

LAPLACIAN-LIKE ENERGY OF TREES¹

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Abstract

A few alternative definitions of (molecular) graph energy have recently appeared in the literature, among others the Laplacian energy-like invariant, or Laplacian-like energy, defined by Liu and Liu. It was already shown that the Laplacian-like energy shares a number of properties with the usual graph energy. Here we exhibit further similarities between them by showing that among the n -vertex trees, $n \in \mathbf{N}$, the star S_n has minimal Laplacian-like energy and the path P_n has maximal Laplacian-like energy.

1 Introduction

Let $G = (V, E)$ be a finite, simple and undirected graph with vertices $V = \{1, 2, \dots, n\}$ and $m = |E|$ edges. The degree of a vertex $u \in V$ will be denoted by d_u . Let G have adjacency matrix A with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, and Laplacian matrix $L = D - A$, where D is the diagonal matrix of vertex degrees, with eigenvalues $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n = 0$. Additional details on the theory of graph spectra may be found in [1].

The energy and the Laplacian-like energy of G are defined as follows

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

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The energy of a graph was defined by Ivan Gutman in [2] and it has a long known chemical applications; for details see the surveys [3, 4, 5]. Much work has appeared in the literature in the last decade, and, in particular, in this journal (see, for instance, [6]-[19]). On the other hand, the Laplacian-like energy has been recently defined in [20], as a counterpart to yet another concept of the Laplacian energy defined in [21], whose further properties may be found in [22]-[25].

Among the trees, it has been long known [26, 27] that, for $n \in \mathbf{N}$, the path P_n has maximum energy and that the star S_n has minimum energy. Our goal here is to show that the analogous result holds for the Laplacian-like energy of trees.

Theorem 1 *If G is a tree on n vertices, $n \geq 4$, then*

$$LEL(S_n) \leq LEL(G) \leq LEL(P_n). \tag{1}$$

Equality holds in first inequality if and only if $G \cong S_n$, and in the second inequality if and only if $G \cong P_n$.

The plan of the paper is as follows: In the next section we will first establish a partial ordering of graphs which perfectly correlates with Laplacian-like energy, and in Section 3 we will use recent results of Mohar [30] to establish Theorem 1. Additional remarks may be found in concluding section.

2 Partial ordering via Laplacian coefficients

Suppose G is connected. Then $n \geq \mu_1$ and $\mu_{n-1} > 0$, so that 0 is a simple eigenvalue of G . Let

$$\Lambda(G, x) = \sum_{k=0}^n (-1)^k c_k x^{n-k}$$

be the characteristic polynomial of the Laplacian matrix L of G . Here $c_k = c_k(G)$, $0 \leq k \leq n$, are the absolute values of the coefficients of $\Lambda(G, x)$. It is easy to see that $c_0 = 1$, $c_1 = 2m$, $c_n = 0$, and $c_{n-1} = n\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of G . Detailed introduction to graph Laplacians may be found in [31]-[33].

The eigenvalues $n \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > 0$ are the roots of $\Lambda(G, x)/x$, so from Viette's formulas we see that the values c_1, c_2, \dots, c_{n-1} are the elementary symmetric functions of $\mu_1, \mu_2, \dots, \mu_{n-1}$:

$$c_k = \sum_{I \subseteq \{1, 2, \dots, n-1\}, |I|=k} \prod_{i \in I} \mu_i. \tag{2}$$

Let us move, for the moment, to a more general setting. Consider the open set in \mathbf{R}^{n-1}

$$\mathcal{M} = \{(\mu_1, \mu_2, \dots, \mu_{n-1}) : n > \mu_1 > \mu_2 > \dots > \mu_{n-1} > 0\}.$$

Let \mathcal{C} denote the set of coefficients of polynomials having roots in \mathcal{M} ,

$$\mathcal{C} = \{(c_1, c_2, \dots, c_{n-1}) : (\exists (\mu_1, \mu_2, \dots, \mu_{n-1}) \in \mathcal{M}) \\ x^{n-1} - c_1 x^{n-2} + c_2 x^{n-3} - \dots + (-1)^{n-1} c_{n-1} = (x - \mu_1)(x - \mu_2) \cdots (x - \mu_{n-1})\}.$$

