n} = \Delta_2 + \frac{\Delta_1 - \Delta_2}{n} \geq \frac{2m}{n}.$$

Subcase 2.2*: $\Delta_1 \geq \Delta_2 + 3$.* From (3.2), we have $g(\Delta_2+1) = \Delta_1 - \Delta_2 - 3 \geq 0$. Similarly, as the above subcase, we have $\mu_2(N^*) \geq \Delta_2 + 1$. Again by Lemma 2.2 with (3.1), we have

$$\mu_2(G) \geq \mu_2(N^*) \geq \Delta_2 + 1 > \frac{2m}{n}.$$

This completes the proof of the result. □

Let T_1 and T_2 be two sets of vertices such that

$$T_1 = \{v_j \in T \mid v_1 v_j \in E(G)\}, \quad T_2 = T \setminus T_1.$$

If $|T_1| = t_1$ and $|T_2| = t_2$, then we have

$$n - k = t_1 + t_2. \tag{3.4}$$

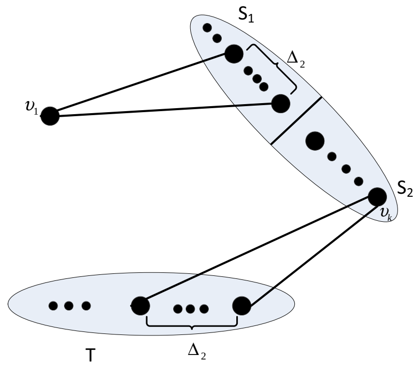
Lemma 3.3. *Let $G \ncong K_{1,n-1}$ be a connected graph of order n with m edges. If there is not any edge in the subgraph induced by S in G and $\Delta_2 < 2m/n$, then $\mu_2(G) > 2m/n$.*

Proof. We have that S is an independent set. Since G is connected and $G \ncong K_{1,n-1}$, we have $\Delta_2 \geq 2$. Again since $\Delta_2 < 2m/n$, by Lemma 3.1, we have that Lemma 3.1(i), (iii) and (iv) hold. From $|S_2| \geq 0$, we consider the following two cases:

Case 1*: $|S_2| \geq 1$.* Let v_k be any one vertex in S_2. Then the degree of v_k is Δ_2. Since S is an independent set, one can easily see that $K_{1,\Delta_2} \cup K_{1,\Delta_2}$ is a subgraph of G with one star K_{1,Δ_2} induced by $\{v_1\}$ with any Δ_2 vertices in S_1 and the other star K_{1,Δ_2} induced by $\{v_k\} \cup N(v_k)$, where $N(v_k) \subseteq T$, $|N(v_k)| = \Delta_2$ (see Figure 3.2), that is, $K_{1,\Delta_2} \cup K_{1,\Delta_2} \subseteq G$ and hence

$$\mu_2(G) \geq \mu_2(K_{1,\Delta_2} \cup K_{1,\Delta_2}) = \Delta_2 + 1 > \frac{2m}{n}$$

by (3.1).



G

Figure 3.2: The graph G contains two vertex-disjoint stars K_{1,Δ_2} with central vertices v_1 and v_k.

Case 2: $|S_2| = 0$. From the definitions, we have $\Delta_1 = k - 1 + t_1$. Using this with Lemma 3.1(iii) and (3.4), we get

$$t_2 < k - 1 - \Delta_2. \tag{3.5}$$

Let G_T be the subgraph of G induced by vertex set T with $|E(G_T)| = m_T \geq 0$. Since $S = S_1$ is an independent set, we have

$$m = \Delta_1 + (k-1)(\Delta_2 - 1) + m_T \leq \sum_{v_i \in T} d_i + k - 1.$$

Since $m_T \geq 0$, from the above with $\Delta_1 = k - 1 + t_1$, we get

$$\begin{aligned} (k-1)(\Delta_2 - 1) &\leq \sum_{v_i \in T} d_i - t_1 \\ &= \sum_{v_i \in T_1} (d_i - 1) + \sum_{v_i \in T_2} d_i \\ &\leq t_1(\Delta_2 - 2) + t_2(\Delta_2 - 1) \quad \text{as } d_i \leq \Delta_2 - 1 \text{ for } v_i \in T \\ &\leq (t_1 + t_2)(\Delta_2 - 1). \end{aligned} \tag{3.6}$$

