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A NOTE ON LAPLACIAN ENERGY OF GRAPHS

Bo Zhou [a], Ivan Gutman [b], Tatjana Aleksić [b]

[a] *Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China*
e-mail: zhoubo@scnu.edu.cn

[b] *Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
e-mail: gutman@kg.ac.yu , taleksic@kg.ac.yu

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Abstract

Let G be a simple graph with n vertices and m edges. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of the adjacency matrix $\mathbf{A}$ of G and $\mu_1, \mu_2, \ldots, \mu_n$ denote the eigenvalues of the Laplacian matrix $\mathbf{L}$ of G. Let $\gamma_i = \mu_i - 2m/n$. The energy $E(G)$, defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$, is a much studied quantity with well known applications in chemistry. In this paper we investigate the properties of the Laplacian energy $LE(G) = \sum_{i=1}^{n} |\gamma_i|$ and its connections to $E(G)$. We establish some new analogies between the properties of $E(G)$ and $LE(G)$.

INTRODUCTION

Let G be a simple graph possessing n vertices and m edges. The ordinary spectrum of G, consisting of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ (arranged in non-increasing order), is the spectrum of the adjacency matrix $\mathbf{A}$ of G [1]. The energy of G is a quantity defined about 30 years ago as [2]

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

Likewise, the Laplacian spectrum of G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$ (arranged in non-increasing order), is the spectrum of the Laplacian matrix $\mathbf{L}$ of G [3]. The Laplacian energy of G is a newer concept, defined as [4]

$$LE(G) = \sum_{i=1}^{n} |\gamma_i|$$

where

$$\gamma_i = \mu_i - \frac{2m}{n} \ , \ i = 1, 2, \ldots, n$$

and where $2m/n$ is the average vertex degree of G. Since $\mu_n = 0$, we have $\gamma_n = -2m/n$.

The energy $E(G)$ of a graph G has a clear connection to chemical problems [2, 5, 6] and there are numerous known results in the theory of the graph energy [7–13]. There is a great deal of analogy between the properties of $E(G)$ and $LE(G)$, but also significant differences [4, 14, 15]. More properties on LE are reported here.

RESULTS

The ordinary graph eigenvalues of G satisfy the following conditions:

$$\sum_{i=1}^{n} \lambda_i = 0 \,, \qquad \sum_{i=1}^{n} \lambda_i^2 = 2m \qquad \text{and} \qquad \prod_{i=1}^{n} \lambda_i = \det \mathbf{A} \ .$$

Analogously, for the Laplacian eigenvalues of G we have

$$\sum_{i=1}^{n} \gamma_i = 0 \,, \qquad \sum_{i=1}^{n} \gamma_i^2 = 2M \qquad \text{and} \qquad \prod_{i=1}^{n} \gamma_i = \det \left(\mathbf{L} - \frac{2m}{n} \mathbf{I} \right)$$

where

$$M = m + \frac{1}{2} \sum_{i=1}^{n} \left(\delta_i - \frac{2m}{n} \right)^2$$

with δ_i denoting the degree of the i-th vertex of G.

In [14] the following inequalities for $LE(G)$ were obtained:

$$\sqrt{2M + n(n-1)D^{\frac{2}{n}}} \leq LE(G) \leq \sqrt{2M(n-1) + nD^{\frac{2}{n}}} \tag{1}$$

where

$$D = \left| \det \left(\mathbf{L} - \frac{2m}{n} \mathbf{I} \right) \right| \ .$$

Analogous inequalities for graph energy were reported much earlier [16].

Lemma 1. *Let $a_1, a_2, \ldots, a_n$ be non-negative numbers. Then*

$$\begin{aligned} n \left[\frac{1}{n} \sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i \right)^{1/n} \right] \ &\leq \ n \sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n} \sqrt{a_i} \right)^2 \\ &\leq \ n(n-1) \left[\frac{1}{n} \sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i \right)^{1/n} \right] \ . \end{aligned}$$

If $a_1, a_2, \ldots, a_n$ are all positive numbers, then Lemma 1 is just Kober's inequality [17]. Otherwise, it is equivalent to

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

The left inequality follows directly from the Cauchy–Schwartz inequality, while the right inequality is obvious.

Theorem 2. *Let G be a graph with $n \geq 2$ vertices and m edges. Then*

$$\frac{2m}{n} + \sqrt{2M - \left(\frac{2m}{n} \right)^2 + (n-1)(n-2) \left(\frac{nD}{2m} \right)^{\frac{2}{n-1}}} \quad \leq LE(G) \leq$$

$$\frac{2m}{n} + \sqrt{(n-2) \left[2M - \left(\frac{2m}{n} \right)^2 \right] + (n-1) \left(\frac{nD}{2m} \right)^{\frac{2}{n-1}}} \ . \tag{2}$$

Proof. Note that

$$\sum_{i=1}^{n-1} |\gamma_i| = LE(G) - \frac{2m}{n} \qquad \text{and} \qquad \sum_{i=1}^{n-1} \gamma_i^2 = 2M - \left(\frac{2m}{n} \right)^2 \ .$$

Using Lemma 1 it can be easily checked that (2) is true if $D = 0$.

