The Laplacian–energy Like Invariant is an Energy Like Invariant

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Abstract

Short time ago Liu and Liu [MATCH Commun. Math. Comput. Chem. 59 (2008) 355–372] put forward a so-called Laplacian–energy like invariant (LEL), defined as the sum of the square roots of the Laplacian eigenvalues. From its name, one could get the impression that the properties of LEL are similar to those of the Laplacian energy \(LE\). However, already the inventors of LEL realized that LEL resembles much more the ordinary graph energy \(E\) than \(LE\). We now provide further arguments supporting this conclusion. In particular, numerous earlier obtained bounds and approximations for \(E\) can be simply “translated” into bounds and approximations for LEL.

1. INTRODUCTION

In this paper we are concerned with some spectrum–based invariants of (molecular) graphs. Let \(G\) be a graph. Its number of vertices and edges will be denoted by \(n\) and \(m\), respectively.

Let \(A(G)\) be the adjacency matrix of \(G\), and let \(\lambda_1, \lambda_2, \ldots, \lambda_n\) be its eigenvalues. These eigenvalues form the (ordinary) spectrum of the graph \(G\) \([1]\). Let \(L(G)\) be the
Laplacian matrix of $G$, and let $\mu_1, \mu_2, \ldots, \mu_n$ be its eigenvalues. These eigenvalues form the Laplacian spectrum of the graph $G$ [2–4].

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

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

This graph invariant, whose origins are in the molecular orbital theory of conjugated $\pi$-electron systems [5–9], has recently attracted much attention of mathematical chemists. For details on the mathematical aspects of the theory of graph energy see the reviews [10, 11] and the references cited therein.

In an attempt to provide a Laplacian–spectral analogue of the graph energy, two of the present authors proposed the so-called Laplacian energy, defined as [12, 13]

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

It could be shown that $LE$ and $E$ have a number of analogous properties [12–17], but there also were some drastic disagreements. In particular, if $G_1 \cup G_2$ is the graph composed of two connected components $G_1$ and $G_2$, then

$$E(G_1 \cup G_2) = E(G_1) + E(G_2)$$

whereas, in the general case it is not true that

$$LE(G_1 \cup G_2) = LE(G_1) + LE(G_2) .$$

If, in addition, $G_1$ is connected and has $n$ vertices and $m$ edges, whereas $G_2$ has $p$ vertices and no edges, then

$$E(G_1 \cup G_2) = E(G_1)$$

whereas for sufficiently large values of $p$,

$$LE(G_1 \cup G_2) = 4m \frac{p+1}{p+n} \quad \text{and} \quad \lim_{p \to \infty} LE(G_1 \cup G_2) = 4m .$$

Thus, in this case, the Laplacian energy of $G_1 \cup G_2$ depends only on the numbers of vertices and edges, and is independent of any other structural detail of $G_1$.

The Laplacian energy is currently much investigated [12–28]. It is worth mentioning that $LE$ found remarkable chemical applications, beyond the molecular orbital theory of conjugated molecules [29].
J. Liu and B. Liu [30] proposed recently another Laplacian–spectrum based “energy”, and called it \textit{Laplacian–energy like invariant, LEL}. It is defined as

\[ LEL(G) := \sum_{i=1}^{n} \sqrt{\mu_i}. \]  

At this point one should recall that all Laplacian eigenvalues of any graph are non-negative real numbers [2, 3]. One Laplacian eigenvalue is necessarily equal to zero; let this be \( \mu_n \). In view of this, we may write Eq. (7) as

\[ LEL(G) := \sum_{i=1}^{n-1} \sqrt{\mu_i}. \]  

After the publication of the paper [30], a number of properties of \( LEL \) have been established [31–33]. Especially intriguing is the recently discovered [34] equality between \( LEL \) and the, seemingly unrelated, incidence energy [35], which holds in the case of bipartite graphs.

