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 $\mathbf{A}(G)$ be the adjacency matrix of G, and let $\lambda_1, \lambda_2, \dots, \lambda_n$ be its eigenvalues. These eigenvalues form the (ordinary) spectrum of the graph G [1]. Let $\mathbf{L}(G)$ 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:

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

This graph invariant, whose origins are in the molecular orbital theory of conjugated π-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]

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

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

$$E(G_1 \cup G_2) = E(G_1) + E(G_2) \tag{3}$$

whereas, in the general case it is not true that

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

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

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

whereas for sufficiently large values of p,

$$LE(G_1 \cup G_2) = 4m \frac{p+1}{p+n} \qquad \text{and} \qquad \lim_{p \to \infty} LE(G_1 \cup G_2) = 4m . \tag{6}$$

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 *Laplacian–energy like invariant*, LEL. It is defined as

$$LEL(G) := \sum_{i=1}^{n} \sqrt{\mu_i} \ . \tag{7}$$

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 μ_n. In view of this, we may write Eq. (7) as

$$LEL(G) := \sum_{i=1}^{n-1} \sqrt{\mu_i} \ . \tag{8}$$

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.

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

$$LEL(G_1 \cup G_2) = LEL(G_1) + LEL(G_2) \tag{9}$$

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

$$LEL(G_1 \cup G_2) = LEL(G_1) \ . \tag{10}$$

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. 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

$$q_i \geq 0 \qquad \text{for all } i = 1, 2, \ldots, N \tag{11}$$

and

$$\sum_{i=1}^{N} (q_i)^2 = 2M \tag{12}$$

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

$$P = P(G) = \prod_{i=1}^{N} q_i \tag{13}$$

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 $Q \equiv LEL(G)$, cf. Eq.

(8). The only difference is that for the latter choice, $P = \sqrt{n\,\Theta}$, where Θ 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 know 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]

$$\sqrt{2MN - (N-1)D} \leq Q \leq \sqrt{2MN - D} \tag{14}$$

where

$$D = 2M - N\,P^{2/N} \tag{15}$$

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

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

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:

$$\sqrt{2m + (n-1)(n-2)(n\,\Theta)^{1/(n-1)}} \leq LEL \leq \sqrt{2m(n-2) + (n-1)(n\,\Theta)^{1/(n-1)}}\ . \tag{16}$$

In particular, for disconnected graphs the bounds (16) reduce to:

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

whereas for trees to:

$$\sqrt{2n - 2 + (n-1)(n-2)\, n^{n/(n-1)}} \leq LEL \leq \sqrt{2(n-1)(n-2) + (n-1)\, n^{1/(n-1)}}\ .$$

$3°$ 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:

$$E \approx a_1 \sqrt{2mn} \tag{17}$$

and

$$E \approx a_2 \sqrt{2mn} + b_2 \tag{18}$$

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

$R(LEL, LE) = 0.99971$. 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 LEL. Now the Nordhaus–Gaddum–type results for E [18, 27] are "translated" into 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 Δ. 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

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

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

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

It follows that

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

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,

$$
\begin{aligned}
LEL(G) + LEL(\overline{G}) &\leq \sqrt{\mu_1} + \sqrt{\overline{\mu_1}} + \sqrt{(n-2)(2m - \mu_1)} + \sqrt{(n-2)(2\overline{m} - \overline{\mu_1})} \\
&\leq \sqrt{2(\mu_1 + \overline{\mu_1})} + \sqrt{2(n-2)\left[n(n-1) - (\mu_1 + \overline{\mu_1})\right]}\,.
\end{aligned}
$$

Consider the function $g(x) = \sqrt{2x} + \sqrt{2(n-2)\left[n(n-1) - x\right]}$. 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 Δ and δ 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

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

Then

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

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

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

References

[1] D. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Pres, New York, 1980.

[2] R. Merris, Laplacian matrices of graphs: A survey, *Lin. Algebra Appl.* **197–198** (1994) 143–176.

[3] R. Merris, A survey of graph Laplacians, *Lin. Multilin. Algebra* **39** (1995) 19–31.

[4] N. Trinajstić, D. Babić, S. Nikolić, D. Plavšić, D. Amić, Z. Mihalić, The Laplacian matrix in chemistry, *J. Chem. Inf. Comput. Sci.* **34** (1994) 368–376.

[5] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambridge Phil. Soc.* **36** (1940) 201–203.

[6] C. A. Coulson, B. O'Leary, R. B. Mallion, *Hückel Theory for Organic Chemists*, Academic Press, London, 1978.

[7] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[8] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology, *J. Serb. Chem. Soc.* **70** (2005) 441–456.

[9] M. Perić, I. Gutman, J. Radić–Perić, The Hückel total π-electron energy puzzle, *J. Serb. Chem. Soc.* **71** (2006) 771–783.