Let $F : \mathcal{M} \rightarrow \mathcal{C}$ be the bijection defined by Viète's formulas (2) which represent polynomial coefficients from \mathcal{C} via the roots from \mathcal{M} . Viète's formulas are continuously differentiable functions and we have

$$\frac{\partial c_k}{\partial \mu_j} = \sum_{j \in I \subseteq \{1, 2, \dots, n-1\}, |I|=k} \prod_{i \in I \setminus \{j\}} \mu_i. \quad (3)$$

Notice that $\partial c_k / \partial \mu_j$ is a polynomial of degree $k - 1$ in variables μ_1, \dots, μ_{n-1} . The Jacobian determinant of the function F is then

$$\det J_F = \begin{vmatrix} 1 & 1 & \dots & 1 \\ \frac{\partial c_2}{\partial \mu_1} & \frac{\partial c_2}{\partial \mu_2} & \dots & \frac{\partial c_2}{\partial \mu_{n-1}} \\ \dots & \dots & \dots & \dots \\ \frac{\partial c_{n-1}}{\partial \mu_1} & \frac{\partial c_{n-1}}{\partial \mu_2} & \dots & \frac{\partial c_{n-1}}{\partial \mu_{n-1}} \end{vmatrix}$$

also a polynomial in variables μ_1, \dots, μ_{n-1} , of degree at most $(n - 1)(n - 2)/2$. This determinant may be calculated in the same way as any other Vandermonde-type determinant: if, for any $i \neq j$, we have that $\mu_i = \mu_j$, then the columns i and j of J_F are identical, and the determinant of J_F becomes equal to 0. Hence, $\mu_i - \mu_j$ is a factor of $\det J_F$, and since there are $(n - 1)(n - 2)/2$ factors of this form, we have

$$\det J_F = c \prod_{1 \leq i < j \leq n-1} (\mu_i - \mu_j), \quad (4)$$

for some nonzero constant c . The value of the constant may be obtained by comparing coefficients of $\mu_1^{n-2} \mu_2^{n-3} \cdots \mu_{n-2}$ on both sides of (4).

Thus, the Jacobian determinant of F is nonzero on whole \mathcal{M} . By the inverse function theorem [34], we conclude that, for every point $\mu \in \mathcal{M}$, F has continuously differentiable inverse function F_μ^{-1} in some neighborhood of $F(\mu)$. However, F is bijection, so the function F_μ^{-1} must coincide with F^{-1} in the neighborhood of $F(\mu)$. Thus, we may conclude that F^{-1} is continuously differentiable on whole \mathcal{C} , and that \mathcal{M} and \mathcal{C} are homeomorphic.

The Laplacian-like energy function $LEL : \mathcal{M} \rightarrow \mathbf{R}$, defined by

$$LEL(\mu_1, \mu_2, \dots, \mu_{n-1}) = \sqrt{\mu_1} + \sqrt{\mu_2} + \dots + \sqrt{\mu_{n-1}},$$

may then be represented as an implicit function of coefficients from \mathcal{C} . By the chain rule, for arbitrary k , $1 \leq k \leq n - 1$, we have

$$\frac{\partial LEL}{\partial c_k} = \sum_{j=1}^{n-1} \frac{\partial LEL}{\partial \mu_j} \cdot \frac{\partial \mu_j}{\partial c_k} = \sum_{j=1}^{n-1} \frac{\partial LEL / \partial \mu_j}{\partial c_k / \partial \mu_j}.$$

Now, $\partial LEL/\partial\mu_j = \frac{1}{2\sqrt{\mu_j}} > 0$, while from (3) it follows that $\partial c_k/\partial\mu_j > 0$ for points of \mathcal{M} . Thus,

$$\frac{\partial LEL}{\partial c_k} > 0$$

and the Laplacian-like energy function LEL is strictly increasing on \mathcal{C} in each coordinate.