\section{2. LEL IS NOT LAPLACIAN–ENERGY LIKE}

Liu and Liu [30] named \( LEL \) “Laplacian–energy like”, which gives the impression that it was expected to be similar to \( LE \). Yet, already in the paper [30] it was recognized that there are fundamental disagreements between \( LEL \) and \( LE \), and that \( LEL \) is more an “energy like” invariant. In particular, in contrast to Eq. (4) which in the general case is violated, the relation

\[ LEL(G_1 \cup G_2) = LEL(G_1) + LEL(G_2) \]  

is always satisfied. In contrast to Eq. (6), in the case of edgeless \( G_2 \) we have

\[ LEL(G_1 \cup G_2) = LEL(G_1). \]  

Not only that the properties of \( LEL \) and \( LE \) disagree in the above specified manner, but the form of Eqs. (9) and (10) precisely agrees with the form of Eqs. (3) and (5). Already this indicates that \( LEL \) is not “Laplacian–energy like”, but “energy like”. More arguments in favor of this claim are given in the subsequent section.
3. \textit{LEL IS ENERGY LIKE}

Starting with the seminal work of McClelland [36], the basic results (bounds and approximations) for graph energy could be deduced by relying to a limited number of simple properties of the graph eigenvalues (for details see [7, 8], the recent works [37, 38], and the references cited therein).

Let \( G \) be a (molecular) graph with \( n \) vertices and \( m \) edges. Let \( N \) and \( M \) be two positive integers. Consider an auxiliary quantity \( Q \), defined as

\[
Q = Q(G) = \sum_{i=1}^{N} q_i
\]

where \( q_i \), \( i = 1, 2, \ldots, N \), are some numbers which somehow can be computed from the graph \( G \), for which we only need to know that they satisfy the conditions

\[
q_i \geq 0 \quad \text{for all } i = 1, 2, \ldots, N
\]

and

\[
\sum_{i=1}^{N} (q_i)^2 = 2M
\]

or, the conditions (11), (12), and

\[
P = P(G) = \prod_{i=1}^{N} q_i
\]

From (11) & (12) it is possible to deduce an upper bound for \( Q \), whereas from (11)–(13) both lower and upper bounds for \( Q \), see below.

What now needs to be observed is that if we choose \( N = n \), \( M = m \), and \( q_i = |\lambda_i| \) for \( i = 1, 2, \ldots, n \), then the auxiliary quantity \( Q \) is the graph energy, cf. Eq. (1). In this case the quantity \( P \) in Eq. (13) is just the determinant of the adjacency matrix (taken with positive sign). In the case of molecular graphs of benzenoid hydrocarbons, \( P \) is equal to the square of the number of Kekulé structures [39]. In the case of molecular graphs of alternant non-benzenoid hydrocarbons, \( P \) is equal to the square of the so-called algebraic structure count [39]. In the case of acyclic systems, \( P = 1 \) for Kekuléan and \( P = 0 \) for non-Kekuléan species.

Now, all the three conditions (11)–(13) are obeyed also for the choice \( N = n - 1 \), \( M = m \), and \( q_i = \sqrt{\mu_i} \) for \( i = 1, 2, \ldots, n - 1 \), in which case \( Q = LEL(G) \), cf. Eq.
The only difference is that for the latter choice, \( P = \sqrt{n\Theta} \), where \( \Theta \) is the number of spanning trees of the underlying graph \( G \) [2, 3]. In particular, if \( G \) is not connected, then \( \Theta = 0 \). If \( G \) is a tree, then \( \Theta = 1 \). If \( G \) is connected and unicyclic, with cycle size \( c \), then \( \Theta = c \). If \( G \) is a molecular graph of a benzenoid system, then \( \Theta = \phi(G, 6) \), where \( \phi(G, x) \) is the characteristic polynomial of \( G \) [40, 41]. For such molecular graphs, \( P(G) = \sqrt{n\phi(G, 6)} \).

Bearing the above in mind, we may simply “translate” various known results for the graph energy into analogous results for \( LEL \). We point out only a few such results.

1° Using the conditions (11) and (12), assuming \( N = n \), \( M = m \), and \( q_i = |\lambda_i| \), one gets [36, 42]

\[
E(G) \leq \sqrt{2mn} .
\]

The \( LEL \)-counterpart of this formula is, of course,

\[
LEL(G) \leq \sqrt{2m(n-1)}
\]

a known result [30].

