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ON LAPLACIAN ENERGY OF GRAPHS

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Abstract

Let G be a graph with n vertices and m edges. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the Laplacian eigenvalues of G. The *Laplacian energy* of G has recently been defined [*Lin. Algebra Appl.* **414** (2006) 29–37] as $LE(G) = \sum_{i=1}^{n} |\mu_i - 2m/n|$. We establish a few new properties of $LE(G)$.

INTRODUCTION

The energy $E(G)$ of a graph G is equal to the sum of the absolute values of the eigenvalues of the adjacency matrix of G. This quantity, introduced almost 30 years ago [1] and having a clear connection to chemical problems [2,3], has in newer times attracted much attention of mathematicians and mathematical chemists [4–15]. We have recently proposed [16] an energy–like quantity $LE(G)$, based on the eigenvalues of the Laplacian matrix of G. The Laplacian energy $LE(G)$ and the ordinary energy $E(G)$ were found [16] to have a number of analogous properties, but also some noteworthy differences between them have been recognized [16]. In this paper we report further properties of LE.

Let G be a simple graph possessing n vertices and m edges. The ordinary spectrum of G, consisting of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, is the spectrum of the adjacency matrix $\mathbf{A}$ of G [17]. Then

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

The Laplacian spectrum of G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$, is the spectrum of the Laplacian matrix $\mathbf{L}$ of G [18–23]. Then

$$LE = LE(G) = \sum_{i=1}^{n} |\gamma_i| \tag{2}$$

where

$$\gamma_i = \mu_i - \frac{2m}{n} \ . \tag{3}$$

The ordinary graph eigenvalues satisfy the conditions

$$\sum_{i=1}^{n} \lambda_i = 0 \qquad \text{and} \qquad \sum_{i=1}^{n} (\lambda_i)^2 = 2m \ . \tag{4}$$

The analogous relations for the Laplacian eigenvalues read

$$\sum_{i=1}^{n} \gamma_i = 0 \qquad \text{and} \qquad \sum_{i=1}^{n} (\gamma_i)^2 = 2M \tag{5}$$

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. It is immediately seen that $M \geq m$ for all graphs G, and that $M = m$ holds if and only if G is a regular graph.

The idea behind the definition (2) of the Laplacian energy is the following. In the theory of graph energy, Eq. (1), there are numerous known results (especially lower and upper bounds) that are obtained by using the relations (4) and that depend on the parameters n and m. Then one could expect analogous results for LE, obtained by means of the relations (5), that would depend on the parameters n and M. Indeed, a number of such results could be deduced [16]; in the subsequent section we point out a few more.

FURTHER (n, M, m)-TYPE BOUNDS FOR THE LAPLACIAN ENERGY

1

If the graph G has p components ($p \geq 1$), and if the Laplacian eigenvalues are labelled so that $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$, then

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

This immediately implies, $\gamma_{n-i} = -2m/n$ for $i = 0, \ldots, p-1$, and thus

$$LE(G) \geq p\,\frac{2m}{n} \ .$$

This upper bound can be improved. If the graph G possesses at least one edge, then [20,21]

$$\mu_1 \geq \frac{2m}{n} + 1$$

and therefore $\gamma_1 \geq 1$, resulting in

$$LE(G) \geq p\,\frac{2m}{n} + 1 \ .$$

2

In [16] we proved (in Theorem 3) that

$$LE(G) \leq \frac{2m}{n}\,p + \sqrt{(n-p)\left[2M - p\left(\frac{2m}{n}\right)^2\right]} \ . \tag{6}$$

We now show that the right–hand side expression in (6) is a decreasing function of the parameter p .

