MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **66** (2011) 713-730

ISSN 0340 - 6253

A Survey on the Laplacian–Energy–Like Invariant*

Bolian Liu†, Yufei Huang, Zhifu You
School of Mathematical Science, South China Normal University, Guangzhou, 510631, P.R. China

(Received February 1, 2011)

Abstract

Let G be a simple graph of order n, and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be the Laplacian spectrum of G. The Laplacian-energy-like invariant of G, LEL for short, is defined as $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$. In this paper, we survey results on LEL, with emphasis on the bounds and extremal graphs of LEL.

1 Introduction

Let $G = (V,\ E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. Let A be the adjacency matrix of G with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and let $D = diag(d_1,\ d_2,\ \ldots\ ,\ d_n)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L = D - A$, with eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ (the Laplacian spectrum of G).

The Laplacian-energy-like invariant of G, LEL for short, is defined as follows:

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

The concept of LEL was first introduced by J. Liu and B. Liu ([20], 2008), where it was shown that it has similar features as graph energy [6]:

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

*This work is supported by NNSF of China (No.11071088).
†Corresponding author. E-mail address: liubl@scnu.edu.cn.

defined by I. Gutman in 1978 (for recent survey on graph energy, see e.g. [8, 10]). In [28], it was shown that LEL describes well the properties which are accounted by the majority of molecular descriptors: motor octane number, entropy, molar volume, molar refraction, particularly the acentric factor AF parameter, but also more difficult properties like boiling point, melting point and partition coefficient *Log P*. In a set of polycyclic aromatic hydrocarbons, LEL was proved [28] to be as good as the Randić χ index (a connectivity index) and better than the Wiener index (a distance based index). Moreover, it is well defined mathematically and shows interesting relations in particular classes of graphs, these recommending LEL as a new and powerful topological index.

This survey is organized as follows. In Section 2, we present some properties and bounds of LEL. In Section 3, by introducing a connection between LEL and the Laplacian coefficients, and using some operations of graphs such that all Laplacian coefficients are monotone, the extremal graphs minimizing (resp. maximizing) LEL among some classes of graphs are discussed. In Section 4, (almost) LEL–equienergetic graphs are investigated.

2 Properties and bounds of LEL

2.1 Fundamental properties of LEL

In [24], the concept of graph energy was extended to any matrix as follows. The singular values of a real (not necessarily square) matrix M are the square roots of the eigenvalues of the (square) matrix MM^T, where M^T denotes the transpose of M. The energy $E(M)$ of the matrix M [24] is defined as the sum of its singular values. Clearly, $E(G) = E(A)$. For more applications in the theory of graph energy, see [32]. Let edges of G be given an arbitrary orientation producing an oriented graph $\overrightarrow{G}$, and let $\overrightarrow{B}$ be the (vertex-edge) incidence matrix of $\overrightarrow{G}$. Then $\overrightarrow{B}\overrightarrow{B}^T = L = D - A$. It follows that

$$LEL(G) = E\left(\overrightarrow{B}\right).$$

This provides a new interpretation of LEL: oriented incidence energy ([31], 2009), and offers a new insight into its possible physical or chemical meaning.

Let B be the (vertex-edge) incidence matrix of G. Motivated by Nikiforov's idea and LEL, Jooyandeh et al. ([18], 2009) introduced the concept of incidence energy of a graph G: if the singular values of B are $\sigma_1,\ \sigma_2,\ \dots,\ \sigma_n$, then the incidence energy of G

$$IE(G) := \sum_{i=1}^{n} \sigma_i = E(B)\ .$$

Notice that $BB^T = A + D := Q$ is the signless Laplacian matrix [2], with eigenvalues $q_1 \geq q_2 \geq \cdots \geq q_n \geq 0$ (the signless Laplacian spectrum of G). Then we have

$$IE(G) = \sum_{i=1}^{n} \sigma_i = \sum_{i=1}^{n} \sqrt{q_i} \quad [4]$$

and

$$LEL(G) = IE\left(\overrightarrow{G}\right) = \sum_{i=1}^{n-1} \sqrt{\mu_i} \quad [5]\ .$$

Note that the spectra of L and Q coincide if and only if the graph G is bipartite [2]. Then for a bipartite graph G, we have

$$LEL(G) = IE(G)\ .$$

The energy $E(G)$, Laplacian–energy–like invariant $LEL(G)$, incidence energy $IE(G)$ of a graph G all have the following basic properties.

Proposition 2.1 ([8, 20, 18]) *Let G be a simple graph with n vertices and m edges.*

(i) $E(G) \geq 0$, $LEL(G) \geq 0$, $IE(G) \geq 0$, and equalities hold if and only if $m = 0$.

(ii) If G consists of components $G_1, G_2, \ldots, G_p$, then $E(G) = \sum_{i=1}^{p} E(G_i)$, $LEL(G) = \sum_{i=1}^{p} LEL(G_i)$, and $IE(G) = \sum_{i=1}^{p} IE(G_i)$.

2.2 Bounds for LEL

Let $\overline{G}$ be the complement of a graph G. Let K_n denote the complete graph of order n, and let $K_{n_1, n_2, \ldots, n_t}$ denote the complete multipartite graph with $n_1, n_2, \ldots, n_t$ vertices in its t partite sets, respectively. Denote by S_n the star of order n, and P_n the path of order n.

Theorem 2.2 ([20]) *Let G be a simple graph with n vertices and m edges. Then*

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

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

Corollary 2.3 ([20]) *Let G be a simple graph of order n. Then*

$$LEL(G) \leq (n-1)\sqrt{n}$$

with equality if and only if $G \cong K_n$.

