CREAT. MATH. INFORM. **24** (2015), No. 2, 183 - 187
Online version at http://creative-mathematics.ubm.ro/
Print Edition: ISSN 1584 - 286X Online Edition: ISSN 1843 - 441X

Remark on the Laplacian-energy-like and Laplacian incidence energy invariants of graphs

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ABSTRACT. Let G be an undirected connected graph with n vertices and m edges, $n \geq 3$, and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ and $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$ be Laplacian and normalized Laplacian eigenvalues of G, respectively. The Laplacian-energy-like (LEL) invariant of graph G is defined as $\mathrm{LEL(G)} = \sum_{\mathrm{i=1}}^{\mathrm{n-1}} \sqrt{\mu_\mathrm{i}}$. The Laplacian incidence energy of graph is defined as $\mathrm{LIE(G)} = \sum_{\mathrm{i=1}}^{\mathrm{n-1}} \sqrt{\rho_\mathrm{i}}$. In this paper, we consider lower bounds of graph invariants LEL(G) and LIE(G) in terms of some graph parameters, that refine some known results.

1. INTRODUCTION AND PRELIMINARIES

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be an undirected connected graph with n vertices and m edges, $n \geq 3$. Denote by $deg(G) = \{d_1, d_2, \ldots, d_n\}$, $d_i = d(i)$, a sequence of vertex degrees in G. If i-th and j-th vertices of graph G are adjacent, we denote it as $i \sim j$. The Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{A}$ is the adjacency matrix of G and $\mathbf{D}$ the diagonal matrix of its vertex degrees. Eigenvalues of $\mathbf{L}$, denoted as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, are called Laplacian eigenvalues of G. Because the graph G is assumed to be connected, the normalized Laplacian matrix is defined as $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$. Its eigenvalues $\rho_1 \geq \rho_2 \cdots \geq \rho_{n-1} > \rho_n = 0$ are called normalized Laplacian eigenvalues of G.

The following results are well known for the Laplacian and normalized Laplacian eigenvalues (see [2, 5])

$$\sum_{i=1}^{n-1} \mu_i = \sum_{i=1}^{n} d_i = 2m, \qquad \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m$$

and

$$\sum_{i=1}^{n-1} \rho_i = n, \qquad \sum_{i=1}^{n-1} \rho_i^2 = n + 2R_{-1},$$

where $M_1 = \sum_{i=1}^{n} d_i^2$ is the first Zagreb index (see [1, 4, 13]) and $R_{-1} = \sum_{i\sim j} \frac{1}{d_i d_j}$ is general Randić index (see [3]).

Liu and Liu [9] defined the quantity, named *Laplacian-energy-like invariant* of a graph G, as

$$\mathrm{LEL(G)} = \sum_{\mathrm{i=1}}^{\mathrm{n-1}} \sqrt{\mu_\mathrm{i}}. \tag{1.1}$$

Received: 24.01.2015. In revised form: 31.07.2015. Accepted: 07.08.2015
2010 *Mathematics Subject Classification.* 15A18, 05C50.
Key words and phrases. *Laplacian spectrum (of graph), normalized Laplacian spectrum, Laplacaian energy like invariant, Laplacian incidence energy.*
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The authors established the following simple upper bound for the invariant LEL(G) in terms of parameters n and m

$$\mathrm{LEL(G)} \leq \sqrt{2m(n-1)}. \tag{1.2}$$

More on this invariant and its bounds one can found in [6] and the references cited therein.

In [11] Shi and Wang introduced graph invariant

$$\mathrm{LIE(G)} = \sum_{\mathrm{i}=1}^{\mathrm{n}-1} \sqrt{\rho_{\mathrm{i}}} \tag{1.3}$$

named *Laplacian incidence energy*. The authors of [11] determine upper bound for LIE(G) in term of parameter n

$$\mathrm{LIE(G)} \leq \sqrt{\mathrm{n(n-1)}}. \tag{1.4}$$

These graph invariants, as well as the others, find their applications not only in spectral graph theory, but also in many other areas, including biology, physics, computer science, and particulary in molecular chemistry (see for example [6, 8, 11]). However, in a small number of cases these invariants can be determined in a closed form. Therefore finding the inequalities that determine upper/lower bounds in terms of some graph parameters are of interest. In this paper we determined upper bound for LEL(G) in terms of n and m that is stronger than the one given by (1.2). Also, we determine upper bound for LIE(G) in terms of n and R_{-1} and prove that it is stronger than the one given by (1.4).