Since $\Delta_2 \geq 2$, therefore from the above $k - 1 \leq t_1 + t_2$. This result with (3.5), we have $t_2 < t_1 + t_2 - \Delta_2$, that is, $t_1 > \Delta_2$. If $t_1(\Delta_2 - 2) + t_2(\Delta_2 - 1) = (t_1 + t_2)(\Delta_2 - 1)$ (see the last inequality of (3.6)), then $t_1 = 0$, a contradiction as $t_1 > \Delta_2 \geq 2$. Hence the last inequality of (3.6) is strict, that is, $k \leq t_1 + t_2$ and hence $k \leq n/2$, by (3.4). Using $k \leq t_1 + t_2$ in (3.5), we get $t_2 < t_1 + t_2 - \Delta_2 - 1$, that is, $t_1 \geq \Delta_2 + 2$. Using this and Lemma 3.1(iv), from $\Delta_1 = k - 1 + t_1$, we get $\Delta_1 \geq 2\Delta_2 + 3$. Also we have

$$\frac{2m}{n} = \frac{\Delta_1 + (k-1)\Delta_2 + \sum_{i=k+1}^{n} d_i}{n} \leq \Delta_2 + \frac{\Delta_1 - \Delta_2 + k - n}{n}.$$

From the above with $k \leq n/2$, one can easily get

$$\frac{2m}{n} < \Delta_2 + \frac{1}{2}. \tag{3.7}$$

We now consider the following two subcases:

Subcase 2.1*: There exists at least one vertex in S non-adjacent to any vertex in T_2.* Suppose that vertex v_i in S is not adjacent to any vertex in T_2. Then the vertex v_i is adjacent to v_1 and $\Delta_2 - 1$ vertices in T_1 as the degree of v_i is Δ_2. Again since vertex v_1 is adjacent to all the vertices in T_1, one can easily see that $K_2 \vee \overline{K}_{\Delta_2-1}$ (see Figure 3.3) is a subgraph of G. Then we have $\mu_2(G) \geq \mu_2(K_2 \vee \overline{K}_{\Delta_2-1}) = \Delta_2 + 1 > 2m/n$, by (3.7).

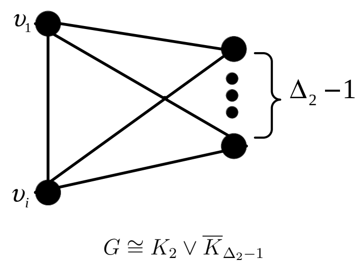


Figure 3.3: The graph $G \cong K_2 \vee \overline{K}_{\Delta_2-1}$.

Subcase 2.2*: Any one vertex in S is adjacent to at least one vertex in T_2.* We have $d_\ell \leq \Delta_2 - 1$ for any $v_\ell \in T_2$. Therefore

$$t_2 \geq \left\lceil \frac{k-1}{\Delta_2 - 1} \right\rceil. \tag{3.8}$$

If $\Delta_2 = 2$, then from the above, $t_2 \geq k - 1$. From (3.5), we have $t_2 < k - 3$, a contradiction. Hence $\Delta_2 \geq 3$. Now we have to prove that $\mu_2(G) > 2m/n$ for $\Delta_2 \geq 3$. Let $X = \{v_i \in T \mid d_i \leq \Delta_2 - 2\}$ and $|X| = x$. Then

$$n\Delta_2 < 2m \leq \Delta_1 + (k-1)\Delta_2 + x(\Delta_2 - 2) + (n - k - x)(\Delta_2 - 1),$$

that is,

$$x < \Delta_1 - \Delta_2 - n + k. \tag{3.9}$$

Let $T' = T \setminus X$. We define two edge sets E_{SX} and $E_{ST'}$, where

$$E_{SX} = \{v_iv_j \in E(G) \mid v_i \in S, v_j \in X\} \quad \text{and} \quad E_{ST'} = \{v_iv_j \in E(G) \mid v_i \in S, v_j \in T'\}.$$