Remark 1 *From Proposition 2.1 (i) and Corollary 2.3, the graph of order n with minimal LEL is the null graph* $\overline{K_n}$, *and the graph of order n with maximal LEL is the complete graph* K_n .

Remark 2 *Note that the Laplacian eigenvalues of an edge-deleted graph* $G-e$ *are interlaced to those of G ([12]), and* $\sum_{i=1}^{n-1}\mu_i(G)-\sum_{i=1}^{n-1}\mu_i(G-e)=2$, *so that we immediately get*

$$LEL(G-e) < LEL(G) \quad [36] \ .$$

This also implies that for a graph $G \ncong K_n$ *and* $\overline{K_n}$ *with n vertices,*

$$LEL\left(\overline{K_n}\right) < LEL(G) < LEL(K_n) \ .$$

Corollary 2.4 (*i*) *Let G be a bipartite graph with r and s vertices in its two partite sets. Then* $LEL(G) \le (s-1)\sqrt{r}+(r-1)\sqrt{s}+\sqrt{r+s}$, *and the equality holds if and only if* $G \cong K_{r,\ s}$.

(*ii*) *Let G be a bipartite graph with* $n\ (\ge 2)$ *vertices. Then* $LEL(G) \le (\lfloor \frac{n}{2} \rfloor - 1)\sqrt{\lceil \frac{n}{2} \rceil} + (\lceil \frac{n}{2} \rceil - 1)\sqrt{\lfloor \frac{n}{2} \rfloor} + \sqrt{n}$, *and the equality holds if and only if* $G \cong K_{\lfloor \frac{n}{2} \rfloor,\ \lceil \frac{n}{2} \rceil}$.

Proof. (*i*) For a bipartite graph $G \ncong K_{r,\ s}$ with r and s vertices in its two partite sets, since $LEL(G-e) < LEL(G)$, and it leads to

$$LEL(G) < LEL(K_{r,\ s}) = (s-1)\sqrt{r}+(r-1)\sqrt{s}+\sqrt{r+s} \ .$$

(*ii*) As a function of r with $1 \le r \le \lfloor \frac{n}{2} \rfloor$, $(n-r-1)\sqrt{r}+(r-1)\sqrt{n-r}+\sqrt{n}$ is increasing for r . So

$$LEL(G) \le \left(\left\lceil \frac{n}{2} \right\rceil - 1\right)\sqrt{\left\lfloor \frac{n}{2} \right\rfloor} + \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\sqrt{\left\lceil \frac{n}{2} \right\rceil} + \sqrt{n},$$

with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor,\ \lceil \frac{n}{2} \rceil}$. □

Theorem 2.5 ([20]) *Let G be a graph with n vertices,* $m\ (\ge 1)$ *edges and maximum degree* Δ . *Then*

$$LEL(G) \le \sqrt{\Delta+1} + \sqrt{(n-2)(2m-\Delta-1)} \ ,$$

with equality if and only if $G \cong K_n$ *or* $G \cong S_n$.

Theorem 2.6 ([20]) *Let G be a simple graph with n vertices and m edges. Then*

$$\sqrt{2m} \leq LEL(G) \leq \sqrt{2}m \ .$$

The first equality is attained if and only if $G \cong \overline{K_n}$ or $K_2 \cup (n-2)K_1$, and the second equality is attained if and only if $G \cong rK_2 \cup (n-2r)K_1$, where $0 \leq r \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Let $(d_1, \ d_2, \ \ldots \ , \ d_n)$ be the non-increasing degree sequence of a graph G of order n . Now the upper and lower bounds for LEL of connected graphs are given, respectively.

Theorem 2.7 ([20]) *Let G be a connected simple graph of order n . Then*

$$LEL(G) \geq \sqrt{n} + (n-2) \, ,$$

with equality if and only if $G \cong S_n$.

Remark 3 *From Corollary 2.3 and Theorem 2.7, the connected graph of order n with minimal LEL is S_n , and the connected graph of order n with maximal LEL is K_n .*

Theorem 2.8 ([20]) *Let G be a connected simple graph on n (> 2) vertices. Then*

$$\sqrt{d_1+1} + \sqrt{d_2} \leq LEL(G) \leq \sqrt{d_1+1} + \sqrt{d_2} + \cdots + \sqrt{d_{n-1}} + \sqrt{d_n - 1} \ .$$

The first equality holds if and only if $G \cong P_3$, and the second one holds if and only if $G \cong S_n$.

Let $G_1 \cup G_2$ denote the graph consisting of two components G_1 and G_2 , and let kG denote the graph consisting of k copies of G . The join $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph with vertex set $V(G_1 \vee G_2) = V(G_1 \cup G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{(u, \ v) \mid u \in V(G_1), \ v \in V(G_2)\}$.

Let $k \geq 1$. We say that a graph G is k-connected if either G is K_{k+1}, or G has at least $k+2$ vertices and contains no $(k-1)$-vertex cut. Similarly, G is k-edge-connected if it has at least two vertices and does not contain $(k-1)$-edge cut. The maximum value of k for which a connected graph G being k-connected is the connectivity of G, denoted by $\kappa(G)$, and the edge-connectivity $\kappa'(G)$ is defined analogously. We denote by $\mathcal{V}_n^k$ the set of graphs of order n with $\kappa(G) \leq k \leq n-1$, and by $\mathcal{E}_n^k$ the set of graphs of order n with $\kappa'(G) \leq k \leq n-1$. In [34], B. Zhu obtained that

Theorem 2.9 ([34]) *Let* $G \in \mathcal{V}_n^k$ *(or* $G \in \mathcal{E}_n^k$*). Then*

$$LEL(G) \leq k\sqrt{n} + \sqrt{k} + (n-k-2)\sqrt{n-1}\,,$$

where equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

A coloring of a graph is an assignment of colors to its vertices such that any two adjacent vertices have different colors. The chromatic number $\chi(G)$ of the graph G is the minimum number of colors in any coloring of G.