2. Main results

Throughout the paper we will use standard notations for the special types of graphs (see [2, 5]). Thus, with K_n we denote a complete graph, i.e. a graph with sequence of vertex degrees $deg(K_n) = \{\underbrace{n-1, n-1, \dots, n-1}_{n-\text{times}}\}$. By C_n we denote a ring, i.e. 2-regular graph with sequence of vertex degrees of the form $deg(C_n) = \{\underbrace{2, 2, \dots, 2}_{n-\text{times}}\}$. Finally, with $K_{1,n-1}$ we denote a star graph, i.e. n-vertex tree in which one vertex has degree $n-1$, that is $deg(K_{1,n-1}) = \{n-1, \underbrace{1, 1, \dots, 1}_{(n-1)-\text{times}}\}$.

In the following theorem we prove the inequality that establishes upper bound for LEL(G) in terms of n, m and M_1.

Theorem 2.1. *Let $G = (V, E)$ be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$\mathrm{LEL(G)} \leq \sqrt{2\mathrm{m(n-1)} - \frac{\mathrm{(n-1)(M_1 + 2m) - 4m^2}}{\mathrm{4m}}}. \tag{2.5}$$

Equality holds if and only if $G \cong K_n$.

Proof. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ be Laplacian eigenvalues of G. Then

$$2m(n-1) - \mathrm{LEL(G)}^2 = (\mathrm{n}-1)\sum_{\mathrm{i}=1}^{\mathrm{n}-1}\mu_{\mathrm{i}} - \left(\sum_{\mathrm{i}=1}^{\mathrm{n}-1}\sqrt{\mu_{\mathrm{i}}}\right)^2$$

$$\begin{aligned}
&= \sum_{1\leq i<j\leq n-1}\left(\sqrt{\mu_i}-\sqrt{\mu_j}\right)^2 \\
&\geq \sum_{i=2}^{n-2}\left((\sqrt{\mu_1}-\sqrt{\mu_i})^2 + \left(\sqrt{\mu_i}-\sqrt{\mu_{n-1}}\right)^2\right) + \left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2 \\
&\geq \frac{n-3}{2}\left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2 + \left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2 \\
&= \frac{n-1}{2}\left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2,
\end{aligned}$$

i.e.,

$$2(2m(n-1) - \mathrm{LEL(G)}^2) \geq (\mathrm{n}-1)\left(\sqrt{\mu_1}-\sqrt{\mu_{\mathrm{n}-1}}\right)^2. \tag{2.6}$$

On the other hand, based on Shisha–Mond inequality [12],

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 - \left(\sum_{i=1}^n a_i b_i\right)^2 \leq \left(\sqrt{\frac{R_1}{r_2}} - \sqrt{\frac{r_1}{R_2}}\right)^2 \sum_{i=1}^n b_i^2 \sum_{i=1}^n a_i b_i,$$

where $0 < r_1 \leq a_i \leq R_1 < +\infty$, $0 < r_2 \leq b_i \leq R_2 < +\infty$, for $i = 1, 2, \ldots, n$, setting $n := n-1$, $b_i := 1$, $a_i := \mu_i$, $i = 1, 2, \ldots, n-1$, $r_1 = \mu_{n-1}$, $R_1 = \mu_1$, $r_2 = R_2 = 1$, we get

$$(n-1)\sum_{i=1}^{n-1}\mu_i^2 - \left(\sum_{i=1}^{n-1}\mu_i\right)^2 \leq \left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2 (n-1)\sum_{i=1}^{n-1}\mu_i$$

i.e.

$$(n-1)\left(\sqrt{\mu_1}-\sqrt{\mu_{n-1}}\right)^2 \geq \frac{(n-1)(M_1+2m)-4m^2}{2m}. \tag{2.7}$$

Using inequalities (2.6) and (2.7) we obtain the desired result.

Equalities in (2.6) and (2.7) hold if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$, so the equality (2.5) holds if and only if $G \cong K_n$. □

Bearing in mind the inequality $M_1 \geq \frac{4m^2}{n}$ for the first Zagreb index [7], Theorem 2.1 yields the following corollary.

Corollary 2.1. *Let $G = (V, E)$ be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$\mathrm{LEL(G)} \leq \sqrt{2\mathrm{m}(\mathrm{n}-1) - \frac{\mathrm{n}(\mathrm{n}-1)-2\mathrm{m}}{2\mathrm{n}}}. \tag{2.8}$$

Equality holds if and only if $G \cong K_n$.

