

Some remarks on Laplacian eigenvalues and Laplacian energy of graphs

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Abstract. Suppose $\mu_1, \mu_2, \dots, \mu_n$ are Laplacian eigenvalues of a graph G . The Laplacian energy of G is defined as $LE(G) = \sum_{i=1}^n |\mu_i - 2m/n|$. In this paper, some new bounds for the Laplacian eigenvalues and Laplacian energy of some special types of the subgraphs of K_n are presented.

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1. Introduction and preliminaries

Let G be a graph of order n with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $\mathcal{E}(G)$. The first Zagreb index $M_1(G)$ is defined as the sum of squares of degrees in G . It is well known that $M_1(G) = \sum_{e=uv \in \mathcal{E}(G)} [d(u) + d(v)]$. The adjacency matrix $A(G) = [a_{ij}]$ of G is a square matrix of order n whose (i, j) -entry is equal to the number of edges between the vertices v_i and v_j .

In the case that G is a simple graph, the adjacency matrix $A(G)$ will be a $(0,1)$ -matrix. The spectrum of G is defined as the set of eigenvalues of $A(G)$, together with their multiplicities. Let $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ be the eigenvalues of G . The energy of G is the sum of absolute values of eigenvalues of G . This quantity, introduced by Ivan Gutman, has noteworthy chemical applications; see [6 – 9, 11] for details.

Let $D(G) = [d_{ij}]$ be a diagonal matrix associated with the graph G , where $d_{ii} = \deg(v_i)$ and $d_{ij} = 0$ if $i \neq j$. Define $L(G) = D(G) - A(G)$. $L(G)$ is called the Laplacian matrix of G . The Laplacian polynomial of G is the characteristic polynomial of its Laplacian matrix, $\phi(G, \mu) = \det(\mu I_n - L(G))$. Let $\mu_1 \leq \mu_2 \leq \dots \leq \mu_n$ be the Laplacian eigenvalues of G , i. e., the roots of $\phi(G, \mu)$. It is well known that $\mu_1 = 0$ and that the multiplicity of 0 equals the number of connected components of G .

The Laplacian energy of G is a very recently defined graph invariant [10], defined as $LE(G) = \sum_{i=1}^n |\mu_i - 2m/n|$, where n and m are the number of vertices and edges of G , respectively. LE is a proper extension of the graph-energy concept. An interested reader should consult the papers [1, 2, 5, 16 – 18, 20 – 22] for the main properties of the Laplacian energy of graphs.

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The complement of a graph G is denoted by \bar{G} , where $e \in E(G)$ if and only if $e \notin E(\bar{G})$. Suppose G and H are two graphs with disjoint vertex and edge sets. The disjoint union of G and H is a graph T such that $V(T) = V(G) \cup V(H)$ and $E(T) = E(G) \cup E(H)$.

For the sake of completeness, we mention below some results which are important throughout the paper.

Theorem A [Polya-Szego Inequality, [15]]. *Suppose a_i and b_i , $1 \leq i \leq n$, are positive real numbers. Then*

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}} \right)^2 \left(\sum_{i=1}^n a_i b_i \right)^2,$$

where

$$M_1 = \max_{1 \leq i \leq n} a_i, M_2 = \max_{1 \leq i \leq n} b_i, m_1 = \min_{1 \leq i \leq n} a_i \text{ and } m_2 = \min_{1 \leq i \leq n} b_i.$$

Theorem B [Ozeki's Inequality, [14]]. *If a_i and b_i , $1 \leq i \leq n$, are nonnegative real numbers, then*

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 - \left(\sum_{i=1}^n a_i b_i \right)^2 \leq \frac{n^2}{4} (M_1 M_2 - m_1 m_2)^2,$$

where M_i and m_i are defined similarly to Theorem A.

Theorem C [Mohar, [13]]. *Let G be a graph and $e \in E(G)$. Then*

$$\mu_1(G - e) \leq \mu_1(G) \leq \mu_2(G - e) \leq \mu_2(G) \leq \dots \leq \mu_n(G - e) \leq \mu_n(G).$$

Theorem D [Biggs, [3]]. *Suppose λ_i and μ_i , $1 \leq i \leq n$, are eigenvalues and Laplacian eigenvalues of G , respectively. Then*

$$\sum \lambda_i = 0, \sum \lambda_i^2 = 2m, \sum \mu_i = 2m \text{ and } \sum \mu_i^2 = 2m + M_1(G).$$

Throughout this paper C_n , P_n and K_n denote the cycle, path and complete graphs on n vertices. The complete bipartite graph with a partition by m and n vertices is denoted by $K_{m,n}$. A graph G is called r -regular, if for any vertex x , $\text{deg}(x) = r$. Our other notations are standard and taken mainly from [3, 4, 12].