Theorem 2.10 ([34]) *Let* G *be a connected graph with* $n \geq 3$ *vertices and chromatic number* χ. *Then*

$$LEL(G) \leq (\chi-1)\sqrt{n} + (\chi-s)(r-1)\sqrt{n-r} + sr\sqrt{n-r-1}$$

with equality if and only if $G \cong K_{\underbrace{r,\,\ldots\,,\,r}_{\chi-s},\,\underbrace{r+1,\,\ldots\,,\,r+1}_{s}}$, *where* $n = r\chi + s$ *and* $0 \leq s < \chi$.

Let G be a simple graph with n vertices and m (≥ 1) edges. The first Zagreb index of G is defined as $Zg(G) = \sum_{i=1}^{n} d_i^2$. Note that $\sum_{i=1}^{n-1} \mu_i = 2m$ and $\sum_{i=1}^{n-1} \mu_i^2 = Zg(G) + 2m$. Then

$$LEL(G) \geq \sqrt{\frac{(2m)^3}{Zg(G)+2m}}\,,$$

with equality if and only if all nonzero Laplacian eigenvalues are equal ([7]). A K_{r+1}-free graph is a graph with no K_{r+1} as its subgraph. From the above inequality, we have

Theorem 2.11 [7]) *Let* G *be a simple graph with* n *vertices and* m *edges. Then*

$$LEL(G) \geq \frac{2m}{\sqrt{n}}$$

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

Theorem 2.12 ([7]) *Let* G *be a* K_{r+1}*-free* $(2 \leq r \leq n)$ *graph with* n *vertices and* m *edges. Then*

$$LEL(G) \geq \frac{2m}{\sqrt{\frac{n(r-1)}{r}+1}}$$

with equality if and only if $G \cong \overline{K_n}$, *or* $r = n$ *and* $G \cong K_n$.

Nordhaus-Gaddum-type [25] results for many graph invariants are known. By Theorems 2.6 and 2.9, we have the following Nordhaus-Gaddum-type result for LEL.

Theorem 2.13 *Let G be a simple graph with n (≥ 2) vertices. Then*

$$\sqrt{n}\,(n-1) \leq LEL(G) + LEL\left(\overline{G}\right) \leq \sqrt{2}\binom{n}{2}\,.$$

The first equality holds if and only if $G \cong K_n$ or $G \cong \overline{K_n}$, and the second one holds if and only if $n = 2$.

The line graph of G is denoted by $\mathcal{L}(G) = \mathcal{L}^1(G)$. The iterated line graphs of G are then defined recursively as $\mathcal{L}^2(G) = \mathcal{L}(\mathcal{L}(G))$, $\mathcal{L}^3(G) = \mathcal{L}(\mathcal{L}^2(G))$, $\ldots$, $\mathcal{L}^k(G) = \mathcal{L}(\mathcal{L}^{k-1}(G))$ for $k = 2,\ 3,\ \ldots$, and it is both consistent and convenient to set $G = \mathcal{L}^0(G)$. For some results on the energy of line graphs, please refer to [11]. The line graph $\mathcal{L}(G)$ of a regular graph G is a regular graph. Let n_t and r_t denote the order and degree of $\mathcal{L}^t(G)$ respectively, where $t = 0,\ 1,\ \ldots$, k. Then we have the following recurrence:

Theorem 2.14 ([20])

$$LEL(\mathcal{L}^k(G)) = LEL(\mathcal{L}^{k-1}(G)) + \sqrt{2r_{k-1}}(n_k - n_{k-1})\ .$$

For a complex $m \times n$ matrix C, we recall that its nonzero singular values correspond to the nonzero eigenvalues of the positive semidefinite matrix $|C| = (C^T C)^{\frac{1}{2}}$. Suppose

$$\mathscr{L}\mathscr{E}\mathscr{L}(C) = \sum_j \sqrt{s_j(C)} \ \ ([27])\,,$$

where $s_j(C)$ are the singular values of C. Then $LEL(G) = \mathscr{L}\mathscr{E}\mathscr{L}(L)$. For $k,\ d \geq 1$, a Bethe tree of k levels, $B_k(d)$, is a rooted tree such that the root vertex has degree d, the vertices from level 2 to $k-1$ have degree $d+1$ and the vertices at level k are leaves. A recurrence relation for LEL of Bethe trees is given as follows. Let T_k be the $k \times k$ tri-diagonal matrix, where the $(i,\ j)$ entry of T_k:

$$T_k(i,\ j) = \begin{cases} 1, & i = j = 1, \\ d+1, & 2 \leq i = j \leq k, \\ \sqrt{d}, & |i-j| = 1, \\ 0, & \text{elsewhere}\ . \end{cases}$$

Theorem 2.15 [27] *Let $k > 2$, and $v_k = \sum_{j=1}^{k-1} \sqrt{d+1+2\sqrt{d}cos\frac{\pi j}{k}}$. Then*

$$LEL(B_k(d)) = dLEL(B_{k-1}(d)) + v_k - dv_{k-1} + (d-1)\mathscr{LEL}(T_{k-1})$$

and

$$(k-2)\sqrt{d} \leq \mathscr{LEL}(T_{k-1}) \leq 1 + v_{k-2} .$$

Denote by $\mathcal{G}_n(p)$ the Erdős-Rényi model of random graphs, which consists of all simple graphs with vertex set $[n]$ in which the edges are chosen independently with probability p, where p is a constant with $0 < p < 1$ for the convenience of description.