Denoted by $|X \cap T_1| = x_1$ and $|X \cap T_2| = x_2$, then we obtain

$$|E_{SX}| \leq (\Delta_2 - 3)x_1 + (\Delta_2 - 2)x_2 \tag{3.10}$$

as all the vertices in T_1 are adjacent to v_1. Note that

$$\sum_{v_i \in S} d_i = (k-1)\Delta_2 = k - 1 + |E_{SX}| + |E_{ST'}|.$$

From the above result with (3.9) and (3.10), we have

$$\begin{aligned}
|E_{ST'}| &= (k-1)(\Delta_2 - 1) - |E_{SX}| \\
&\geq (k-1)(\Delta_2 - 1) - ((\Delta_2 - 3)x_1 + (\Delta_2 - 2)x_2) \\
&\geq (k-1)(\Delta_2 - 1) - x_1(\Delta_2 - 1) - x_2(\Delta_2 - 1) \\
&= (k - 1 - x)(\Delta_2 - 1) \quad \text{as } x = x_1 + x_2 \\
&> (n - \Delta_1 + \Delta_2 - 1)(\Delta_2 - 1) \quad \text{as } \Delta_2 \geq 2.
\end{aligned} \tag{3.11}$$

Claim 3.4. $(n - \Delta_1 + \Delta_2 - 1)(\Delta_2 - 1) > k - 1$.

Proof. By contradiction, we assume that $(n - \Delta_1 + \Delta_2 - 1)(\Delta_2 - 1) \leq k - 1$. From the above and using (3.8), we have

$$n - \Delta_1 + \Delta_2 - 1 \leq \frac{k-1}{\Delta_2 - 1} \leq t_2.$$

Since $n = \Delta_1 + 1 + t_2$, from the above, we get $\Delta_2 \leq 0$, a contradiction. Hence the proof is finished. $\square$

From Claim 3.4 with (3.11), we get $|E_{ST'}|/(k-1) > 1$. Suppose that all the vertices in S are adjacent to at most one vertex in T'. Then $k - 1 < |E_{ST'}| \leq k - 1$, a contradiction. Hence we conclude that there is at least one vertex in S (say, v_2) adjacent to at least two vertices (say, $v_i, v_j \in N(v_2)$, $i, j \neq 1$) of degrees $\Delta_2 - 1$ in T'. Thus vertex v_2 is adjacent to vertices v_1, v_i and v_j. Then the 4×4 leading principal submatrix L^* corresponding to vertices v_1, v_2, v_i, v_j (six possibilities up to permutation) is of the form

$$L^* = \begin{pmatrix} \Delta_1 & -1 & a & b \\ -1 & \Delta_2 & -1 & -1 \\ a & -1 & \Delta_2 - 1 & c \\ b & -1 & c & \Delta_2 - 1 \end{pmatrix}, \quad \text{where } a, b, c \in \{0, -1\}.$$

Let $f(x) = \det(xI - L^*)$ be the characteristic polynomial of L^*. Then

$$\begin{aligned}
f(\Delta_2 + 1) &= \det((\Delta_2 + 1)I - L^*) \\
&= \begin{vmatrix} \Delta_2 - \Delta_1 + 1 & 1 & -a & -b \\ 1 & 1 & 1 & 1 \\ -a & 1 & 2 & -c \\ -b & 1 & -c & 2 \end{vmatrix} = \begin{vmatrix} \Delta_2 - \Delta_1 & 1 & -a-1 & -b-1 \\ 0 & 1 & 0 & 0 \\ -a-1 & 1 & 1 & -c-1 \\ -b-1 & 1 & -c-1 & 1 \end{vmatrix}
\end{aligned}$$