2. The Laplacian eigenvalues of some subgraphs of complete graphs

A matching or edge-independent set of a graph G is a set of edges without common vertices in G . In this section, the Laplacian eigenvalues and Laplacian energy of some subgraphs of K_n are investigated.

Lemma 1. *If G is a subgraph of K_n with $n' < n$ vertices, then the Laplacian eigenvalues of $K_n - \mathcal{E}(G)$ are as follows:*

$$0, n - \mu_1(G), \dots, n - \mu_{n'}(G), \underbrace{n, \dots, n}_{n-n'-1 \text{ times}}.$$

Proof. Suppose $G'_n = G \cup \{V(K_n) - V(G)\}$. Then $K_n - \mathcal{E}(G) = \bar{G}'_n$ and by [4, 2.6], $\phi(\bar{G}'_n, x) = (-1)^n \frac{x}{x-n} \phi(G'_n, n-x)$. We now apply [4, 2.4] to prove $\phi(G'_n, x) = \phi(G, x)x^{n-n'}$. Therefore,

$$\phi(\bar{G}'_n, x) = (-1)^n \frac{x}{x-n} \phi(G, n-x)(n-x)^{n-n'} = (-1)^n x \phi(G, n-x)(n-x)^{n-n'-1}$$

and a direct calculation implies the theorem. □

Corollary 1. *Suppose $E_i \subseteq \mathcal{E}(K_n)$ is a matching with i elements. Then the Laplacian eigenvalues of $K_n - E_i$ are as follows:*

$$0, \underbrace{n-2, \dots, n-2}_{i \text{ times}}, \underbrace{n, \dots, n}_{n-i-1 \text{ times}}.$$

Proof. The complement of $K_n - E_i$ consists of i copies of K_2 and $n - 2i$ copies of K_1 . Thus its spectrum is 0 ($n - i$ times) and 2 (i times). So the result follows from the Lemma 1 and [4, 2.6]. □

Corollary 2. *If G_{2s} is a Cocktail-Party graph with $2s$ vertices, then the Laplacian eigenvalues of G_{2s} are $0, \underbrace{2s-2, \dots, 2s-2}_{s \text{ times}}, \underbrace{2s, \dots, 2s}_{s-1 \text{ times}}$.*

Corollary 3. $LE(K_n - E_i) = 2(n - i - 1) - (4i/n)(i + 1)$.

Lemma 2. *The Laplacian eigenvalues of $K_{n,n} - e$ are computed as follows:*

$$0, \frac{3n-2-\sqrt{n^2+4n-4}}{2}, \underbrace{n, \dots, n}_{n-3 \text{ times}}, \frac{3n-2+\sqrt{n^2+4n-4}}{2}.$$

Therefore, $LE(K_{n,n} - e) = n + 2 - 4/n + \sqrt{n^2 + 4n - 4}$.

Proof. We know that

$$0, \underbrace{n, n, \dots, n}_{n-2 \text{ times}}, 2n$$

are the Laplacian eigenvalues of $K_{n,n}$ [3]. By Theorem C, the Laplacian eigenvalues of $K_{n,n} - e$ satisfy the following inequalities:

$$0 = \mu_1 \leq \mu_2 \leq \mu_3 = n = \dots = \mu_{2n-1} \leq \mu_{2n}.$$

Since

$$\sum \mu_i = 2m, \sum \mu_i^2 = 2m + M_1(G), \mu_2 + \mu_{2n} = 3n - 2 \text{ and } \mu_2^2 + \mu_{2n}^2 = 5n^2 - 4n, \mu_2 \mu_{2n} = 2(n - 1)^2.$$

This concludes that

$$\mu_2 = \frac{3n-2-\sqrt{n^2+4n-4}}{2} \text{ and } \mu_{2n} = \frac{3n-2+\sqrt{n^2+4n-4}}{2}.$$

For the second part, we notice that $LE(K_{n,n} - e) = \sum_{i=1}^{2n} |\mu_i - n + 1/n| = n + 2 - 4/n + \sqrt{n^2 + 4n - 4}$, proving the result. □

Theorem 1. *Suppose G is a graph. Then $|LE(G - e) - LE(G)| < 4$ and 4 is the best possible bound.*