Theorem 2.16 ([3]) *Almost every graph $G_n(p)$ in $\mathcal{G}_n(p)$ enjoys the following*

$$LEL(G_n(p)) = (\sqrt{p} + o(1))\, n^{\frac{3}{2}} .$$

Let α be a non-zero real number. As a natural extension of LEL, the sum of the αth power of the non-zero Laplacian eigenvalues of graph G is introduced in [36], i.e.,

$$s_\alpha(G) = \sum_{i=1}^{h} \mu_i^\alpha ,$$

where h is the number of non-zero Laplacian eigenvalues of G. Obviously, the case $\alpha = 1$ is trivial as $s_1(G) = 2m$ (where m is the number of edges), and $LEL(G) = s_{\frac{1}{2}}(G)$.

Theorem 2.17 ([36]) *Let α be a real number with $\alpha \neq 0,\ 1$, and let G be a connected graph with $n \geq 3$ vertices, t spanning trees and maximum degree Δ. Then*

$$s_\alpha(G) \geq (1+\Delta)^\alpha + (n-2)\left(\frac{tn}{1+\Delta}\right)^{\frac{\alpha}{n-2}} ,$$

with equality if and only if $G \cong K_n$ or $G \cong S_n$.

Let $V(G) = \{v_1,\ v_2,\ \dots,\ v_n\}$. For $v_i \in V(G)$, the degree of v_i and the sum of the degrees of the vertices adjacent to v_i are denoted by d_i and t_i, respectively. Denote by $i \sim j$ if the vertices v_i and v_j are adjacent. Let $w_i := d_i(d_i^2 + t_i) + \sum_{j\sim i}(d_j^2 + t_j)$ for all $i \in \{1,\ 2,\ \dots,\ n\}$.

Theorem 2.18 ([33]) *Let α be a real number with $\alpha \neq 0,\ 1$, and let G be a connected bipartite graph with $n \geq 3$ vertices, and t spanning trees. Then*

$$s_\alpha(G) \geq \left(\sqrt{\frac{\sum_{i=1}^n w_i^2}{\sum_{i=1}^n (d_i^2+t_i)^2}}\right)^\alpha + (n-2)(tn)^{\frac{\alpha}{n-2}} \left(\sqrt{\frac{\sum_{i=1}^n (d_i^2+t_i)^2}{\sum_{i=1}^n w_i^2}}\right)^{\frac{\alpha}{n-2}} ,$$

with equality if and only if $G \cong K_{\frac{n}{2},\ \frac{n}{2}}$ or $G \cong S_n$, where n is even.

Theorem 2.19 ([33]) *Let α be a real number with $0 < \alpha < 1$, and let G be a connected bipartite graph with $n \geq 3$ vertices, and m edges. Then*

$$s_\alpha(G) \leq \left(\sqrt{\frac{\sum_{i=1}^n w_i^2}{\sum_{i=1}^n (d_i^2 + t_i)^2}} \right)^\alpha + (n-2)^{1-\alpha} \left(2m - \sqrt{\frac{\sum_{i=1}^n w_i^2}{\sum_{i=1}^n (d_i^2 + t_i)^2}} \right)^\alpha ,$$

with equality if and only if $G \cong K_{\frac{n}{2},\, \frac{n}{2}}$ or $G \cong S_n$, where n is even.

There is also a relation between LEL and incidence energy.

Theorem 2.20 ([1]) *Let G be a graph of order n. Then*

$$LEL(G) \leq IE(G) .$$

3 The Laplacian coefficients and LEL

Denote by I_n the unit matrix of order n. The Laplacian characteristic polynomial $P(G,\ \mu)$ of a graph G with n vertices is the characteristic polynomial of its Laplacian matrix L,

$$P(G,\ \mu) = det(\mu I_n - L) = \sum_{k=0}^{n} (-1)^k c_k \mu^{n-k} .$$

Here c_k $(0 \leq k \leq n)$ are the absolute values of the coefficients of $P(G,\ \mu)$. Note that Laplacian coefficients c_k can be expressed in terms of subtree structures of G. Let F be a spanning forest of G with components T_i $(i = 1,\ 2,\ \ldots,\ k)$ having n_i vertices each, and let $\gamma(F) = \prod_{i=1}^k n_i$. Then the Laplacian coefficient c_{n-k} of graph G is given by

$$c_{n-k} = \sum_{F \in \mathscr{F}_k} \gamma(F) \quad ([19]) ,$$

where $\mathscr{F}_k$ is the set of all spanning forests of G with exactly k components.

Moreover, from Viète's formulas, $c_k = \sigma_k(\mu_1,\ \mu_2,\ \ldots,\ \mu_{n-1})$ is a symmetric polynomial of order $n-1$. In particular, $c_0 = 0$, $c_1 = 2n$, $c_n = 0$, $c_{n-1} = n\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of G. If G is a tree, then c_{n-2} is equal to its Wiener index, while c_{n-3} is its modified hyper-Wiener index, introduced by I. Gutman [9].

Let $m_k(G)$ be the number of matchings of G containing exactly k independent edges. The subdivision graph $S(G)$ of G is obtained by inserting a new vertex of degree two on each edge of G. Zhou et al. in [35] showed that for every acyclic graph T of order n,

$$c_k(T) = m_k(S(T)), \ \textit{where}\ 0 \leq k \leq n$$

.

