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RELATION BETWEEN ENERGY AND LAPLACIAN ENERGY

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Abstract

For a graph G with n vertices and m edges, with ordinary spectrum λ_i, $i = 1, 2, \ldots, n$, and with Laplacian spectrum μ_i, $i = 1, 2, \ldots, n$, the energy and the Laplacian energy are defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ and $LE(G) = \sum_{i=1}^{n} |\mu_i - 2m/n|$, respectively. It is known that $E(G) = LE(G)$ if G is regular. We now show that there are non-regular graphs with the same property. We provide numerous examples for the inequality $E(G) \leq LE(G)$ and conjecture that it holds for all graphs.

INTRODUCTION

The concept of the *energy of a graph* was introduced long time ago by one of the present authors [1], motivated by (much older) chemical applications [2–5]. The basic mathematical properties of graph energy are outlined in the review [6]. Research on graph energy is nowadays very active, as seen from the recent papers [7–19] and the references quoted therein.

The energy $E(G)$ of a graph G is defined as follows.

Let G be a graph on n vertices, and let its ordinary spectrum (i. e., the spectrum of its adjacency matrix) consist of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then

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

Details on the spectral theory of graphs can be found in the seminal book [20].

In addition to the ordinary graph spectrum [20], in the mathematical literature the spectra of several other graph matrices were studied. Of these, the spectrum of the Laplacian matrix attracted the greatest attention [21–27] and the Laplacian spectral graph theory is nowadays also well developed.

In order to formulate an energy–like quantity, based on Laplacian eigenvalues, the concept of *Laplacian energy of a graph* was recently put forward [28]. It is denoted by LE and is defined as follows.

Let G be a graph with n vertices and m edges, and let its Laplacian spectrum (i. e., the spectrum of its Laplacian matrix) consist of the numbers $\mu_1, \mu_2, \ldots, \mu_n$. Then

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

The form of Eq. (2) has been chosen bearing in mind the fact that whereas the sum of the ordinary graph eigenvalues is equal to zero, all Laplacian eigenvalues are non-negative, and therefore their sum is non-zero. On the other hand, $\sum_{i=1}^{n} (\mu_i - 2m/n) = 0$. As a consequence, E and LE have numerous analogous properties [28,29].

As an easy result it has been pointed out [28] that the equality

$$LE(G) = E(G) \tag{3}$$

holds whenever the graph G is regular. Curiously, however, Eq.(3) seems to be the only hitherto established relation between the energy and Laplacian energy. The present paper is aimed at contributing towards the filling of this gap, and towards a better understanding of the relations between these two graph–spectrum–based quantities.

NON-REGULAR GRAPHS SATISFYING EQ. (3)

Let $G_1 \cup G_2$ denote the graph consisting of two (disconnected) components G_1 and G_2. For the graph energy the equality

$$E(G_1 \cup G_2) = E(G_1) + E(G_2) \tag{4}$$

is always satisfied. In [28] it has been pointed out that the analogous equality

$$LE(G_1 \cup G_2) = LE(G_1) + LE(G_2) \tag{5}$$

does not hold in the general case. It is easy to verify [28] that the relation (5) holds if G_1 and G_2 have equal average vertex degrees, i. e., if $2m(G_1)/n(G_1) = 2m(G_2)/n(G_2)$.

We now provide an example showing that the above statement is not of "if and only if" type. Namely, there exist graphs G_1 and G_2, such that $2m(G_1)/n(G_1) \neq 2m(G_2)/n(G_2)$, but for which Eq. (5) holds.

As usual, by C_n and K_n are denoted the n-vertex cycle and the n-vertex complete graph, respectively. Let $G_1 \cong C_6$ and $G_2 \cong K_2$. The Laplacian spectra of these graphs are well known [21–27]: $\{4,3,3,1,1,0\}$ and $\{2,0\}$, respectively. Therefore, by Eq. (2), $LE(G_1) = 8$ and $LE(G_2) = 2$.

Consider now the graph $G = C_6 \cup K_2$. Its Laplacian spectrum is the union of the Laplacian spectra of C_6 and K_2, viz., $\{4,3,3,2,1,1,0,0\}$. The graph G has 8 vertices and 7 edges, and thus its average vertex degree is $2m/n = 14/8$. By direct calculation we now obtain

$$\begin{aligned} LE(G) &= \left|4-\frac{14}{8}\right| + 2\cdot\left|3-\frac{14}{8}\right| + \left|2-\frac{14}{8}\right| + 2\cdot\left|1-\frac{14}{8}\right| + 2\cdot\left|0-\frac{14}{8}\right| \\ &= \left(4-\frac{14}{8}\right) + 2\cdot\left(3-\frac{14}{8}\right) + \left(2-\frac{14}{8}\right) + 2\cdot\left(\frac{14}{8}-1\right) + 2\cdot\frac{14}{8} \\ &= 10 \end{aligned}$$

that is,

$$LE(C_6 \cup K_2) = LE(C_6) + LE(K_2)$$

although $2m(G_1)/n(G_1) = 2$ and $2m(G_2)/n(G_2) = 1$.

