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Some remarks on Laplacian eigenvalues and Laplacian energy of graphs

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Abstract. Suppose $\mu_1, \mu_2, \ldots, \mu_n$ 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 $V(G) = \{v_1, v_2, \cdots, v_n\}$ 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 $M_1(G) = \sum_{e=uv \in E(G)}[d(u) + d(v)]$. 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 $\lambda_1 \leq \lambda_2 \cdots \leq \lambda_n$ 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 $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$ 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 $V(T) = V(G) \bigcup V(H)$ and $E(T) = E(G) \bigcap E(H)$.

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*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \leq \frac{1}{4}(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}})^2(\sum_{i=1}^{n} a_ib_i)^2,$$

where

$M_1 = \max_{1\leq i\leq n} a_i$, $M_2 = \max_{1\leq i\leq n} b_i$, $m_1 = \min_{1\leq i\leq n} a_i$ *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*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - (\sum_{i=1}^{n} a_ib_i)^2 \leq \frac{n^2}{4}(M_1M_2 - m_1m_2)^2,$$

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*

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

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, $deg(x) = r$. 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:*

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

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:*

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

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 $0, \underbrace{2s-2, \cdots, 2s-2}_{s \text{ times}}, \underbrace{2s, \cdots, 2s}_{s-1 \text{ times}}$.*

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:*

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

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

Proof. We know that

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

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

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

Since
$\sum \mu_i = 2m$, $\sum \mu_i^2 = 2m + M_1(G)$, $\mu_2 + \mu_{2n} = 3n - 2$ 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:

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

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

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 $\lambda_i^{,}s$. In particular, if G is $k-$regular, then

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

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

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

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

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

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,

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

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

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

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. □

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

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

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

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

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

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

$$LE(T) > \frac{2(n-1)}{n} + \sqrt{M_1(T) + (n-1)(6 - \frac{4}{n^2}) + \frac{(n-1)(n-2)}{n}\sqrt[n-1]{\frac{n}{4(n-1)^2}}}. \quad (3)$$

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

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

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

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

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 $\mu_2 = \mu_3 = \cdots = \mu_n = 2m/n$. To prove this, we assume that one of μ_i is equal to $2m/n$.

Then by a simple calculation, $\mu_2 = \mu_3 = \cdots = \mu_n = 2m/n$. 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

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

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

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

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 $\mu_2 = \mu_3 = \cdots = \mu_n = 2m/n$ 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 $\phi(G, x) = x^n + b_{n-1}x^{n-1} + \cdots + b_1x$. Then

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

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. □

Suppose G is an $n-$vertex tree. Since $\sqrt[n]{n} \longrightarrow 1$ and for any positive constant c, $\sqrt[n]{c} \longrightarrow 1$, 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 $|\phi(G, \frac{2m}{n})| \geq \frac{1}{n^n}$. □

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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