$$= (\Delta_2 - \Delta_1)(1 - c_1^2) + 2a_1b_1c_1 - a_1^2 - b_1^2 \le 0,$$

where $(a_1, b_1, c_1) = (-a-1, -b-1, -c-1) \in \{0, -1\}^3$. Similarly,

$$\begin{aligned} f(\Delta_2 + 1/2) &= \det((\Delta_2 + 1/2)I - L^*) \\ &= \begin{vmatrix} \Delta_2 - \Delta_1 + 1/2 & 1 & -a & -b \\ 1 & 1/2 & 1 & 1 \\ -a & 1 & 3/2 & -c \\ -b & 1 & -c & 3/2 \end{vmatrix} \\ &= -a_2b_2c_2 + \frac{1}{4}(a_2^2 + b_2^2) + \frac{1}{16}(4c_2^2 - 1)(2\Delta_1 - 2\Delta_2 + 3) \ge 0, \end{aligned}$$

where $a_2 = a + 2$, $b_2 = b + 2$, $c_2 = c + 2$ and $a, b, c \in \{0, -1\}$.

One can easily see that $\mu_1(L^*) \ge \Delta_1 \ge 2\Delta_2 + 3$ and consequently $\mu_2(L^*) \ge \Delta_2 + 1/2$. By Lemma 2.2 with (3.7), we conclude that

$$\mu_2(G) \ge \mu_2(L^*) \ge \Delta_2 + \frac{1}{2} > \frac{2m}{n}.$$

This completes the proof of the lemma. □

We are now ready to give a lower bound on μ_2 of connected graph G and characterize the extremal graphs.

Theorem 3.5. *Let G be a connected graph of order $n > 2$ with m edges. If $G \cong K_{1,n-1}$, then $\mu_2(G) = 1$. Otherwise,*

$$\mu_2(G) \ge \frac{2m}{n} \tag{3.12}$$

with equality holding if and only if $G \cong K_{n/2,n/2}$ (n is even).

Proof. If $G \cong K_{1,n-1}$, then from the Laplacian spectrum of $K_{1,n-1}$, we have $\mu_2(G) = 1$. Otherwise, $G \ncong K_{1,n-1}$. Thus we have $\Delta_2 \ge 2$. If $\Delta_2 \ge 2m/n$, then by (1.2), we have

$$\mu_2(G) \ge \Delta_2 \ge \frac{2m}{n}$$

and (3.12) holds. Otherwise, $\Delta_2 < 2m/n$. By Lemma 3.1(iv), we conclude that there are at least $\Delta_2 + 1$ vertices of degree Δ_2. From Lemma 3.1(iii), we get $\Delta_1 \ge \Delta_2 + 1 + |T|$. Since $S \cup T \cup \{v_1\} = V(G)$, therefore there are at least $\Delta_2 + 1$ vertices in S, adjacent to v_1. Hence $|S_1| \ge \Delta_2 + 1 \ge 3$ and $|S_2| \ge 0$. If there is an edge in the subgraph induced by S in G, then by Lemma 3.2, we get the required result in (3.12). Otherwise, there is not any edge in the subgraph induced by S in G. By Lemma 3.3, again we get the required result in (3.12). The first part of the theorem is done.

Suppose that equality holds in (3.12). By Lemmas 3.2 and 3.3, we must have $\mu_2(G) = \Delta_2 = 2m/n$. By Lemma 2.7, we have $\Delta_1 = \Delta_2$ as $G \ncong K_{1,n-1}$. Thus we have $\Delta_1 = 2m/n$ and hence G is a regular graph. Again from $n\mu_2(G) = 2m$, we have

$$\mu_1(G) - 2\mu_2(G) = \sum_{i=3}^{n-1} (\mu_2(G) - \mu_i(G)) \geq 0,$$

i.e., $\mu_1(G) \geq 2\mu_2(G) = 4m/n$. On the other hand, by Lemma 2.5, we have

$$\mu_1(G) \leq \Delta_1 + \Delta_2 = 2\Delta_2 = \frac{4m}{n}.$$

From the above results, we conclude that

$$\mu_1(G) = \frac{4m}{n} \quad \text{and} \quad \mu_2(G) = \mu_3(G) = \cdots = \mu_{n-1}(G) = \frac{2m}{n}.$$

By Lemma 2.6, we get $G \cong K_{n/2,n/2}$ (n is even) as $G \ncong K_{1,n-1}$ and $\mu_1(G) \neq \mu_2(G)$.