In a fully analogous manner one can verify that for any two positive integers p and q,

$$LE(p\,C_6 \cup q\,K_2) = p\,LE(C_6) + q\,LE(K_2) \tag{6}$$

where $p\,C_6 \cup q\,K_2$ is the (non-regular) graph consisting of p copies of C_6 and q copies of K_2.

Now, both C_6 and K_2 are regular graphs (of degree two and one, respectively). Therefore, by Eq. (3), $LE(C_6) = E(C_6)$ and $LE(K_2) = E(K_2)$, which substituted back into (6) and by taking into account (4) yields

$$LE(p\,C_6 \cup q\,K_2) = E(p\,C_6 \cup q\,K_2) \ .$$

Thus, relation (3) holds also for some non-regular graphs.

It would be interesting to characterize either all non-regular graphs that satisfy Eq. (3), or to determine necessary and sufficient conditions that a graph must obey in order that Eq. (3) be valid.

ENERGY AND LAPLACIAN ENERGY OF COMPLETE BIPARTITE GRAPHS

As usual, by $K_{a,b}$ we denote the complete bipartite graph on $a+b$ vertices. In what follows, we assume that $a \leq b$. The spectrum and Laplacian spectrum of $K_{a,b}$ are well known: $\{\sqrt{ab}, -\sqrt{ab},\ 0\ \ (n-2 \text{ times})\}$ and $\{0, a+b,\ a\ \ (b-1 \text{ times}),\ b\ \ (a-1 \text{ times})\}$. From these data, and the fact that $K_{a,b}$ has ab edges, it straightforwardly follows:

$$E(K_{a,b}) = 2\sqrt{ab} \qquad ; \qquad LE(K_{a,b}) = 2a + 2ab\,\frac{b-a}{a+b} \ . \tag{7}$$

From $(\sqrt{a} - \sqrt{b})^2 \geq 0$ we get $a + b - 2\sqrt{ab} \geq 0$. Then in view of (7),

$$E(K_{a,b}) \leq a + b \tag{8}$$

with equality if and only if $a = b$.

From $ab \geq a$ and $ab \geq b$ follows $2ab - a - b \geq 0$ and therefore

$$\frac{(b-a)(2ab-a-b)}{a+b} \geq 0 \ . \tag{9}$$

Because

$$(b-a)(2ab-a-b) = 2a(a+b) + 2ab(b-a) - (a+b)^2$$

from the inequality (9) we get

$$2a + 2ab\,\frac{b-a}{b+a} - (a+b) \geq 0$$

which in view of (7) yields

$$LE(K_{a,b}) \geq a+b \ . \tag{10}$$

From the above considerations it is evident that equality in (10) occurs if and only if $a = b$.

Comparing (8) and (10) we see that $E(K_{a,b}) \leq LE(K_{a,b})$, with equality if and only if $a = b$.

A more detailed analysis reveals that for $a + b = n$ having a fixed value, $E(K_{a,b})$ is a monotonically increasing function of the parameter a , $a = 1, 2, \ldots, \lfloor n/2 \rfloor$. In contrast to this, $LE(K_{a,b})$ monotonically increases for $a = 1, 2, \ldots, a_0$ and then decreases for $a = a_0 + 1, a_0 + 2, \ldots, \lfloor n/2 \rfloor$, where a_0 is either $\lfloor (3 - \sqrt{3\,n^2 - 6})/6 \rfloor$ or $\lceil (3 - \sqrt{3\,n^2 - 6})/6 \rceil$, depending on the actual value of n.

Anyway, the complete bipartite graphs $K_{a,b}$ provide an example for the inequality

$$E(G) \leq LE(G) \ . \tag{11}$$

SEARCH FOR A VIOLATION OF INEQUALITY (11)

After recognizing the simple result outlined in the preceding section, we intended to find a graph G whose energy would exceed the Laplacian energy, i. e., a graph that would violate inequality (11). Initially we expected that this will be an easy task. However, the quest continued without any result. In this section we describe a few classes of graphs for which we could establish that inequality (11) is satisfied.