So far we have dealt with the case of distinct eigenvalues only. The remaining step is to consider the closures of \mathcal{M} and \mathcal{C} : first, the closure of \mathcal{M} is the compact set

$$\bar{\mathcal{M}} = \{(\mu_1, \mu_2, \dots, \mu_{n-1}) : n \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq 0\}.$$

Its image under equations (2) is the set $\bar{\mathcal{C}}$ of coefficients of polynomials having roots in $\bar{\mathcal{M}}$. The continuously differentiable bijection F between \mathcal{M} and \mathcal{C} extends to the bijection \bar{F} between $\bar{\mathcal{M}}$ and $\bar{\mathcal{C}}$, showing that $\bar{\mathcal{C}}$ is the closure of \mathcal{C} . Then the Laplacian-like energy function LEL , which is strictly increasing on \mathcal{C} in each coordinate, must be strictly increasing on $\bar{\mathcal{C}}$ as well.

Restoring our setting back to the Laplacian coefficients of graphs, and noting that $\bar{\mathcal{C}}$ contains the Laplacian coefficients of disconnected graphs as well, we arrive at the following

Lemma 2 *Let G and H be two n -vertex graphs. If $c_k(G) \leq c_k(H)$ for $k = 1, \dots, n-1$, then $LEL(G) \leq LEL(H)$. Furthermore, if a strict inequality $c_{k'}(G) < c_{k'}(H)$ holds for some k' , $1 \leq k' \leq n-1$, then $LEL(G) < LEL(H)$.*

We may now introduce relations \preceq_c and \prec_c on the set of n -vertex graphs by defining

$$G \preceq_c H \iff (\forall k = 1, \dots, n-1) c_k(G) \leq c_k(H)$$

and

$$G \prec_c H \iff G \preceq_c H \text{ and } c_k(G) < c_k(H) \text{ for some } 1 \leq k \leq n-1.$$

The above lemma may then be restated as: *If $G \prec_c H$, then $LEL(G) < LEL(H)$.*

3 Proof of Theorem 1

Recently, Zhou and Gutman [35] proved a conjecture from [36] that the extreme values of Laplacian coefficients among all n -vertex trees are attained on one side by the path P_n of length $n-1$, and on the other side by the star $S_n = K_{1,n-1}$ of order n . In other words,

$$c_k(S_n) \leq c_k(T) \leq c_k(P_n), \quad 0 \leq k \leq n$$

holds for all trees T of order n . Applying Lemma 2 to these inequalities, we immediately obtain Theorem 1, except for the case of equality.

In order to settle the case of equality, we may use a recent strengthening of the above result by Mohar [30], who proved that all Laplacian coefficients are monotone under two operations called π and σ .

Let u_0 be a vertex of tree T . Suppose that $P = u_0u_1 \dots u_p$ ($p \geq 1$) is a path in T whose internal vertices u_1, \dots, u_{p-1} all have degree 2 in T and where u_p is a leaf (i.e., a vertex of degree 1 in T). Then we say that P is a *pendant path* of length p attached at u_0 . Suppose that $\deg_T(u_0) \geq 3$ and that $P = u_0u_1 \dots u_p$ and $Q = u_0v_1 \dots v_q$ are distinct pendant paths attached at u_0 . Then we form a tree $T' = \pi(T, u_0, P, Q)$ by removing the paths P and Q and replacing them with a longer path $R = u_0u_1 \dots u_pv_1v_2 \dots v_q$. We say that T' is a π -transform of T .

Mohar proved that every tree which is not a path contains a vertex of degree at least three at which (at least) two pendant paths are attached, and, in particular, that every tree can be transformed into a path by a sequence of π -transformations. He also proved the following

Theorem 3 ([30]) *Let $T' = \pi(T, u_0, P, Q)$ be a π -transform of a tree T of order n . For $d = 1, \dots, k - 1$, let n_d be the number of vertices in $T - P - Q$ that are at distance d from u_0 in T . Then*

$$c_k(T) \leq c_k(T') - \sum_{d=1}^{k-1} n_d \binom{n-3-d}{k-1-d} \quad \text{for } 2 \leq k \leq n-2$$

and $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$.

Next, let u_0 be a vertex of a tree T of degree $p + 1$. Suppose that $u_0u_1, u_0u_2, \dots, u_0u_p$ are pendant edges incident with u_0 , and that v_0 is the neighbor of u_0 distinct from u_1, \dots, u_p . Then we form a tree $T' = \sigma(T, u_0)$ by removing the edges u_0u_1, \dots, u_0u_p from T and adding p new pendant edges v_0v_1, \dots, v_0v_p incident with v_0 . We say that T' is a σ -transform of T .

