Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

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COMPARISON BETWEEN THE LAPLACIAN–ENERGY–LIKE INVARIANT AND THE KIRCHHOFF INDEX*

S. PIRZADA†, HILAL A. GANIE†, AND IVAN GUTMAN‡

Abstract. For a simple connected graph G of order n, having Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_{n-1}, \mu_n = 0$, the Laplacian–energy–like invariant (LEL) and the Kirchhoff index (Kf) are defined as $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$ and $Kf(G) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}$, respectively. In this paper, LEL and Kf are compared, and sufficient conditions for the inequality $Kf(G) < LEL(G)$ are established.

Key words. Laplacian spectrum, Laplacian-energy-like invariant, Kirchhoff index.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Let G be finite, undirected and simple graph with n vertices and m edges having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix $A = (a_{ij})$ of G is the $(0,1)$-square matrix of order n whose (i,j)-entry is equal to one if v_i is adjacent to v_j, and is equal to zero otherwise. Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix, where d_i is the degree of the vertex v_i of G. Then $L(G) = D(G) - A(G)$ is the Laplacian matrix, and its spectrum $Sp_L(G) = \{\mu_1, \mu_2, \ldots, \mu_{n-1}, \mu_n\}$ is the Laplacian spectrum of the graph G. For the sake of simplicity, we use $\mu_i^{t_j}$ to denote that the eigenvalue μ_i is repeated t_j times in the spectrum. In what follows, we assume that $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. For other undefined notations and terminology from spectral graph theory, the readers are referred to [6, 32]

It is well known that the Laplacian eigenvalues are non-negative real numbers and that eigenvalue zero has multiplicity equal to the number of connected components of the underlying graph G, for more details on Laplacian eigenvalues, see [16, 18, 19, 29, 30, 33, 34, 36, 37]. Thus, $\mu_n = 0$ for all graphs, and $\mu_{n-1} > 0$ if and only if G is connected. The eigenvalue μ_{n-1} is called the *algebraic connectivity* of the graph G [10, 12].

The concept of resistance distance was introduced by Klein and Randić [23]. In a graph G, the resistance distance between vertices v_i and v_j, denoted by r_{ij}, is defined

*Received by the editors on March 31, 2015. Accepted for publication on December 31, 2015. Handling Editor: Bryan L. Shader.

†Department of Mathematics, University of Kashmir, Srinagar, India (pirzadasd@kashmiruniversity.ac.in, hilahmad1119kt@gmail.com).

‡Faculty of Science, University of Kragujevac, Kragujevac, Serbia, and State University of Novi Pazar, Novi Pazar, Serbia (gutman@kg.ac.rs).

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

to be the effective resistance between nodes v_i and v_j as computed by Kirchhoff's laws, when all the edges of G are considered to be unit resistors.

The traditional distance between vertices v_i and v_j, denoted by d_{ij}, is the length of a shortest path connecting them. The Wiener index $W(G)$ is defined as $W(G) = \sum_{i<j} d_{ij}$. As an analogue to the Wiener index, the sum $Kf(G) = \sum_{i<j} r_{ij}$ was considered [23], later named the *Kirchhoff index* [5]. In [23], it was shown that $r_{ij} \leq d_{ij}$ and $Kf(G) \leq W(G)$ with equality if and only if G is a tree.

The Kirchhoff index has a nice purely mathematical interpretation. Mohar and one of the present authors [21] demonstrated that the Kirchhoff index of a connected graph satisfies the relation

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

Noteworthy applications in chemistry of the Kirchhoff index as a molecular structure descriptor have been found [5, 7, 11, 31, 43]. For details on the extensive mathematical research of the Kirchhoff index, see the recent papers [2, 3, 4, 14, 15, 24, 35, 38, 40, 42] and the references cited therein.

Another Laplacian–spectrum–based graph invariant was put forward by Liu and Liu [27], defined as

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

and named this as *Laplacian–energy–like invariant*. The motivation for introduction of the LEL was in its analogy to the earlier studied graph energy [25] and Laplacian energy [22, 25]; for more details see the survey [26] and the references cited therein. Recently, several mathematical investigations of the LEL were communicated [8, 20, 28, 35, 38, 39, 41, 44, 45].

Motivated by the papers [3, 9] in which two sufficient conditions were established for the inequality $Kf(G) > LEL(G)$, and the relations between $Kf(G)$ and $LEL(G)$ were completely solved for trees, unicyclic graphs, bicyclic graphs, tricyclic graphs, and tetracyclic graphs, we now obtain sufficient conditions under which $LEL(G) > Kf(G)$ holds. Complete comparisons are only given for these graphs if they have a sufficient number of vertices.

Electronic Journal of Linear Algebra ISSN 1081-3810
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2. Main results. In order to compare the Kirchhoff index and the Laplacian-energy-like invariant of a graph G, we need the following lemmas [12, 17, 18].