1

We first examined the graph $K_a \cup K_b$ on $a+b$ vertices, $a \leq b$, which is just the complement of the earlier considered complete bipartite graph $K_{a,b}$. Its spectrum is $\{a-1, b-1, \ -1 \ \ (a+b-2 \text{ times})\}$ whereas its Laplacian spectrum is $\{a \ \ (a-1 \text{ times}), \ b \ \ (b-1 \text{ times}), 0, 0\}$. Therefore

$$E(K_a \cup K_b) = 2(a+b) - 4 \tag{12}$$

and

$$LE(K_a \cup K_b) = 2d + (a-1) \cdot |a-d| + (b-1) \cdot |b-d|$$

where d is the average vertex degree, equal to $[a(a-1)+b(b-1)]/(a+b)$.

Because $a \leq b$, it is always $b-d \geq 0$ and therefore $|b-d| = b-d$. With regard to $|a-d|$ two cases need to be distinguished.

Case 1: $a-d \geq 0$. Then by a lengthy calculation we obtain

$$LE(K_a \cup K_b) = 4\,\frac{a^2+b^2}{a+b} - 4$$

which combined with (12) gives

$$LE(K_a \cup K_b) - E(K_a \cup K_b) = 2\,\frac{(a-b)^2}{a+b}$$

and therefore relation (11) is obeyed.

Case 2: $a-d \leq 0$. Then,

$$LE(K_a \cup K_b) = 2(a+b) - 2 + (b-a-2)\,\frac{2ab}{a+b}$$

and

$$LE(K_a \cup K_b) - E(K_a \cup K_b) = (b-a-2)\,\frac{2ab}{a+b} + 2\,. \tag{13}$$

The condition $a-d \leq 0$ is tantamount to $a \leq b(b-1)/(b+1)$. This, in turn, means that it must be $b \geq a-2$ i. e., $b-a-2 \geq 0$. Then, evidently, the right–hand side of (13) is positive–valued.

Therefore, relation (11) is satisfied also in Case 2, i. e., it is satisfied for all graphs of the form $K_a \cup K_b$.

2

In the paper [30], the energies of certain graphs with large number of edges were studied. In particular, in [30] were examined the graphs $Kb_n(k)$ obtained by deleting k independent edges from the complete graph K_n, and $Kc_n(k)$ obtained by deleting the $k(k-1)/2$ edges of a complete graph K_k from the complete graph K_n. It was shown that [30]

$$E(Kb_n(k)) = n - 3 + \sqrt{(n+1)^2 - 8k} \quad , \quad 0 \leq k \leq \lfloor n/2 \rfloor$$

and that

$$E(Kb_n(k)) \leq 2n - 2 \quad , \quad 0 \leq k \leq \lfloor n/2 \rfloor \ . \tag{14}$$

Also [30],

$$E(Kc_n(k)) = n - k - 1 + \sqrt{(n-k-1)^2 + 4k(n-k)} \quad , \quad 0 \leq k \leq n$$

and

$$E(Kc_n(k)) < 2n - 2 \quad , \quad 2 \leq k \leq n \ .$$

The analogous expressions for the Laplacian energy read:

$$LE(Kb_n(k)) = 2n - 2 + 2k - \frac{4k(k+1)}{n}$$

and

$$LE(Kc_n(k)) = 2n + 2\,k^2 - 4k - \frac{2\,k^2(k-1)}{n} \ .$$

If $0 \leq k \leq \lfloor (n-2)/2 \rfloor$, then $2k - 4k(k+1)/n \geq 0$, and therefore $LE(Kb_n(k)) \geq 2n - 2$. In view of (14) we then have $E(Kb_n(k)) \leq LE(Kb_n(k))$.

Direct computation shows that $E(Kb_n(k)) < LE(Kb_n(k))$ holds also in the case when $k > \lfloor (n-2)/2 \rfloor$.

We have also that $E(Kc_n(k)) \leq LE(Kc_n(k))$, for all k , $k = 2, \ldots, n$. (For $n \geq 6$ and $k = 3, \ldots, n-2$, it suffices to verify that $2\,k^2 - 4k - 2\,k^2(k-1)/n \geq 0$ is true.) The verification that (11) holds for $Kc_n(k)$ also for $n < 6$ was accomplished by computer–aided numerical calculations.

3

The extremal Hakimi graphs H_n on n vertices are the graphs with the least number of edges among the graphs G for which $a(G) = k(G) = \lambda(G)$, where $a(G)$, $k(G)$, and $\lambda(G)$ respectively denote the algebraic connectivity, the vertex connectivity, and the edge connectivity of G. They were characterized by Lima *et al.* in [31]. If n is even, then H_n is obtained by deleting $n/2$ independent edges from the complete graph K_n. If n is odd, then H_n is obtained from K_n by deleting two incident edges and additional $(n-3)/2$ independent edges.

If n is even, then H_n is a regular graph (of degree $n-2$), also known under the name "cocktail–party graph". Therefore, by Eq. (3), $E(H_n) = LE(H_n)$ and condition (11) is obeyed. Note also that if n is even, then $H_n \cong Kb_n(k)$ for $k = n/2$.