In 2009, Stevanović [30] presented a connection between LEL and the Laplacian coefficients, which provides a method to study the extremal graphs for LEL.

Lemma 3.1 ([30]) *Let G and H be two n-vertex graphs. If $c_k(G) \leq c_k(H)$ for $k = 1,\ 2,\ \dots,\ n-1$, then $LEL(G) \leq LEL(H)$. Furthermore, if a strict inequality $c_k(G) < c_k(H)$ holds for some $1 \leq k \leq n-1$, then $LEL(G) < LEL(H)$.*

Remark 4 *Recently, A. Ilić et al. in [14] corrected the original proof of Lemma 3.1.*

From Lemma 3.1, it is natural to consider the extreme values of Laplacian coefficients for finding the extremal graphs of LEL among various classes of graphs. By introducing some operations of trees (e.g. π-transformation [23], σ-transformation [23], δ-transformation [17], ρ-transformation [15]) such that all Laplacian coefficients are monotone under these transformations, the authors in [30, 17, 15] obtained the extremal trees minimizing or maximizing LEL among some classes of trees as follows.

Theorem 3.2 ([30]) *If T is a tree on n $(n \geq 4)$ vertices, then*

$$LEL(S_n) \leq LEL(T) \leq LEL(P_n)\ .$$

The first equality holds if and only if $T \cong S_n$, and the second one holds if and only if $T \cong P_n$.

Theorem 3.3 ([30]) *If T is a tree with n vertices and maximum degree Δ $(2 \leq \Delta \leq n-1)$, then*

$$LEL(T) \leq LEL(S(n-\Delta,\ 1,\ \dots,\ 1))\,,$$

with equality if and only if $T \cong S(n-\Delta,\ 1,\ \dots,\ 1)$, where $S(p_1,\ p_2,\ \dots,\ p_\Delta)$ is a starlike tree with paths of lengths $p_1,\ p_2,\ \dots,\ p_\Delta$, and $p_1 + p_2 + \cdots + p_\Delta = n-1$.

The balanced starlike tree $S(n,\ k)$ $(2 \leq k \leq n-1)$ is a tree of order n with just one center vertex v, and each of the k branches of T at v is a path of length $\left\lceil \frac{n-1}{k} \right\rceil$ or $\left\lfloor \frac{n-1}{k} \right\rfloor$. Notice that the starlike trees are determined by their Laplacian spectrum [26]. By repetitive applying δ-transformation and π-transformation, it follows from Lemma 3.1 that

Theorem 3.4 ([17]) *Among trees on n vertices and $2 \le k \le n-1$ leaves, the balanced starlike tree $S(n,\ k)$ has minimal Laplacian coefficient c_i for every $i = 0,\ 1,\ \dots\ ,\ n$, and $S(n,\ k)$ is the unique tree that has minimal LEL.*

Theorem 3.5 ([17]) *Among trees on n vertices and $0 \le p \le n-4$ vertices of degree two, the balanced starlike tree $S(n,\ n-p-1)$ has minimal Laplacian coefficient c_i for every $i = 0,\ 1,\ \dots\ ,\ n$, and $S(n,\ n-p-1)$ is the unique tree that has minimal LEL.*

Remark 5 *Note that there is no tree of order n with $n-3$ vertices of degree two, and the tree with n vertices and $n-2$ vertices of degree two is P_n. Hence the original restriction $0 \le p \le n-2$ in [17] is revised to $0 \le p \le n-4$ in Theorem 3.5.*

Let $n,\ m$ be positive integers with $n \ge 2m$. Define a tree $A(n,\ m)$ with n vertices as follows: $A(n,\ m)$ is obtained from S_{n-m+1} by attaching a pendant edge to each of certain $m-1$ non-central vertices of S_{n-m+1}. Notice that $A(n,\ m)$ has an m-matching.

Theorem 3.6 ([15]) *Among trees with n vertices and matching number m $(1 \le m \le \frac{n}{2})$, the tree $A(n,\ m)$ has minimal Laplacian coefficient c_i for every $i = 0,\ 1,\ \dots\ ,\ n$, and $A(n,\ m)$ is the unique tree that has minimal LEL.*

Corollary 3.7 ([15]) *Among trees with n vertices and independence number α $(\frac{n}{2} \le \alpha \le n-1)$, the tree $A(n,\ n-\alpha)$ is the unique tree that has minimal LEL.*

Let $T(p,\ q)$ be the tree of order n by joining an edge between two centers of S_{p+1} and S_{q+1} with $p+q+2 = n$. Denote by $T(n,\ q,\ k,\ p_1,\ \dots\ ,\ p_k)$ the tree of order n obtained from $S_{q+1},\ S_{p_1+1},\ \dots\ ,\ S_{p_k+1}$ by identifying the pendent vertices of S_{q+1} and the centers of $S_{p_1+1}, \dots, S_{p_k+1}$ respectively, where $q \ge k \ge 2$, $1+q+p_1+\cdots+p_k = n$, and $p_i \ge 1$ for $i = 1,\ 2,\ \dots\ ,\ k$. In [37], X. Zhang et al. ordered trees by Laplacian coefficients in the class of all trees with n vertices and diameter 3 (resp. diameter 4), and proved that for $i = 0,\ 1,\ \dots\ ,\ n$, (1) $c_i(T(p,\ q))$ is an increasing function of p for $1 \le p \le \lfloor \frac{n}{2} \rfloor - 1$; (2) if $n \ge 5$, then $c_i(T(n,\ n-3,\ 2,\ 1,\ 1)) \le c_i(T(n,\ q,\ k,\ p_1,\ \dots\ ,\ p_k))$, with equality if and only if $T(n,\ q,\ k,\ p_1,\ \dots\ ,\ p_k) \cong T(n,\ n-3,\ 2,\ 1,\ 1)$; (3) if $n \ge 8$, then $c_i(S_n) \le c_i(T(1,\ n-3)) \le c_i(T(2,\ n-4)) \le c_i(T(n,\ n-3,\ 2,\ 1,\ 1)) < c_i(T)$, where T is a tree of order n such that $T \ncong S_n,\ T(1,\ n-3), T(2,\ n-4),\ T(n,\ n-3,\ 2,\ 1,\ 1)$.