Proof. Define $\mu'_i = \mu_i(G - e)$. By Theorem C, $\mu_i - \mu'_i \geq 0$ and $\sum_{i=1}^n [\mu_i - \mu'_i] = 2$. So, there exists i , $1 \leq i \leq n$, such that $\mu_i > \mu'_i$. This implies that

$$\sum_{i=1}^n \left| \mu_i - \mu'_i - \frac{2}{n} \right| < \sum_{i=1}^n \left[|\mu_i - \mu'_i| + \frac{2}{n} \right]$$

and we have:

$$\begin{aligned} |LE(G - e) - LE(G)| &= \left| \sum_{i=1}^n \left| \mu_i - 2\frac{m}{n} \right| - \left| \mu'_i - 2\frac{m-1}{n} \right| \right| \\ &= \left| \sum_{i=1}^n \left[\left| \mu_i - 2\frac{m}{n} \right| - \left| \mu'_i - 2\frac{m-1}{n} \right| \right] \right| \\ &\leq \sum_{i=1}^n \left| \left| \mu_i - 2\frac{m}{n} \right| - \left| \mu'_i - 2\frac{m-1}{n} \right| \right| \\ &\leq \sum_{i=1}^n \left| \mu_i - \mu'_i - \frac{2}{n} \right| \\ &< \sum_{i=1}^n \left[|\mu_i - \mu'_i| + \frac{2}{n} \right] \\ &= \sum_{i=1}^n \left[\mu_i - \mu'_i + \frac{2}{n} \right] = 4. \end{aligned}$$

To complete the argument we construct a sequence $\{G_n\}_{n \geq 2}$ of graphs such that $|LE(G_n - e) - LE(G_n)| \rightarrow 4$. Define $G_n = \bar{K}_n + e$. Then $LE(G_n) = 4 - \frac{4}{n}$ and $LE(G_n - e) = 0$ and so $|LE(G_n - e) - LE(G_n)| = 4 - \frac{4}{n} \rightarrow 4$. This completes the argument. \square

3. Bounds on the Laplacian eigenvalues and the Laplacian energy of graphs

In this section, a variety of upper and lower bounds for the Laplacian eigenvalues of a graph G and its Laplacian energy are presented. At first, we apply Ozeki's theorem to obtain a simple inequality on the energy of graphs. By Theorem B,

$$E(G) \geq \sqrt{2mn - \frac{n^2}{4}(a_n - a_1)^2},$$

where a_1 and a_n are minimum and maximum values of the set $\{|\lambda_i| \mid 1 \leq i \leq n\}$.

Theorem 2. *Suppose zero is not an eigenvalue of G . Then*

$$E(G) \geq \frac{2\sqrt{2mn}\sqrt{a_1a_n}}{a_1 + a_n},$$

where a_1 and a_n are minimum and maximum of the absolute value of λ_i s. In particular, if G is k -regular, then

$$LE(G) = E(G) \geq \frac{2nk\sqrt{2a_1}}{a_1 + k}.$$

Proof. Suppose $\lambda_i, 1 \leq i \leq n$, are the eigenvalues of G . We also assume that $a_i = |\lambda_i|$, where $a_1 \leq a_2 \leq \dots \leq a_n$ and $b_i = 1, 1 \leq i \leq n$. Apply Theorem A to show that

$$\sum_{i=1}^n |\lambda_i|^2 \sum_{i=1}^n 1^2 \leq \frac{1}{4} \left(\sqrt{\frac{|\lambda_n|}{|\lambda_1|}} + \sqrt{\frac{|\lambda_1|}{|\lambda_n|}} \right)^2 \left(\sum_{i=1}^n |\lambda_i| \right)^2.$$

Therefore, by $\sum_{i=1}^n |\lambda_i|^2 = 2m$ and a simple calculation,

$$E(G) \geq \frac{2\sqrt{2mn}\sqrt{a_1a_n}}{a_1 + a_n}.$$

To prove the second part, it is enough to notice that $a_n = k$ and $2m = nk$ for k -regular graphs. □

Theorem 3. Let G be a connected graph with the smallest and largest positive Laplacian eigenvalues μ_2 and μ_n , respectively. Then

$$\sqrt{\mu_n/\mu_2} + \sqrt{\mu_2/\mu_n} \geq (\sqrt{n-1}/m)\sqrt{2m + M_1(G)}.$$

In particular, if G is an n -vertex tree, then $\sqrt{\mu_n/\mu_2} + \sqrt{\mu_2/\mu_n} \geq \sqrt{(6n-8)/(n-1)}$.