Conversely, one can easily see that the equality holds in (3.12) for $K_{n/2,n/2}$ (n is even). $\square$

We now generalize our result in Theorem 3.5 as follows. For this let Γ_1 be the class of graphs H of order $n > 2$ such that $H \cong K_{1,n-1}$ or $H \cong K_2 \cup (n-2)K_1$ or $H \cong K_{1,n-r-1} \cup rK_1$ ($1 \leq r \leq \lceil n/2 \rceil - 2$). For $G \in \Gamma_1$, $\mu_2(G) = 0$ when $G \cong K_2 \cup (n-2)K_1$, and $\mu_2(G) = 1$ when $G \in \Gamma_1 \setminus \{K_2 \cup (n-2)K_1\}$. Otherwise, we have the following result:

Theorem 3.6. *Let $G \notin \Gamma_1$ be a graph of order $n > 2$ with m edges. Then*

$$\mu_2(G) \geq \frac{2m}{n} \tag{3.13}$$

with equality holding if and only if $G \cong nK_1$ or $G \cong K_{n/2,n/2}$ (n is even) or $G \cong K_{1,n/2} \cup (n/2-1)K_1$ (n is even).

Proof. Suppose that G is a connected graph. Since $G \notin \Gamma_1$, we have $G \ncong K_{1,n-1}$ and by Theorem 3.5, we get the required result in (3.13). Next suppose that G is a disconnected graph. For $G \cong nK_1$, (3.13) holds. Then there exists an edge in G. We can assume that G_i is the i-th connected component of order n_i with $m_i > 0$ edges in G for $1 \leq i \leq k$ such that $G \cong \bigcup_{i=1}^{k} G_i \cup sK_1$ ($s \geq 0$). First we assume that $k = 1$ and then $s > 0$. For $G_1 \cong K_{1,n-r-1}$, $\lceil n/2 \rceil - 1 \leq r \leq n-3$, then

$$\mu_2(G) = \mu_2(G_1) = 1 \geq \frac{2m}{n} \quad \text{as } 2 \leq m = n-r-1 \leq \lfloor n/2 \rfloor. \tag{3.14}$$

Otherwise, $G_1 \ncong K_{1,n-r-1}$ for $1 \leq r \leq n-2$ as $G \notin \Gamma_1$. By Theorem 3.5, we have

$$\mu_2(G) = \mu_2(G_1) \geq \frac{2m_1}{n_1} = \frac{2m}{n_1} > \frac{2m}{n} \quad \text{as } n > n_1.$$

Next we assume that $k \geq 2$. Without loss of generality we can assume that

$$\frac{2m_1}{n_1} \geq \frac{2m_2}{n_2} \geq \cdots \geq \frac{2m_k}{n_k}. \tag{3.15}$$

We now prove $2m/n \leq 2m_1/n_1$ by contradiction. For this, we suppose that $2m/n > 2m_1/n_1$. Then we have

$$\frac{2m}{n} > \frac{2m_1}{n_1} \geq \frac{2m_2}{n_2} \geq \cdots \geq \frac{2m_k}{n_k},$$

that is, $2mn_i > 2nm_i$, $i = 1, 2, \dots, k$, that is,

$$2m \sum_{i=1}^{k} n_i > 2n \sum_{i=1}^{k} m_i,$$

that is, $2m(n - s) > 2mn$, a contradiction.

If $G_1 \ncong K_{1,n_1-1}$ for some $n_1 \geq 2$, then by Theorem 3.5 we have

$$\mu_2(G) \geq \mu_2(G_1) \geq \frac{2m_1}{n_1} \geq \frac{2m}{n}. \tag{3.16}$$

Otherwise, $G_1 \cong K_{1,n_1-1}$ for some $n_1 \geq 2$ and we have $\mu_1(G_1) = n_1 \geq 2$. Since G_2 is a connected graph of order at least 2, we have $K_2 \subseteq G_2$ (K_2 is a subgraph of G_2) and therefore $\mu_1(G_2) \geq \mu_1(K_2) = 2$. From the above, we get

$$\mu_2(G) \geq 2 > \frac{2(n_1 - 1)}{n_1} = \frac{2m_1}{n_1} \geq \frac{2m}{n}.$$

The first part of the theorem is proved.