Furthermore, A. Ilić [16] showed that among trees on n vertices and diameter d $(2 \le d \le n-1)$, $C_{n,\ d}$ has minimal Laplacian coefficient c_i for every $i = 0,\ 1,\ \dots\ ,\ n$, where

$C_{n,\ d}$ denotes the caterpillar obtained from a path P_d with vertices $\{v_0,\ v_1,\ \ldots,\ v_d\}$ by attaching $n-d-1$ pendent edges to vertex $v_{\lfloor \frac{d}{2} \rfloor}$. Note that the starlike trees are determined by their Laplacian spectrum [26], then by Lemma 3.1, we have the following corollaries.

Corollary 3.8 (1) *Any tree of order* n $(n \geq 4)$ *with diameter* 3 *can be regarded as* $T(p,\ q)$ *with* $p+q+2=n$ *and* $1 \leq p \leq q$. *Moreover,*

$$LEL(T(1,\ n-3)) < LEL(T(2,\ n-4)) < \cdots < LEL\left(T\left(\left\lfloor \frac{n}{2} \right\rfloor - 1,\ \left\lceil \frac{n}{2} \right\rceil - 1\right)\right) .$$

(2) *Let* $T \ncong T(n,\ n-3,\ 2,\ 1,\ 1)$ *be a tree of order* n *with diameter* 4, *where* $n \geq 5$. *Then*

$$LEL(T(n,\ n-3,\ 2,\ 1,\ 1)) < LEL(T) .$$

(3) *Let* T *be a tree of order* n *with* $T \ncong S_n,\ T(1,\ n-3), T(2,\ n-4),\ T(n,\ n-3,\ 2,\ 1,\ 1)$, *where* $n \geq 8$. *Then*

$$\begin{aligned} LEL(S_n) &< LEL(T(1,\ n-3)) < LEL(T(2,\ n-4)) \\ &< LEL(T(n,\ n-3,\ 2,\ 1,\ 1)) < LEL(T) . \end{aligned}$$

Corollary 3.9 *Among trees on* n *vertices and diameter* d $(2 \leq d \leq n-1)$, *the tree* $C_{n,\ d}$ *is the unique tree that has minimal LEL.*

Denote by $A_{n,\ \Delta}$ a starlike tree consisting of a central vertex v, a pendent edge, a pendent path of length $n-2\Delta+2$ and $\Delta-2$ pendent paths of length 2, all attached at v. A. Ilić in [16] proved that $A_{n,\ \Delta}$ has minimal Laplacian coefficients among trees with perfect matching and maximum degree Δ. By Lemma 3.1 and the results in [26], we obtain that

Corollary 3.10 *Among trees with perfect matching and maximum degree* Δ $(2 \leq \Delta \leq n-1)$, *the tree* $A_{n,\ \Delta}$ *is the unique tree that has minimal LEL.*

Recently, D. Stevanović and A. Ilić [29] generalized π and σ transformations of trees [23] to general graphs, and introduced γ and τ transformations of unicyclic graphs, such that all Laplacian coefficients are monotone under these transformations. Using these transformations, and by Lemma 3.1, the extremal unicyclic graphs of order n minimizing (resp. maximizing) LEL are obtained as follows.

Denote by C_n the cycle of order n, and S_n^+ the graph obtained from S_n by joining two of its pendent vertices with an edge.

Theorem 3.11 ([29]) *Let G be a connected unicyclic graph of order n $(n \geq 3)$, and let i be an integer with $2 \leq i \leq n-2$. Then*

$$c_i(S_n^+) < c_i(G) < c_i(C_n) \text{ if } G \ncong S_n^+ \text{ and } G \ncong C_n\,,$$

and

$$n + \sqrt{n} - 3 + \sqrt{3} \leq LEL(G) \leq 2\cot\frac{\pi}{2n}\ .$$

The first equality holds if and only if $G \cong S_n^+$ $(LEL(S_n^+) = n + \sqrt{n} - 3 + \sqrt{3})$, and the second equality holds if and only if $G \cong C_n$ $(LEL(C_n) = 2cot\frac{\pi}{2n})$.

Generalizing the approach in [29] on graph transformations, C. He and H. Shan [13] showed that among all bicyclic graphs of order n, the Laplacian coefficient c_k is smallest when the graph is B_n, where B_n is obtained from C_4 by adding one edge connecting two non-adjacent vertices and adding $n-4$ pendent vertices attached to the vertex of degree 3. It leads to

Theorem 3.12 ([13]) *Let G be a connected bicyclic graph on n $(n \geq 4)$ vertices. Then $LEL(B_n) < LEL(G)$ if $G \ncong B_n$.*

4 LEL–equienergetic graphs

Two non-isomorphic graphs G_1 and G_2 of the same order are said to be LEL-equienergetic if $LEL(G_1) = LEL(G_2)$. Two non-isomorphic graphs G_1 and G_2 of the same order are said to be almost-LEL-equienergetic if the difference $LEL(G_1) - LEL(G_2)$ is nonzero, but negligibly small, i.e. $|LEL(G_1) - LEL(G_2)| < 10^{-k}$ (we take $k = 8$ in the following).