Proof. Suppose $a_i = 1$ and $b_i = \mu_i, 2 \leq i \leq n$. Apply Theorem B to show that,

$$\sum_{i=2}^n 1^2 \sum_{i=2}^n \mu_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{\mu_n}{\mu_2}} + \sqrt{\frac{\mu_2}{\mu_n}} \right)^2 \left(\sum_{i=2}^n \mu_i \right)^2.$$

Since

$$\sum_{i=2}^n \mu_i^2 = 2m + M_1(G), \quad \sqrt{\mu_n/\mu_2} + \sqrt{\mu_2/\mu_n} \geq (\sqrt{n-1}/m)\sqrt{2m + M_1(G)}.$$

When G is a tree with at least three vertices, $d(u)+d(v) \geq 3$ and so $M_1(G) \geq 3(n-1)$, as desired. □

Corollary 4. With notation of Theorem 3, $\mu_n/\mu_2 + \mu_2/\mu_n \geq \frac{n-1}{m}(2 + \frac{4m}{n}) - 2$. In particular, when G is an n -vertex tree, $\mu_n/\mu_2 + \mu_2/\mu_n \geq 4 - \frac{4}{n}$.

Theorem 4. Suppose G is a graph without isolated vertices. Then

$$\mu_n - \mu_2 \geq \frac{4}{(n-1)^2} [(n-1)(2m + M_1(G)) - 4m^2].$$

Proof. Suppose $a_i = 1$ and $b_i = \mu_i$, $2 \leq i \leq n$. Apply Theorem B to show that

$$(n-1) \sum_{i=2}^n \mu_i^2 - \left(\sum_{i=2}^n \mu_i \right)^2 \leq \frac{(n-1)^2}{4} (\mu_n - \mu_2)^2.$$

Since

$$\sum_{i=2}^n \mu_i^2 = 2m + M_1(G), \quad \mu_n - \mu_2 \geq \frac{4}{(n-1)^2} [(n-1)(2m + M_1(G)) - 4m^2],$$

which proves the theorem. \square

We now prove some new bounds for the energy and Laplacian energy of graphs.

Theorem 5. *Suppose G is a graph. Then*

$$\begin{aligned} & {}^{2(n-1)}\sqrt{4m^2} \left[LE(G) - \frac{2m}{n} \right] \\ & \geq \sqrt{{}^{n-1}\sqrt{4m^2} \left[M_1 + 2m - (n+1) \frac{4m^2}{n^2} \right] + 2 \binom{n-1}{2} {}^{n-1}\sqrt{n^2 \phi(G, \frac{2m}{n})^2}}, \end{aligned} \quad (1)$$

with equality if and only if G is an empty graph. In particular, if G is a non-empty graph, then

$$LE(G) > \frac{2m}{n} + \sqrt{2m - \frac{4m^2}{n^2} + 2 \binom{n-1}{2} {}^{n-1}\sqrt{\frac{n^2}{4m^2} \phi(G, \frac{2m}{n})^2}}. \quad (2)$$

Moreover, if T is an n -vertex tree, $n \geq 3$, then

$$\begin{aligned} LE(T) & > \frac{2(n-1)}{n} \\ & + \sqrt{M_1(T) + (n-1) \left(6 - \frac{4}{n^2} \right) + \frac{(n-1)(n-2)}{n} {}^{n-1}\sqrt{\frac{n}{4(n-1)^2}}}. \end{aligned} \quad (3)$$

Proof. By a well-known theorem of algebraic graph theory, $\mu_1 = 0$ and so,

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

If $x = \sum_{i=2}^n |\mu_i - \frac{2m}{n}|$, then by the arithmetic-geometric mean inequality,

$$\begin{aligned}
 x^2 &= \sum_{i=2}^n |\mu_i - \frac{2m}{n}|^2 + 2 \sum_{i \neq j, i, j=2,3,\dots,n} |\mu_i - \frac{2m}{n}| |\mu_j - \frac{2m}{n}| \\
 &= M_1 + 2m - \frac{4m^2}{n} - \frac{4m^2}{n^2} + 2 \sum_{i \neq j, i, j=2,3,\dots,n} |\mu_i - \frac{2m}{n}| |\mu_j - \frac{2m}{n}| \\
 &\geq M_1 + 2m - \frac{4m^2}{n} - \frac{4m^2}{n^2} + 2 \binom{n-1}{2} (\prod_{i=2}^n |\mu_i - \frac{2m}{n}|^{2(n-2)})^{1/(n-1)(n-2)} \\
 &= M_1 + 2m - \frac{4m^2}{n} - \frac{4m^2}{n^2} + 2 \binom{n-1}{2} (\prod_{i=2}^n (\mu_i - \frac{2m}{n}))^{2/(n-1)} \\
 &= M_1 + 2m - (n+1) \frac{4m^2}{n^2} + 2 \binom{n-1}{2} \sqrt[n-1]{\frac{n^2}{4m^2} \phi(G, \frac{2m}{n})^2}. \tag{5}
 \end{aligned}$$

Equation (1) is a direct consequence of (4) and (5) with equality if and only if $|\mu_i - 2m/n| |\mu_j - 2m/n| = |\mu_r - 2m/n| |\mu_s - 2m/n|, 2 \leq i, j \leq n, 2 \leq r, s \leq n$. We claim that these equalities hold if and only if $\mu_2 = \mu_3 = \dots = \mu_n = 2m/n$. To prove this, we assume that one of μ_i is equal to $2m/n$.