Let $a = 2m/n$ and consider the function

$$f(x) := ax + \sqrt{(n-x)(2M - a^2\,x)} \quad , \quad 0 \leq x \leq n \ .$$

Then

$$f'(x) = a - \frac{2M + a^2\,n - 2a^2\,x}{2\sqrt{(n-x)(2M - a^2\,x)}} \ .$$

It is easy to see that $2M + a^2 n - 2a^2 x \geq 0$ since $x \leq n$. Therefore $f'(x) \leq 0$ if and only if

$$2a\sqrt{(n-x)(2M-a^2 x)} \leq 2M + a^2 n - 2a^2 x$$

i. e.,

$$4a^2 (n-x)(2M-a^2 x) \leq (2M + a^2 n - 2a^2 x)^2$$

which is transformed into the obvious inequality

$$4Ma^2 n \leq 4M^2 + a^4 n^2 \ .$$

Because the upper bound (6) increases with decreasing p, by setting $p = 1$ we obtain the estimate

$$LE(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]} \tag{7}$$

which holds for all (n,m)-graphs.

3

In [16] we proved (in Theorem 2) that

$$LE \leq \sqrt{2Mn} \ . \tag{8}$$

We now show that the bound (7) is better than (8).

Indeed,

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

holds if and only if

$$(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right] \leq \left(\sqrt{2Mn} - \frac{2m}{n}\right)^2$$

which is directly transformed into

$$2m\sqrt{2Mn} \leq 2m^2 + Mn$$

i. e.,

$$\sqrt{(2m^2)(Mn)} \leq \frac{1}{2}\left[(2m^2) + (Mn)\right]$$

which is just the relation between the geometric and arithmetic means.

Another way to arrive at the same conclusion is based on the result of the previous point **2**. There we showed that the right–hand side of (6) is a decreasing function of the parameter p for $0 \leq p \leq n$. Setting $p = 0$ in (6) we obtain (8). Thus, the estimate (7), pertaining to $p = 1$, is better than the estimate (8), pertaining to $p = 0$.

4

Proposition 1. Let G be an (n,m)-graph with $n \geq 3$. Then

$$LE(G) \leq \sqrt{\frac{2M - (2m/n)^2}{n-1}} + \frac{2m}{n} + \sqrt{(n-2) + \left[2M - \frac{2M-(2m/n)^2}{n-1} - \left(\frac{2m}{n}\right)^2\right]} \, .$$

Proof. By the Cauchy–Schwartz inequality, bearing in mind that $\gamma_n = -2m/n$,

$$\sum_{i=2}^{n-1} |\gamma_i| \leq \sqrt{(n-2)\sum_{i=2}^{n-1} \gamma_i^2} = \sqrt{(n-2)\left[2M - (\gamma_1)^2 - \left(\frac{2m}{n}\right)^2\right]} \, .$$

Hence, recalling that $\gamma_1 \geq 0$,

$$LE(G) \leq \gamma_1 + \frac{2m}{n} + \sqrt{(n-2)\left[2M - (\gamma_1)^2 - \left(\frac{2m}{n}\right)^2\right]} \, .$$

The function

$$f(x) = x + \frac{2m}{n} + \sqrt{(n-2)\left[2M - x^2 - \left(\frac{2m}{n}\right)^2\right]}$$

decreases if and only if

$$x \geq \sqrt{[2M - (2m/n)^2]/(n-1)} \, .$$

Therefore

$$LE(G) \leq f\left(\sqrt{[2M - (2m/n)^2]/(n-1)}\right) \, .$$

The result follows. $\Box$

5

In [16] we proved (in Theorem 4) that

$$LE(G) \geq 2\sqrt{M} \tag{9}$$

with equality if and only if $G \cong K_{n/2,n/2}$. Because $M \geq m$, we have

$$LE(G) \geq 2\sqrt{m}\,. \tag{10}$$

Equality $M = m$ holds only for regular graphs, whereas the only (regular) graph for which equality in (9) holds is $K_{n/2,n/2}$. Therefore, also the equality in (10) holds if and only if $G \cong K_{n/2,n/2}$.