Certainly, cospectral graphs are LEL–equienergetic, and in what follows we concern with pairs of non-cospectral LEL–equienergetic graphs. The minimal examples of connected, non-cospectral LEL–equienergetic graphs are given in [21] (for all connected graphs up to 7 vertices, there are no connected, non-cospectral LEL–equienergetic graphs).

Example 1 ([21]) *Let G_{801} and G_{802} be the graphs shown in Fig. 1 of [21]. Their Laplacian spectra are $\{6,\ 6,\ 4,\ 4,\ 4,\ 2,\ 2,\ 0\}$ and $\{8,\ 6,\ 6,\ 4,\ 4,\ 1,\ 1,\ 0\}$, respectively. It is easy to verify that $LEL(G_{801}) = LEL(G_{802}) = 2\sqrt{6} + 2\sqrt{2} + 6$.*

Example 2 ([21]) *Let* G_{803} *and* G_{804} *be the graphs shown in Fig. 2 of [21]. Their Laplacian spectra are* $\{6,\ 4,\ 4,\ 4,\ 2,\ 2,\ 2,\ 0\}$ *and* $\{8,\ 6,\ 4,\ 4,\ 2,\ 1,\ 1,\ 0\}$*, respectively. It is straightforward to check that* $LEL(G_{803}) = LEL(G_{804}) = \sqrt{6} + 3\sqrt{2} + 6$ *.*

The authors in [21] also gave an example of connected, non-cospectral LEL–equienergetic graphs with 12 vertices and irrational Laplacian eigenvalues (see Example 2.3 of [21]). Moreover, by direct computing, they found that up to 14 vertices, there are no non-cospectral LEL–equienergetic or almost–LEL–equienergetic trees [21]. For $n = 15$ there exist two pairs of almost–LEL–equienergetic trees, depicted in Fig. 4 of [21].

It is also claimed that the connected, non-cospectral LEL–equienergetic graphs are relatively rare ([21]). However, the number of the connected, non-cospectral LEL–equienergetic graphs is infinite ([22]). Liu et al. in [22] constructed some pairs of connected, non-cospectral LEL–equienergetic graphs of order n for $n \geq 12$.

Let $H_1 = (K_3 \cup S_7 \cup (n-11)K_1) \vee K_1$ and $H_2 = (S_8 \cup S_3 \cup (n-12)K_1) \vee K_1$, where $n \geq 12$. Let $H_3 = (7K_3 \cup (n-22)K_1) \vee K_1$ and $H_4 = (K_8 \cup (n-9)K_1) \vee K_1$, where $n \geq 22$. Let $H_5 = (4K_7 \cup 4K_3 \cup (n-41)K_1) \vee K_1$ and $H_6 = (K_{17} \cup (n-18)K_1) \vee K_1$, where $n \geq 41$. Let $H_7 = (20K_2 \cup 5K_3 \cup (n-56)K_1) \vee K_1$ and $H_8 = (K_{11} \cup (n-12)K_1) \vee K_1$, where $n \geq 56$.

Theorem 4.1 ([22]) H_1 *and* H_2 *(resp.* H_3 *and* H_4 *,* H_5 *and* H_6 *,* H_7 *and* H_8*) are a pair of connected, non-cospectral LEL-equienergetic graphs of order* n *.*

A graph is decomposable if it can be constructed from isolated vertices by the operations of union and complement. D. Stevanović et al. [31] provided a set of n mutually LEL-equienergetic decomposable graphs with $O(n)$ vertices for any given $n \in N$.

Let $A = \{a_1,\ \ldots\ ,\ a_k\}$ be a multiset of positive integers such that $a_i \geq 3$ for $i = 1,\ \ldots\ ,\ k$. The graph S_A^* , formed from the union of stars $S_{a_1-1},\ \ldots\ ,\ S_{a_k-1}$ by adding a vertex adjacent to all other vertices, has $n = \left(\sum_{i=1}^{k} a_i\right) - k + 1$ vertices and $m = 2n - k - 2$ edges. It is decomposable since it can be represented as

$$S_A^* = \overline{\overline{K_1 \cup \bigcup_{i=1}^{k} \overline{\overline{K_1 \cup \overline{a_{i-2}K_1}}}}}\ .$$

The Laplacian spectrum and LEL of S_A^* is given by

$$\{n,\ a_1,\ \ldots\ ,\ a_k,\ 2^{n-2k-1},\ 1^{k-1},\ 0\}\ ,\ LEL(S_A^*) = \sqrt{n} + \sum_{i=1}^{k} \sqrt{a_i} + (n-2k-1)\sqrt{2} + k - 1\ .$$

Let $\mathcal{S}$ be the set of finite multisets of positive integers each of which is at least three. Let ρ be an equivalence relation on $\mathcal{S}$ defined by

$$A \;\rho\; B \Longleftrightarrow |A| = |B|,\;\; \sum_{i=1}^{k} a_i = \sum_{i=1}^{k} b_i \text{ and } \sum_{i=1}^{k} \sqrt{a_i} = \sum_{i=1}^{k} \sqrt{b_i}\;.$$

It can be seen that if A and B are distinct equivalent multisets, then the graphs S_A^* and S_B^* are a pair of connected, non-cospectral LEL-equienergetic graphs. Therefore, some nontrivial equivalence classes of ρ in $\mathcal{S}$ were found in [31].