Remark 2.1. Since for each $n \geq 3$ we have that

$$0 \leq 2m(n-1) - \frac{n(n-1)-2m}{2n} \leq 2m(n-1)$$

the inequality (2.8) is stronger than (1.2).

TABLE 1

n	Exact value	Ineq. (1.2)	Ineq.(2.5)	Ineq.(2.8)
3	2.732050808	2.828427125	2.828427125	2.768874621
4	4	4.242640687	4.153311931	4.153311931
5	5.236067977	5.656854249	5.477225575	5.54977477
10	11.16227766	12.72792206	12.09338662	12.58570618
50	55.07106781	69.29646456	65.00961467	69.12655062
100	108	140.0071427	131.153536	139.8337942
1000	1029.622777	1412.799349	1321.741749	1412.622915

Table 1 shows the exact values of LEL(G) invariant for the graph $G = K_{1,n-1}$, and upper bounds obtained according to inequalities (1.2), (2.5) and (2.8), for various n.

By using similar arguments as in the proof of Theorem 2.1, we obtain our second main result:

Theorem 2.2. *Let G be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$\mathrm{LIE(G)} \leq \sqrt{\mathrm{n(n-1)} - \frac{\mathrm{2(n-1)R_{-1} - n}}{\mathrm{2n}}}. \tag{2.9}$$

Equality in (2.9) holds if and only if $G \cong K_n$.

Denote by Δ maximal vertex degree in G. It was proved in [10] that $R_{-1} \geq \frac{n}{2\Delta}$. According to this and inequality (2.9), it is possible to determine upper bound for invariant $\mathrm{LIE(G)}$ in terms of n and Δ.

Corollary 2.2. *Let G be an undirected connected graph with n, $n \geq 3$, vertices and m edges. Then*

$$\mathrm{LIE(G)} \leq \sqrt{\mathrm{n(n-1)} - \frac{\mathrm{n} - 1 - \Delta}{2\Delta}}. \tag{2.10}$$

Equality holds if and only if $G \cong K_n$.

Remark 2.2. Since

$$0 \leq n(n-1) - \frac{2(n-1)R_{-1} - n}{2n} \leq n(n-1),$$

and

$$0 \leq n(n-1) - \frac{(n-1) - \Delta}{2\Delta} \leq n(n-1)$$

the inequalities (2.9) and (2.10) are stronger than (1.4). Also, since $R_{-1} \geq \frac{n}{2(n-1)}$ [8] and $\Delta \leq n-1$, from inequalities (2.9) and (2.10), respectively the inequality (1.4) follows. However, the upper bound for graph invariant $\mathrm{LIE(G)}$ that depends only on n, obtained in (1.4) is the best possible.

Table 2 shows upper bounds of invariant LIE(G) obtained according to inequalities (1.4) and (2.9) for the graph $G = C_n$ for various n.

According to (2.7) the following results are also valid.

Theorem 2.3. *Let $G = (V, E)$ be an undirected connected graph with $n, n \geq 3$, vertices and m edges. Then*

$$\sqrt{\mu_1} - \sqrt{\mu_{n-1}} \geq \sqrt{\frac{(n-1)(M_1 + 2m) - 4m^2}{2m(n-1)}} \geq \sqrt{1 - \frac{2m}{n(n-1)}}.$$

TABLE 2

n	Ineq. (1.4)	Ineq. (2.9)
3	2.44948	2.41522
4	3.46410	3.42782
5	4.47213	4.43846
10	9.48683	9.46572
50	49.49747	49.49262
100	99.49874	99.49628
1000	999.49987	999.49962

Equality holds if and only if $G \cong K_n$.

Theorem 2.4. *Let* $G = (V, E)$ *be an undirected connected graph with* $n, n \geq 3$, *vertices and* m *edges. Then*

$$\sqrt{\rho_1} - \sqrt{\rho_{n-1}} \geq \sqrt{\frac{2(n-1)(R_{-1}-n}{n(n-1)}} \geq \sqrt{\frac{1}{\Delta} - \frac{1}{n-1}}.$$

Equality holds if and only if $G \cong K_n$.

Acknowledgements. This work was supported by the Serbian Ministry of Education and Science, Project No TR32012 and TR32009.

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