2° If all the three conditions (11)–(13) are taken into account, then [43]

\[
\sqrt{2MN - (N-1)D} \leq Q \leq \sqrt{2MN - D}
\]

where

\[
D = 2M - N \frac{P^{2/N}}{N}
\]

For the graph energy (namely, by setting into (14) and (15) \( N = n \), \( M = m \), and \( P = |\det A| \)), this yields [43]

\[
\sqrt{2m + n(n-1) |\det A|^{2/n}} \leq E \leq \sqrt{2m(n-1) + n |\det A|^{2/n}} .
\]

The \( LEL \)-counterpart of the above estimates is obtained by by setting into (14) and (15) \( N = n-1 \), \( M = m \), and \( P = \sqrt{n\Theta} \), resulting in:

\[
\sqrt{2m + (n-1)(n-2)(n\Theta)^{1/(n-1)}} \leq LEL \leq \sqrt{2m(n-2) + (n-1)(n\Theta)^{1/(n-1)}}.
\]
In particular, for disconnected graphs the bounds (16) reduce to:

\[ \sqrt{2m} \leq LEL \leq \sqrt{2m(n - 2)} \]

whereas for trees to:

\[ \sqrt{2n - 2 + (n - 1)(n - 2) \frac{n^{n/(n-1)}}{n}} \leq LEL \leq \sqrt{2(n - 1)(n - 2) + (n - 1) \frac{n^{1/(n-1)}}{n}} \]

3° In the chemical literature there are countless approximate expressions for \( E \), in which the only variables are \( n \) and \( m \). Several systematic comparative studies of such \((n, m)\)-type formulas were reported [44–47]. The final conclusion of these examinations was somewhat surprising: no \((n, m)\)-type approximation can reproduce \( E \) better than the simple McClelland formula:

\[ E \approx a_1 \sqrt{2mn} \]  

and

\[ E \approx a_2 \sqrt{2mn} + b_2 \]  

where \( a_1, a_2, b_2 \) are empirically determined fitting constants. In fact, a number of other, algebraically much more complicated, \((n, m)\)-type expressions yield approximations for \( E \) of comparable accuracy, but none is superior to (17) and (18).

For the usually employed standard set of 106 benzenoid hydrocarbons [44–47], one gets \( a_1 = 0.908 \pm 0.002 \), \( a_2 = 0.898 \pm 0.002 \), \( b_2 = 0.44 \pm 0.07 \), correlation coefficient \( R = 0.99982 \), and average relative error of (18) equal to 0.30\%. If in (17) and (18) \( E \) is replaced by \( LEL \), and \( n \) by \( n - 1 \), then we arrive at an even more accurate approximation: \( a_1 = 0.9334 \pm 0.0002 \), \( a_2 = 0.9256 \pm 0.0007 \), \( b_2 = 0.33 \pm 0.03 \), \( R = 0.99997 \), and average relative error of modified Eq. (18) equal to 0.13\%.

Knowing the above, it is no surprise that an excellent linear correlation is found between \( E \) and \( LEL \), whose correlation coefficient is \( R(E, LEL) = 0.99980 \).

As explained above, \( E \) and \( LEL \) have similar properties, which significantly differ from the analogous properties of \( LE \). In spite of this, for benzenoid molecules both \( E \) and \( LE \), as well as \( LEL \) and \( LE \) are well linearly correlated. For the standard set of 106 benzenoid hydrocarbons [44–47] we found \( R(E, LE) = 0.99967 \) and
\( R(\text{LEL}, LE) = 0.99971 \). Thus, as far as benzenoid molecular are concerned, there is essentially no difference in the structure–dependency of energy, Laplacian energy, and the Laplacian–energy like invariant.

4. NORDHAUS–GADDUM–TYPE RESULTS

Recall that Nordhaus and Gaddum [48] gave bounds for the sum of the chromatic numbers of a graph \( G \) and its complement \( \overline{G} \). We have pointed out that earlier obtained bounds and approximations for \( E \) can be simply “translated” into bounds and approximations for \( \text{LEL} \). Now the Nordhaus–Gaddum–type results for \( E \) [18, 27] are “translated” into \( \text{LEL} \) as follows. Let \( K_n \) be the complete graph with \( n \) vertices and \( K_{a,b} \) be the complete bipartite graph with \( a \) and \( b \) vertices in its two partite sets, respectively. We first need a lemma.