Suppose that equality holds in (3.13). Then all inequalities in the above argument must be equalities. For connected graph G, by Theorem 3.5, $G \cong K_{n/2,n/2}$ (n is even). For disconnected graph G, the equality holds in (3.14) and (3.16). From the equality in (3.14), we get

$$\mu_2(G) = \mu_2(G_1) = 1 = \frac{2m}{n}, \quad 2 \leq m = n - r - 1 \leq \left\lfloor \frac{n}{2} \right\rfloor,$$

that is, $m = n - r - 1 = n/2$. In this case $G \cong K_{1,n/2} \cup (n/2 - 1)K_1$ (n is even).

From the equality in (3.16), we get

$$\mu_2(G) = \mu_2(G_1) = \frac{2m_1}{n_1} = \frac{2m}{n}. \tag{3.17}$$

We now consider the following two cases:

Case 1*:* $2m_1/n_1 = 2m_k/n_k$. Then

$$\mu_2(G) = \mu_2(G_1) = \frac{2m_1}{n_1} = \frac{2m_2}{n_2} = \cdots = \frac{2m_k}{n_k} = \frac{2m}{n}.$$

From the second equality, by Theorem 3.5, we have $G_1 \cong K_{n_1/2,n_1/2}$. Since $\mu_1(G_1) = n_1 > 2m_1/n_1 = 2m/n = \mu_2(G)$, from the above, we must have

$$\mu_1(G_i) \leq \mu_2(G) = \frac{2m_i}{n_i}, \quad i = 2, 3, \ldots, k.$$

But we have

$$\mu_1(G_i) \geq \Delta(G_i) + 1 > \frac{2m_i}{n_i}, \quad i = 2, 3, \ldots, k,$$

which gives a contradiction.

Case 2: $2m_1/n_1 > 2m_k/n_k$. From (3.15), we have

$$2m_i \leq \frac{2m_1}{n_1} n_i, \quad i = 2, 3, \ldots, k-1.$$

Thus we have

$$2m = 2\sum_{i=1}^{k} m_i < \frac{2m_1}{n_1} \sum_{i=1}^{k} n_i = \frac{2m_1}{n_1}(n-s),$$

i.e., $2m/n \leq 2m/(n-s) < 2m_1/n_1$, a contradiction by (3.17).

Conversely, one can easily see that the equality holds in (3.13) for nK_1 or $K_{n/2,n/2}$ (n is even) or $K_{1,n/2} \cup (n/2-1)K_1$. □

We now give an upper bound on the third smallest Laplacian eigenvalue $\mu_{n-2}(G)$ in terms of m and n. For this let Γ_2 be the class of graphs H of order $n > 2$ such that $H \cong 2K_1 \vee K_{n-2}$ or $H \cong K_1 \cup K_{n-1}$ or $H \cong (K_1 \cup K_{n-r-1}) \vee K_r$ $(1 \leq r \leq \lceil n/2 \rceil - 2)$. One can easily see that $H \in \Gamma_2 \Leftrightarrow \overline{H} \in \Gamma_1$, which is equivalent to $H \notin \Gamma_2 \Leftrightarrow \overline{H} \notin \Gamma_1$. For $G \in \Gamma_2$, $\mu_{n-2}(G) = n$ when $G \cong 2K_1 \vee K_{n-2}$, and $\mu_{n-2}(G) = n-1$ when $G \in \Gamma_2 \setminus \{2K_1 \vee K_{n-2}\}$. Otherwise, we have the following result:

Theorem 3.7. *Let $G \notin \Gamma_2$ be a graph of order $n > 2$ with m edges. Then*

$$\mu_{n-2}(G) \leq \frac{2m}{n} + 1 \tag{3.18}$$

with equality holding if and only if $G \cong K_n$ or $G \cong 2K_{n/2}$ (n is even) or $G \cong (K_1 \cup K_{n/2}) \vee K_{n/2-1}$ (n is even).