THE CASE $LE = 4m/n$

Proposition 2. Let G be an (n,m)-graph with $m > 0$. Then

$$LE(G) = \frac{4m}{n} \tag{11}$$

if and only if G is a complete multipartite graph $K_{n_1,n_2,\ldots,n_k}$ where $n_i = n/k$ for all i and $1 < k \leq n$.

Proof. First note that the complete graph K_n satisfies condition (11). Namely, the Laplacian eigenvalues of K_n are n [$(n-1)$-times] and 0. Consequently, $LE(K_n) = 2(n-1)$ which, in view of $m = n(n-1)/2$, is equal to the right–hand side of (11).

If $G \cong K_n$, then $\mu_{n-1} = n > n-1 = 2m/n$. If $G \ncong K_n$ then $\mu_{n-1} \leq \delta$, where δ denotes the minimum vertex degree of G [24]. Therefore $\mu_{n-1} \leq 2m/n$, since $2m/n$ is the average vertex degree. If $\mu_{n-1} = 2m/n$, then G must be regular. Then, however, $\lambda_2 = 2m/n - \mu_{n-1} = 0$, which means that the graph G has exactly one positive ordinary eigenvalue. This, in turn, implies (cf. Theorem 6.7, p. 163 in [17]) that G is a complete multipartite graph $K_{n_1,n_2,\ldots,n_k}$ where $n_i = n/k$ for all i and $1 < k \leq n$. (Recall that if $k = n$, then $K_{n_1,n_2,\ldots,n_k}$ is just the complete graph K_n.)

Thus $\mu_{n-1} \geq 2m/n$ if and only if $G \cong K_{n_1,n_2,\ldots,n_k}$ with $n_i = n/k$ for all i and $1 < k \leq n$.

Now,

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

holds if and only if

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

i. e., if and only if $\mu_{n-1} \geq 2m/n$. $\square$

Remark. The equality (11) holds also for the graphs without edges.

MORE ANALOGIES BETWEEN E AND LE

There are known bounds for graph energy (for instance, [25–27]), obtained by using the conditions (4) and

$$\prod_{i=1}^{n} \lambda_i = \det \mathbf{A} \ .$$

For chemical applications it is often of great importance that the determinant of the adjacency matrix is related to the Kekulé structures [28–30], and in some cases (e. g. for benzenoid hydrocarbons) is equal to the square of the Kekulé structure count.

Analogous results for Laplacian graph energy can be obtained by combining the conditions (5) with

$$\prod_{i=1}^{n} \gamma_i = D$$

where D is a pertinent graph invariant. It is easy to show that, in view of (3),

$$D = \det \left(\mathbf{L} - \frac{2m}{n} \mathbf{I} \right) \ . \tag{12}$$

Proposition 3. For any (n,m)-graph G, whose invariant D is given by Eq. (12),

$$2M - n\,|D|^{2/n} \leq 2nM - LE(G)^2 \leq (n-1) \left[2M - n\,|D|^{2/n} \right] \ .$$

Proof is analogous to what earlier was reported for $E(G)$ [26].

Proposition 4. Let the graph G be same as in Proposition 3, except that D is required to be non-zero. Consider the system of equations

$$\alpha^2 + (n-1)\,\beta^2 = 2M$$

$$\alpha\,\beta^{n-1} = |D| \ .$$

Let α_1, β_1 be the solution of this system, such that $\alpha_1 \geq \beta_1 > 0$. Let α_2, β_2 be another solution of the system, such that $\beta_2 \geq \alpha_2 > 0$. Let $LE_{min} = \alpha_1 + (n-1)\,\beta_1$ and $LE_{max} = \alpha_2 + (n-1)\,\beta_2$. Then

$$LE_{min} \leq LE(G) \leq LE_{max} \ . \tag{13}$$

Proof is analogous to what earlier was reported for $E(G)$ [27]. According to Theorem 2 of [16], equality on both sides of (13) is attained if and only if G consists of p copies of complete graphs of order k and and $(k-2)p$ isolated vertices, $p \geq 1$, $k \geq 2$.

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