Mohar proved that every tree which is not a star contains a vertex u_0 such that $p = \deg_T(u_0) - 1$ neighbors of u_0 are leaves of T , while the remaining neighbor of u_0 is not a leaf. Consequently, every tree can be transformed into a star by a sequence of σ -transformations. He also proved the following

Theorem 4 ([30]) *Let $T' = \sigma(T, u_0)$ be a σ -transform of a tree T of order n . For $d = 2, \dots, k$, let n_d be the number of vertices in $T - u_0$ that are at distance d from u_0 in T . Then*

$$c_k(T) \geq c_k(T') + \sum_{d=2}^k n_d p \binom{n-2-d}{k-d} \quad \text{for } 2 \leq k \leq n-2$$

and $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$.

From Theorems 3 and 4, we see that the set of n -vertex trees possess a unique minimal element S_n and a unique maximal element P_n under partial ordering \preceq_c . This characterizes the case of equality in Theorem 1 as well: if $LEL(S_n) = LEL(T)$, then $c_k(S_n) = c_k(T)$ for all k , and, consequently, $S_n \cong T$; if $LEL(T) = LEL(P_n)$, then $c_k(T) = c_k(P_n)$ for all k , and, consequently, $T \cong P_n$.

4 Concluding remarks

The fact that S_n has minimal Laplacian-like energy among all connected graphs (not only trees) on n vertices has already been shown in [20, Theorem 4.2], as a consequence of a lower bound on $LEL(G)$.

However, our proof via Lemma 2 is of entirely different nature. Moreover, its basic ingredient, Lemma 2, together with π and σ -transformations may be used to yield other extremal results on the Laplacian-like energy of trees, in conjunction with existing results on the numbers of matchings, which are already used to prove a myriad of results on usual graph energy.

For example, if we consider an arbitrary n -vertex tree T with a given maximum degree Δ , then applying π -transformation at each vertex of degree ≥ 3 , except at one vertex of degree Δ , yields a starlike tree $S(p_1, \dots, p_\Delta)$, with paths of lengths p_1, \dots, p_Δ , $p_1 + \dots + p_\Delta = n - 1$, emanating from a vertex of degree Δ . Moreover,

$$LEL(T) < LEL(S(p_1, \dots, p_\Delta)). \tag{5}$$

Next, for a graph G , let $m_k(G)$ be the number of matchings of G containing precisely k edges, and let $S(G)$ denote the *subdivision* graph of G . Zhou and Gutman [35] proved that for every acyclic graph T of order n ,

$$c_k(T) = m_k(S(T)), \quad 0 \leq k \leq n. \tag{6}$$

Moreover, in this particular case, we have $S(S(p_1, \dots, p_\Delta)) = S(2p_1, \dots, 2p_\Delta)$, where the first S denotes the subdivision graph, and the second and third S refer to corresponding starlike trees.

Using (6) our problem of comparing Laplacian coefficients of starlike trees may be reduced to the problem of comparing matchings of their subdivisions. From that point on, we need a similar partial ordering to \preceq_c , which has been used for a long time in literature on graph energy: for two n -vertex graphs G and H we define

$$G \preceq_m H \iff (\forall k = 1, \dots, n - 1) m_k(G) \leq m_k(H)$$

and

$$G \prec_m H \iff G \preceq_m H \text{ and } m_k(G) < m_k(H) \text{ for some } 1 \leq k \leq n - 1.$$

Let us recall a particular result on \preceq_m . Denote the vertices of the path P_n by v_1, v_2, \dots, v_n so that v_i and v_{i+1} are adjacent. Let two graphs G and H have disjoint vertex sets. If v is a vertex of G and w a vertex of H , then let $GvwH$ denote the graph obtained by identifying vertices v and w . In this notation, Gutman and Zhang [37] have shown the following result:

Lemma 5 ([37]) *For an arbitrary vertex v of the graph G having $n = 4k + i$ vertices, where $i \in \{-1, 0, 1, 2\}$, we have*

$$P_n v_2 v G \prec_m P_n v_4 v G \prec_m \dots \prec_m P_n v_{2k} v G \\ \prec_m P_n v_{2k+1} v G \prec_m P_n v_{2k-1} v G \prec_m \dots \prec_m P_n v_3 v G \prec_m P_n v_1 v G.$$

Applying previous lemma to any pair of paths from $S(2p_1, \dots, 2p_\Delta)$, whose lengths are $p_i, p_j \geq 4$, we easily get that

$$S(2p_1, \dots, 2p_i, \dots, 2p_j, \dots, 2p_\Delta) \prec_m S(2p_1, \dots, 2p_i + 2p_j - 2, \dots, 2, \dots, 2p_\Delta).$$

Iterating the application of Lemma 5 as long as there are at least two paths of length at least four in corresponding starlike trees, we get that

$$S(2p_1, \dots, 2p_\Delta) \prec_m S(2n - 2\Delta, 2, \dots, 2),$$

from (6)

$$S(p_1, \dots, p_\Delta) \prec_c S(n - \Delta, 1, \dots, 1),$$

and finally from Lemma 2

$$LEL(S(p_1, \dots, p_\Delta)) < LEL(S(n - \Delta, 1, \dots, 1)).$$

Thus, we have just shown

Theorem 6 *If T is a tree with n vertices and maximum degree Δ , then $LEL(T) \leq LEL(S(n - \Delta, 1, \dots, 1))$, with equality if and only if $T \cong S(n - \Delta, 1, \dots, 1)$.*

The equation (6) thus represents a strong link between the energy and Laplacian-like energy, which may be used, up to certain degree, to carry over existing results on the energy of trees to the Laplacian-like energy. So, it appears as if the energy and Laplacian-like energy behave in quite a similar way, at least when trees are considered.

However, the Laplacian-like energy may be even more natural from graph-theoretical point of view. After the trees, the next simple class of graphs are unicyclic graphs. Let P_n^l be the unicyclic graph obtained by connecting a vertex of a cycle C_l with a pendant vertex of P_{n-l} . There is a conjecture of Caporossi, Cvetković, Gutman and Hansen, obtained with the use of system AutoGraphiX [38]:

Conjecture 7 ([39]) *Among unicyclic graphs on n vertices, the cycle C_n has maximal energy if $n \leq 7$ and $n = 9, 10, 11, 13$ and 15 . For all other values of n , the unicyclic graph with maximum energy is P_n^6 .*

Best result so far is by Hou, Gutman and Woo [40], who showed that $E(P_n^6)$ is maximal within the class of connected unicyclic bipartite n -vertex graphs that differ from C_n . In particular, they proved that among bipartite unicyclic graphs either C_n or P_n^6 have maximal energy.

However, when the system AutoGraphiX is put to work on the Laplacian-like energy of unicyclic graphs, we obtain a more natural conjecture:

Conjecture 8 *Among unicyclic graphs on n vertices, the cycle C_n has maximal Laplacian-like energy.*

When it comes to general graphs, the Laplacian-like energy behaves in a nicer way than the ordinary energy. Namely, from the interlacing theorem [1] it follows that $E(G - u) \leq E(G)$ for any vertex u , which then extends to any induced subgraph of G . However, it is not known under what conditions on the edge e holds that

$$E(G - e) \leq E(G)?$$

Best result so far by Day and So [41, Theorem 2.6] only claims that

$$E(G) - 2 \leq E(G - e) \leq E(G) + 2.$$

On the other hand, Laplacian eigenvalues of an edge-deleted graph $G - e$ are interlaced to those of G [42],

$$\mu_1(G) \geq \mu_1(G - e) \geq \mu_2(G) \geq \mu_2(G - e) \geq \dots \geq \mu_{n-1}(G) \geq \mu_{n-1}(G - e),$$

so that we immediately get

$$LEL(G - e) \leq LEL(G).$$

All these remarks are in some favour of theoretical properties of Laplacian-like energy when compared to ordinary energy. However, the motivation for the definition of energy comes from the approximations used in Hückel's molecular orbital theory, while the Laplacian-like energy is a pure mathematical fiction. Thus, it would be quite interesting to see whether the Laplacian-like energy can find its place in chemical applications as well.

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