Proof. Since $G \notin \Gamma_2$, we have $\overline{G} \notin \Gamma_1$. Let $\overline{m}$ be the number of edges in $\overline{G}$. Then, by Lemma 2.8 and Theorem 3.6, we have

$$\mu_2(\overline{G}) \geq \frac{2\overline{m}}{n}, \quad \text{or} \quad n - \mu_{n-2}(G) \geq \frac{n(n-1) - 2m}{n}, \quad \text{or} \quad \mu_{n-2}(G) \leq \frac{2m}{n} + 1.$$

By Theorem 3.6, the equality holds in (3.18) if and only if $\overline{G} \cong nK_1$ or $\overline{G} \cong K_{n/2,n/2}$ (n is even) or $\overline{G} \cong K_{1,n/2} \cup (n/2-1)K_1$ (n is even), that is, $G \cong K_n$ or $G \cong 2K_{n/2}$ (n is even) or $G \cong (K_1 \cup K_{n/2}) \vee K_{n/2-1}$ (n is even). □

4. Solution of Problem 1.1 and application to Laplacian energy

In this section, we provide the answer to Problem 1.1. Using this solution, we give an upper bound for Laplacian energy of graphs.

By the definition of $\sigma(G)$, we can rewrite Theorem 3.6 as follows:

Theorem 4.1. *Let $G \notin \Gamma_1$ be a graph of order $n > 2$. Then $\sigma(G) \geq 2$.*

If $G \in \Gamma_1$, then one can easily see that $\mu_2(G) < 2m/n$. This result with Theorem 4.1 leads to the following result which is a complete solution to Problem 1.1.

Theorem 4.2. *Let G be a graph. Then $\sigma = 1$ if and only if $G \in \Gamma_1$.*

Using the above result, we can improve an upper bound on Laplacian energy of graphs. The following upper bound on Laplacian energy of graphs is obtained in [6]:

Theorem 4.3. *Let G be a graph of order n with $m \geq n/2$ edges and maximum degree Δ_1. Then*

$$\mathrm{LE}(G) \leq 4m - 2\Delta_1 - \frac{4m}{n} + 2. \tag{4.1}$$

Now we improve this upper bound in the following:

Theorem 4.4. *Let $G \notin \Gamma_1$ be a graph of order n with $m \geq n/2$ edges and maximum degree Δ_1. Then*

$$\mathrm{LE}(G) \leq 4m - 2\Delta_1 - \frac{8m}{n} + 4. \tag{4.2}$$

Proof. By Theorem 4.1, we have $\sigma \geq 2$. From Lemma 2.1, one can easily see that

$$\sum_{i=1}^{\sigma} \lambda_i(L(G)) \leq \sum_{i=1}^{\sigma} \lambda_i(L(K_{1,\Delta_1})) + \sum_{i=1}^{\sigma} \lambda_i(L(G \setminus K_{1,\Delta_1})),$$

where Δ_1 is the maximum degree of G (For subgraph H of G, let $G \setminus H$ be a subgraph of G such that $V(G \setminus H) = V(G)$ and $E(G \setminus H) = E(G) \setminus E(H)$). Since

$$\sum_{i=1}^{\sigma} \lambda_i(L(K_{1,\Delta_1})) = \sum_{i=1}^{\sigma} \mu_i(K_{1,\Delta_1}) \leq \Delta_1 + \sigma$$

and

$$\sum_{i=1}^{\sigma} \lambda_i(L(G \setminus K_{1,\Delta_1})) = \sum_{i=1}^{\sigma} \mu_i(G \setminus K_{1,\Delta_1}) \leq 2(m - \Delta_1),$$

from the above, we get

$$S_\sigma(G) = \sum_{i=1}^{\sigma} \mu_i(G) \leq 2m - \Delta_1 + \sigma.$$

Using the above result in (1.1), we get

$$\mathrm{LE}(G) = 2S_\sigma(G) - \frac{4m\sigma}{n} \leq 4m - 2\Delta_1 - 2\sigma\left(\frac{2m}{n} - 1\right),$$

which gives the required result in (4.2) by $\sigma \geq 2$ and $m \geq n/2$. $\square$

Remark 4.5. For graph $G \notin \Gamma_1$ with $m \geq n/2$, the upper bound in (4.2) is always better than the upper bound in (4.1).

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