Now we assume that $D \neq 0$. By setting $a_i = \gamma_i^2$, $i = 1, 2, \ldots, n-1$, in Lemma 1, we have

$$F \leq (n-1) \sum_{i=1}^{n-1} \gamma_i^2 - \left(\sum_{i=1}^{n-1} |\gamma_i| \right)^2 \leq (n-2)F$$

which can further be written as

$$F \le (n-1)\left(2M-\gamma_n^2\right) - \left[LE(G)-|\gamma_n|\right]^2 \le (n-2)F$$

i. e.,

$$(n-1)\left(2M-\gamma_n^2\right) - (n-2)F \le \left[LE(G)-|\gamma_n|\right]^2 \le (n-1)\left(2M-\gamma_n^2\right) - F$$

where

$$\begin{aligned} F &= (n-1)\left[\frac{1}{n-1}\sum_{i=1}^{n-1}\gamma_i^2 - \left(\prod_{i=1}^{n-1}\gamma_i^2\right)^{\frac{1}{n-1}}\right] = (n-1)\left[\frac{2M-\gamma_n^2}{n-1} - \left(\frac{D}{|\gamma_n|}\right)^{\frac{2}{n-1}}\right] \\ &= 2M-\gamma_n^2-(n-1)\left(\frac{D}{|\gamma_n|}\right)^{\frac{2}{n-1}} . \end{aligned}$$

Note that $\gamma_n = -2m/n$. Then (2) follows easily. ■

Using the relation between the arithmetic and geometric means,

$$\left(\frac{D}{|\gamma_n|}\right)^2 \le \left(\frac{2M-\gamma_n^2}{n-1}\right)^{n-1}$$

and bearing in mind the upper bound in (2), we arrive at

$$LE(G) \le \frac{2m}{n} + \sqrt{(n-1)\left[2M-\left(\frac{2m}{n}\right)^2\right]} \tag{3}$$

which is same as inequality (10) in [4].

If we know μ_1 and denote

$$2M - \left(\mu_1 - \frac{2m}{n}\right)^2 - \left(\frac{2m}{n}\right)^2 \qquad \text{and} \qquad \left(\frac{n^2\,D}{2m(n\mu_1-2m)}\right)^{\frac{2}{n-2}}$$

by a and b, respectively, then by similar arguments, for $n \ge 3$, we obtain

$$\mu_1 + \sqrt{a+(n-2)(n-3)b} \le LE(G) \le \mu_1 + \sqrt{(n-3)a+(n-2)b} . \tag{4}$$

In an analogous manner as before, the upper bound in (4) implies:

$$LE(G) \le \mu_1 + \sqrt{(n-2)\left[2M-\left(\mu_1-\frac{2m}{n}\right)^2-\left(\frac{2m}{n}\right)^2\right]} . \tag{5}$$

Let K_n be the complete graph on n vertices and $\overline{K_n}$ its edgeless complement. Let K_{n_1,n_2} be the complete bipartite graph on $n_1 + n_2$ vertices.

Theorem 3. *Let G be a graph with $n \geq 2$ vertices. Then $LE(G) + E(G) \geq 2\mu_1$, with equality if and only if $G \cong \overline{K}_n$ or $G \cong K_{n/2,n/2}$.*

Proof. Let m be the number of edges of G. Recall that $\lambda_1 \geq 2m/n$ with equality if and only G is a regular graph. Further, if G is a regular graph with exactly two nonzero eigenvalues, then $G \cong K_{n/2,n/2}$. In view of this we have

$$\begin{aligned} LE(G) + E(G) &= \mu_1 + \sum_{i=2}^{n-1} |\gamma_i| + \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \geq \mu_1 + \left| \sum_{i=2}^{n-1} \gamma_i \right| + \lambda_1 + \left| \sum_{i=2}^{n} \lambda_i \right| \\ &= \mu_1 + \left| \mu_1 - \frac{4m}{n} \right| + 2\lambda_1 \geq 2(\mu_1 + \lambda_1) - \frac{4m}{n} \geq 2\mu_1 \ . \end{aligned}$$

Suppose that $LE(G) + E(G) = 2\mu_1$. Then $\lambda_1 = 2m/n$ and so G is a regular graph. Thus $E(G) = \mu_1 = 2m/n - \lambda_n$, implying that either $G \cong \overline{K}_n$ or $G \cong K_{n/2,n/2}$. Conversely, it is easy to see that $LE(G) + E(G) = 2\mu_1$ if $G \cong \overline{K}_n$ or $G \cong K_{n/2,n/2}$.
■

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