Then by a simple calculation, $\mu_2 = \mu_3 = \dots = \mu_n = 2m/n$. Otherwise, $\mu_i \neq 2m/n, 2 \leq i \leq n$. If $\mu_i, \mu_j \geq 2m/n$ or $\mu_i, \mu_j \leq 2m/n$, then $\mu_i = \mu_j$. Otherwise, $\mu_i + \mu_j = 4m/n$. Thus Laplacian eigenvalues of G are

$$0, \underbrace{\mu_1, \dots, \mu_1}_{k_1 \text{ times}}, \underbrace{\mu_2, \dots, \mu_2}_{k_2 \text{ times}},$$

where $k_1 + k_2 = n - 1$ and $\mu_1 + \mu_2 = 4m/n$. Since $\sum_{i=1}^n \mu_i = 2m, k_1 \mu_1 + k_2 \mu_2 = 2m$. Thus

$$\mu_1 = \frac{2m}{n} \left(\frac{2k_1 - n + 2}{2k_1 - n + 1} \right) = \frac{2m}{n} \left(\frac{k_1 - k_2 + 3}{k_1 - k_2 + 2} \right).$$

Since $(k_1 - k_2 + 3)/(k_1 - k_2 + 2) > 1, \mu_1 > 2m/n$, a contradiction. Thus, in Equation (1) equality holds if and only if $\mu_2 = \mu_3 = \dots = \mu_n = 2m/n$ if and only if G is an empty graph.

It is a well-known fact that $M_1 \geq \frac{4m^2}{n}$. Equation (2) is now derived from Equation (1) by this inequality.

To prove (3), suppose $\phi(G, \frac{2m}{n}) = 0$. Thus $2m/n$ is a Laplacian eigenvalue and so it is an algebraic integer. So, by a well-known result in algebraic number theory $\frac{2m}{n}$ is an integer. But for tree $\frac{2m}{n} = \frac{2(n-1)}{n}$, a contradiction. Thus $\phi(G, \frac{2m}{n}) \neq 0$. Suppose $\phi(G, x) = x^n + b_{n-1}x^{n-1} + \dots + b_1x$. Then

$$\phi(G, \frac{2m}{n}) = (\frac{2m}{n})^n + b_{n-1}(\frac{2m}{n})^{n-1} + \dots + b_1 \frac{2m}{n} \neq 0.$$

This implies that $n^n |\phi(G, \frac{2m}{n})|$ is an integer and so $|\phi(G, \frac{2m}{n})| \geq \frac{1}{n^n}$. This completes the third part of the theorem. \square

Suppose G is an n -vertex tree. Since $\sqrt[n]{n} \rightarrow 1$ and for any positive constant c , $\sqrt[n]{c} \rightarrow 1$, one can see that for large n ,

$$LE(G) \geq \frac{2(n-1)}{n} + \sqrt{\frac{(n-1)(n^2+4)}{n^2} + \frac{(n-1)(n-2)}{2n}}.$$

Corollary 5. *If $\frac{2m}{n} \notin Z$, then*

$$LE(G) \geq \frac{2m}{n} + \sqrt{M_1 + 2m - (n+1)\frac{4m^2}{n^2} + \frac{(n-1)(n-2)}{n} \sqrt[n-1]{\frac{n}{4m^2}}}.$$

In particular, for large n , the Laplacian energy of G is greater than or equal to

$$\frac{2m}{n} + \sqrt{2m - \frac{4m^2}{n^2} + \frac{(n-1)(n-2)}{2n}}.$$

Proof. Apply part (2) of Theorem 5 and this fact that $|\phi(G, \frac{2m}{n})| \geq \frac{1}{n^n}$. \square

Corollary 6. *If G is tree, then*

$$LE(G) \geq \frac{2(n-1)}{n} + \sqrt{M_1 + \frac{2(n-1)(2-n^2)}{n^2} + \frac{(n-1)(n-2)}{n} \sqrt[n-1]{\frac{n}{4(n-1)^2}}}.$$

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