Proposition 4.2 ([31]) *For a given $k \in N$, let $a_i,\ b_i,\ c_i,\ d_i,\ e_i,\ f_i$ be positive integers with $\sum_{i=1}^{k} a_i b_i c_i = \sum_{i=1}^{k} d_i e_i f_i$. Then the multisets*

$$A = \left\{a_i^2 c_i,\; b_i^2 c_i,\; (d_i + e_i)^2 f_i\right\},\;\; B = \left\{(a_i + b_i)^2 c_i,\; d_i^2 f_i,\; e_i^2 f_i\right\}$$

belong to the same equivalence class of ρ.

Let α be a positive integer and $A \in \mathcal{S}$. The product αA is defined as $\alpha A = \{\alpha a \mid a \in A\}$. Denote by $A \uplus B$ the union of A and B, which preserves multiplicities of their elements.

Proposition 4.3 ([31]) *For any $\alpha \in N$ and $A,\ B,\ C,\ D \in \mathcal{S}$,*

$$A \;\rho\; B \Longrightarrow (\alpha A)\;\rho\;(\alpha B) \quad \text{and} \quad A \;\rho\; B,\; C \;\rho\; D \Longrightarrow (A \uplus C)\;\rho\;(B \uplus D)\;.$$

Acknowledgements

The authors would like to thank Professor I. Gutman for his valuable suggestions.

References

[1] S. Akbari, E. Ghorbani, J. H. Koolen, M. R. Oboudi, A relation between the Laplacian and signless Laplacian eigenvalues of a graph, *J. Alg. Comb.* **32** (2010) 459–464.

[2] D. Cvetković, P. Rowlinson, S. Simić, Signless Laplacians of finite graphs, *Lin. Algebra Appl.* **423** (2007) 155–171.

[3] W. Du, X. Li, Y. Li, Various energies of random graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 251–260.

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

[5] I. Gutman, B. Zhou, B. Furtula, The Laplacian–energy–like invariant is an energy like invariant, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 85–96.

[6] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sekt. Forschungsz. Graz* **103** (1978) 1–22.

[7] I. Gutman, D. Kiani, M. Mirzakhah, B. Zhou, On incidence energy of a graph, *Lin. Algebra Appl.* **431** (2009) 1223–1233.

[8] 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.

[9] I. Gutman, Hyper–Wiener index and Laplacian spectrum, *J. Serb. Chem. Soc.* **68** (2003) 949–952.

[10] 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.

[11] I. Gutman, M. Robbiano, E. Andrade Martins, D. M. Cardoso, L. Medina, O. Rojo, Energy of line graphs, *Lin. Algebra Appl.* **433** (2010) 1312–1323.

[12] W. Haemers, Interlacing eigenvalues and graphs, *Lin. Algebra Appl.* **226-228** (1995) 593–616.

[13] C. He, H. Shan, On the Laplacian coefficients of bicyclic graphs, *Discr. Math.* **310** (2010) 3404–3412.

[14] A. Ilić, D. Krtinić, M. Ilić, On Laplacian–like energy of trees, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 111–122.

[15] A. Ilić, Trees with minimal Laplacian coefficients, *Comput. Math. Appl.* **59** (2010) 2776–2783.

[16] A. Ilić, On the ordering of trees by the Laplacian coefficients, *Lin. Algebra Appl.* **431** (2009) 2203–2212.

[17] A. Ilić, M. Ilić, Laplacian coefficients of trees with given number of leaves or vertices of degree two, *Lin. Algebra Appl.* **431** (2009) 2195–2202.

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

[19] A. K. Kelmans, V. M. Chelnokov, A certain polynomial of a graph and graphs with extremal number of trees, *J. Combin. Theory Ser. B* **16** (1974) 197–214.

[20] J. Liu, B. Liu, A Laplacian–energy–like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 397–419.

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

[22] M. Liu, B. Liu, A note on the LEL–equienergetic graphs, *ARS Comb.*, to appear.

[23] B. Mohar, On the Laplacian coefficients of acyclic graphs, *Lin. Algebra Appl.* **722** (2007) 736–741.

[24] V. Nikiforov, The energy of graphs and matrices, *J. Math. Anal. Appl.* **326** (2007) 1472–1475.

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

[26] G. R. Omidi, K. Tajbakhsh, Starlike trees are determined by their Laplacian spectrum, *Lin. Algebra Appl.* **422** (2007) 654–658.

[27] M. Robbiano, V. Trevisan, Applications of recurrence relations for the characteristic polynomials of Bethe trees, *Comput. Math. Appl.* **59** (2010) 3039–3044.

[28] D. Stevanović, A. Ilić, C. Onisor, M. Diudea, LEL – A newly designed molecular descriptor, *Acta Chim. Slov.* **56** (2009) 410–417.

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

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

[31] D. Stevanović, N. M. M. de Abreu, M. A. A. de Freitas, C. Vinagre, R. D. Vecchio, On the oriented incidence energy and decomposable graphs, *Filomat* **23** (2009) 243–249.

[32] 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.* **432** (2010) 2163–2169.

[33] G. Tian, T. Huang, B. Zhou, A note on sum of powers of the Laplacian eigenvalues of bipartite graphs, *Lin. Algebra Appl.* **430** (2009) 2503–2510.

[34] B. Zhu, The Laplacian–energy like of graphs, *Appl. Math. Lett.*, to appear.

[35] B. Zhou, I. Gutman, A connection between ordinary and Laplacian spectra of bipartite graphs, *Lin. Multilin. Algebra* **56** (2008) 305–310.

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

[37] X. D. Zhang, X. P. Lv, Y. H. Chen, Ordering trees by the Laplacian coefficients, *Lin. Algebra Appl.* **431** (2009) 2414–2424.