[10] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[11] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert–Streib (Eds.), *Analysis of Complex Networks. From Biology to Linguistics*, Wiley–VCH, Weinheim, 2009, pp. 145–174.

[12] I. Gutman, B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.* **414** (2006) 29–37.

[13] B. Zhou, I. Gutman, On Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 211–220.

[14] S. Radenković, I. Gutman, Total π-electron energy and Laplacian energy: How far the analogy goes?, *J. Serb. Chem. Soc.* **72** (2007) 1343–1350.

[15] I. Gutman, N. M. M. de Abreu, C. T. M. Vinagre, A. S. Bonifácio, S. Radenković, Relation between energy and Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 343–354.

[16] D. Stevanović, I. Stanković, M. Milošević, More on the relation between energy and Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 395–401.

[17] J. Liu, B. Liu, On relation between energy and Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 403–406.

[18] B. Zhou, I. Gutman, Nordhaus–Gaddum–type relations for the energy and Laplacian energy of graphs, *Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.)* **134** (2007) 1–11.

[19] B. Zhou, On the sum of powers of the Laplacian eigenvalues of graphs, *Lin. Algebra Appl.* **429** (2008) 2239–2246.

[20] H. Wang, H. Hua, Note on Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 373–380.

[21] T. Aleksić, Upper bounds for Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 435–439.

[22] B. Zhou, I. Gutman, T. Aleksić, A note on Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 441–446.

[23] N. N. M. de Abreu, C.T. M. Vinagre, A. S. Bonifácio, I. Gutman, The Laplacian energy of some Laplacian integral graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 447–460.

[24] G. H. Fath-Tabar, A. R. Ashrafi, I. Gutman, Note on Laplacian energy of graphs, *Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.)* **137** (2008) 1–10.

[25] D. Stevanović, Large sets of noncospectral graphs with equal Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 463–470.

[26] M. Robbiano, R. Jiménez, Applications of a theorem by Ky Fan in the theory of Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 537-552.

[27] B. Zhou, New upper bounds for Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 553–560.

[28] W. So, M. Robbiano, N. M. M. de Abreu, I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Lin. Algebra Appl.*, in press.

[29] V. Consonni, R. Todeschini, New spectral index for molecule description, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 3–14.

[30] J. Liu, B. Liu, A Laplacian–energy like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 355–372.

[31] J. Liu, B. Liu, S. Radenković, I. Gutman, Minimal LEL–equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 471–478.

[32] D. Stevanović, Laplacian–like energy of trees, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 407–417.

[33] D. Stevanović, A. Ilić, On the Laplacian coefficients of unicyclic graphs, *Lin. Algebra Appl.* **430** (2009) 2290–2300.

[34] I. Gutman, D. Kiani, M. Mirzakhah, On incidence energy of graphs, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 573–580.

[35] M. R. Jooyandeh, D. Kiani, M. Mirzakhah, Incidence energy of a graph, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 561–572.

[36] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, *J. Chem. Phys.* **54** (1971) 640–643.

[37] I. Gutman, The McClelland approximation and the distribution of π-electron molecular orbital energy levels, *J. Serb. Chem. Soc.* **72** (2007) 967–973.

[38] I. Gutman, G. Indulal, R. Todeschini, Generalizing the McClelland bounds for total π-electron energy, *Z. Naturforsch.* **63a** (2008) 280–282.

[39] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer–Verlag, Berlin, 1977.

[40] D. M. Cvetković, I. Gutman, A new spectral method for determining the number of spanning trees, *Publ. Inst. Math. (Beograd)* **29** (1981) 49–52.

[41] I. Gutman, R. B. Mallion, J. W. Essam, Counting the spanning trees of a labelled molecular–graph, *Mol. Phys.* **50** (1983) 859–877.

[42] I. Gutmanm, New approach to the McClelland approximation, *MATCH Commun. Math. Comput. Chem.* **14** (1983) 71–81.

[43] I. Gutman, Bounds for total π-electron energy, *Chem. Phys. Lett.* **24** (1974) 283–285.

[44] I. Gutman, L. Nedeljković, A. V. Teodorović, Topological formulas for total π-electron energy of benzenoid hydrocarbons – a comparative study, *J. Serb. Chem. Soc.* **48** (1983) 495–500.

[45] I. Gutman, A. V. Teodorović, Ž. Bugarčić, On some topological formulas for total π-electron energy of benzenoid molecules, *J. Serb. Chem. Soc.* **49** (1984) 521–525.

[46] I. Gutman, Total π-electron energy of benzenoid hydrocarbons, *Topics Curr. Chem.* **162** (1992) 29–63.

[47] I. Gutman, T. Soldatović, (n, m)-Type approximations for total π-electron energy of benzenoid hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **44** (2001) 169–182.

[48] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Amer. Math. Monthly* **63** (1956) 175–177.

[49] R. Grone, R. Merris, The Laplacian spectrum of a graph II, *SIAM J. Discrete Math.* **7** (1994) 221–229.