**Lemma 1.** [49] Let \( G \) be a graph with at least one edge and maximum vertex degree \( \Delta \). Then

\[
\mu_1 \geq 1 + \Delta
\]

with equality for connected graphs if and only if \( \Delta = n - 1 \).

**Proposition 2.** Let \( G \) be a graphs with \( n \geq 2 \) vertices. Then

\[
\sqrt{n(n - 1)} \leq \text{LEL}(G) + \text{LEL}(\overline{G}) < \sqrt{2(n + 1)} + \sqrt{2(n - 2)(n^2 - 2n - 1)}
\]

with left equality if and only if \( G \cong K_n \) or \( G \cong \overline{K_n} \).

**Proof.** Let \( m \) and \( m' \) be respectively the number of edges of \( G \) and \( \overline{G} \). Let \( \mu_1, \mu_2, \ldots, \mu_n \) be the Laplacian eigenvalues of \( \overline{G} \) arranged in an non-increasing order. Then \( \mu_i = n - \mu_{n-i} \) for \( i = 1, 2, \ldots, n - 1 \).

It follows that

\[
\text{LEL}(G) + \text{LEL}(\overline{G}) = \sum_{i=1}^{n-1} (\sqrt{\mu_i} + \sqrt{n - \mu_i}) \geq \sum_{i=1}^{n-1} \sqrt{n} = (n - 1)\sqrt{n}
\]

with equality if and only if either \( \mu_1 = \cdots = \mu_{n-1} = n \) and then \( G \cong K_n \), or (by Lemma 1) \( \mu_1 = \cdots = \mu_{n-1} = 0 \) and then \( G \cong \overline{K_n} \).
On the other hand, by the Cauchy–Schwarz inequality,

$$LEL(G) + LEL(\overline{G}) \leq \sqrt{\mu_1} + \sqrt{\overline{\mu_1}} + \sqrt{(n-2)(2m-\mu_1)} + \sqrt{(n-2)(2\overline{m}-\overline{\mu_1})}$$

$$\leq \sqrt{2(\mu_1 + \overline{\mu_1})} + \sqrt{2(n-2)[n(n-1) - (\mu_1 + \overline{\mu_1})]}.$$  

Consider the function $g(x) = \sqrt{2x} + \sqrt{2(n-2)[n(n-1) - x]}$. It is decreasing for $x \geq n$.

If one of $G$ or $\overline{G}$ is empty, then $\mu_1 + \overline{\mu_1} = n$. Otherwise, since one of $G$ and $\overline{G}$ is connected, we have by Lemma 1 that $\mu_1 + \overline{\mu_1} \geq 1 + \Delta + 1 + (n-1-\delta) = n + 1 + \Delta - \delta > n + 1$, where $\Delta$ and $\delta$ are respectively the maximum and minimum vertex degree of $G$. Thus,

$$LEL(G) + LEL(\overline{G}) < g(n+1) = \sqrt{2(n+1)} + \sqrt{2(n-2)(n^2 - 2n - 1)},$$

as desired.  ■

Note that

$$LEL(K_{n/2,n/2}) = \sqrt{n} + \frac{\sqrt{2}}{2}(n-1)\sqrt{n} \text{ and } LEL(K_{n/2,n/2}) = \frac{\sqrt{2}}{2}(n-2)\sqrt{n}.$$  

Then

$$LEL(K_{n/2,n/2}) + LEL(K_{n/2,n/2}) = \sqrt{n} + \sqrt{2} \left(n - \frac{3}{2}\right) \sqrt{n}.$$  

This example shows that the upper bound in the previous proposition is asymptotically best possible. More precisely: Let $\max LEL_{NG}(n)$ be the maximum value of $LEL(G) + LEL(\overline{G})$ over all graphs with $n$ vertices. Then

$$\lim_{n \to \infty} \frac{\max LEL_{NG}(n)}{n^{3/2}} = \sqrt{2}.$$  

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References