If n is odd, then the ordinary spectrum of H_n consists of the numbers 0 $((n-3)/2$ times), -2 $((n-5)/2$ times), -1, and the three solutions of the equation

$$x^3 - (n-4)\,x^2 - 2(n-2)\,x + (n-3) = 0 \ .$$

The Laplacian spectrum is calculated by observing that the complement of H_n consists of a copy of $K_{1,2}$ (whose Laplacian spectrum is $\{3,1,0\}$) and $(n-3)/2$ copies of K_2 (whose Laplacian spectrum is $\{2,0\}$).

If $\mu_1, \mu_2, \ldots, \mu_{n-1}, 0$ are the Laplacian eigenvalues of a graph, then the Laplacian eigenvalues of its complement are [21–27] $n-\mu_1, n-\mu_2, \ldots, n-\mu_{n-1}, 0$.

Therefore the Laplacian spectrum of H_n is

$$\left\{ n-3\,,\, n-1\,,\, n-2\ \left(\frac{n-3}{2}\ \text{times}\right)\,,\, n\ \left(\frac{n-3}{2}\ \text{times}\right)\,,\, 0 \right\}$$

and the respective Laplacian energy is directly calculated as:

$$LE(H_n) = 2n - 2 - \frac{4}{n} \ .$$

By numerical calculation it is now easily to check that for all odd values of n, $n \geq 5$, $E(H_n) < LE(H_n)$. For the first few values of n we have:

n	$E(H_n)$	$LE(H_n)$	$LE(H_n) - E(H_n)$
5	6.3548	7.2000	0.845200
7	10.4916	11.4286	0.936971
9	14.5662	15.5556	0.989356
11	18.6135	19.6364	1.022864
13	22.6462	23.6923	1.046108
15	26.6702	27.7333	1.063133
17	30.6886	31.7647	1.076076
19	34.7032	35.7895	1.086284
21	38.7150	39.8095	1.094534
23	42.7248	43.8261	1.101327
25	46.7330	47.8400	1.107030

4

Suppose we have two graphs G_1 and G_2 with $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$; the *coalescence of* G_1 *and* G_2 *with respect to* v_1 *and* v_2 is the graph formed by identifying v_1 and v_2 and is denoted by $G_1 \bullet G_2$. In other words, $V(G_1 \bullet G_2) = V(G_1) \cup V(G_2) \cup \{v^*\} - \{v_1, v_2\}$, and two vertices in $G_1 \bullet G_2$ are adjacent if they are adjacent in G_1 or G_2, or if one is v^* and the other is adjacent to v_1 or v_2 in G_1 or G_2. The characteristic polynomial of $G_1 \bullet G_2$ is given by [20]:

$$\phi(G_1 \bullet G_2) = \phi(G_1)\,\phi(G_2 - v_2) + \phi(G_1 - v_1)\,\phi(G_2) - \lambda\,\phi(G_1 - v_1)\,\phi(G_2 - v_2)\;. \quad (15)$$

The eigenvalues of $K_n \bullet K_n$ are easily obtained from Eq. (15). The spectrum of $K_n \bullet K_n$ is

$$\left\{ n-2\,,\ \frac{n-2-\sqrt{n^2+4n-4}}{2}\,,\ \frac{n-2+\sqrt{n^2+4n-4}}{2}\,,\ -1\ \ (2n-4 \text{ times}) \right\}$$

Thus, $E(K_n \bullet K_n) = 3n - 6 + \sqrt{n^2+4n-4}\,$.

The Laplacian spectrum is calculated by observing that the complement of $K_n \bullet K_n$ consists of a copy of $K_{n-1,n-1}$ (whose Laplacian spectrum is $\{0, 2n-2,\ n-1\ \ (2n-4 \text{ times})\}$ and one isolated vertex.

Therefore the Laplacian spectrum of $K_n \bullet K_n$ is

$$\{1\,,\ 2n-1\,,\ n\ \ (2n-4 \text{ times})\ ,\ 0\}$$

and the respective Laplacian energy is directly calculated as:

$$LE(K_n \bullet K_n) = (3n-6) + (n+2) - \frac{2}{2n-1}\;.$$

For any $n > 1$, one can easily verify that

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

Thus, (11) holds also for $G \cong K_n \bullet K_n$.

5

The validity of inequality (11) was verified also for all trees with 10 and fewer vertices, and for a set of over 100 hexagonal systems (from the book [32]).

* * *

Bearing in mind all the above outlined results, we deem that it is justified to formulate the following:

Conjecture. *The energy of any graph is smaller than or equal to its Laplacian energy.*

Disproving this conjecture would be simple: a single counterexample would suffice. Proving the conjecture (in case it happens to be correct) may be a much more difficult task. Both remain a problem to be resolved in the future.

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