LEMMA 2.1. *Let G be a connected graph of order n and let Δ be its maximum degree. Then $\Delta + 1 \leq \mu_1 \leq n$. Equality holds on the left if $\Delta = n - 1$ and on the right if and only if G is the join of two graphs.*

LEMMA 2.2. *Let $G \ncong K_n$ be a connected graph of order n and let δ be its smallest vertex degree. Then $\mu_{n-1} \leq \delta$.*

LEMMA 2.3. *If $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_1$ are the Laplacian eigenvalues of the graph G, then the Laplacian eigenvalues of its complement $\overline{G}$ are $0 = \mu_n < n - \mu_1 \leq n - \mu_2 \leq \cdots \leq n - \mu_{n-1}$.*

Our first result is as follows.

THEOREM 2.4. *Let G be a connected graph with algebraic connectivity $\mu_{n-1} \geq k$ and let m be the number of edges and Δ the maximum degree of G. If*

$$2m > \frac{k(\sqrt{n}+\sqrt{k})}{k+\sqrt{n}+\sqrt{k}} \left(\frac{(n+k)(n-1)}{k} - \frac{(n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}} \right), \tag{2.1}$$

then $Kf(G) < LEL(G)$.

Proof. Let $0 = \mu_n < \mu_{n-1} \leq \cdots \leq \mu_1$ be the Laplacian eigenvalues of the connected graph G, and let $\mu_{n-1} \geq k$. Then

$$\begin{aligned}
LEL(G) &= \sum_{i=1}^{n-1} \sqrt{\mu_i} = \sum_{i=1}^{n-1} \left(\sqrt{\mu_i} - \sqrt{\mu_{n-1}}\right) + (n-1)\sqrt{\mu_{n-1}} \\
&= \sum_{i=1}^{n-1} \left(\frac{\mu_i - \mu_{n-1}}{\sqrt{\mu_i} + \sqrt{\mu_{n-1}}} \right) + (n-1)\sqrt{\mu_{n-1}} \\
&\geq \sum_{i=1}^{n-1} \left(\frac{\mu_i - \mu_{n-1}}{\sqrt{\mu_1} + \sqrt{\mu_{n-1}}} \right) + (n-1)\sqrt{\mu_{n-1}} \\
&= \frac{2m + (n-1)\sqrt{\mu_1 \mu_{n-1}}}{\sqrt{\mu_1} + \sqrt{\mu_{n-1}}} \\
&\geq \frac{2m + (n-1)\sqrt{(\Delta+1)\mu_{n-1}}}{\sqrt{n} + \sqrt{\mu_{n-1}}}.
\end{aligned}$$

For $k \leq x \leq \delta$, consider the function

$$f(x) = \frac{2m + (n-1)\sqrt{(\Delta+1)x}}{\sqrt{n} + \sqrt{x}}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
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for which

$$f'(x) = \frac{(n-1)\sqrt{n(\Delta+1)} - 2m}{2\sqrt{x}(\sqrt{n}+\sqrt{x})^2}.$$

Since $\Delta + 1 \geq \frac{2m}{n} + 1 \geq \frac{2m}{n-1}$ and $n - 1 \geq \frac{2m}{n}$, it follows that

$$(\Delta+1)(n-1) \geq \frac{2m}{n-1}\frac{2m}{n} = \frac{1}{n}\left(\frac{4m^2}{n-1}\right);$$

that is, $(n-1)\sqrt{n(\Delta+1)} - 2m \geq 0$, implying $f'(x) \geq 0$. Thus, $f(x)$ is an increasing function for $k \leq x \leq \delta$. Therefore, $f(x) \geq f(k)$, giving

$$\frac{2m + (n-1)\sqrt{(\Delta+1)x}}{\sqrt{n}+\sqrt{x}} \geq \frac{2m + (n-1)\sqrt{(\Delta+1)k}}{\sqrt{n}+\sqrt{k}};$$

that is,

$$LEL(G) \geq \frac{2m + (n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}}. \tag{2.2}$$

We also have

$$\begin{aligned}
Kf(G) &= n\sum_{i=1}^{n-1}\frac{1}{\mu_i} = n\sum_{i=1}^{n-1}\left(\frac{1}{\mu_i} - \frac{1}{\mu_1}\right) + \frac{n(n-1)}{\mu_1} \\
&= n\sum_{i=1}^{n-1}\left(\frac{\mu_1 - \mu_i}{\mu_1\,\mu_i}\right) + \frac{n(n-1)}{\mu_1} \\
&\leq n\sum_{i=1}^{n-1}\left(\frac{\mu_1 - \mu_i}{\mu_1\,\mu_{n-1}}\right) + \frac{n(n-1)}{\mu_1} \\
&= \frac{n(n-1)\mu_1 - 2mn}{\mu_1\mu_{n-1}} + \frac{n(n-1)}{\mu_1} \\
&\leq \frac{kn(n-1) - 2mn}{k\mu_1} + \frac{n(n-1)}{k}.
\end{aligned}$$

For $\Delta + 1 \leq x \leq n$, consider the function $g(x) = \frac{kn(n-1)-2mn}{kx}$, for which $g'(x) = \frac{2mn - kn(n-1)}{kx^2} > 0$. As G is connected, so $2m > k(n-1)$. Therefore, $g(x)$ is an increasing function of x, implying $g(x) \leq g(n)$, that is,

$$\frac{kn(n-1) - 2mn}{kx} \leq \frac{k(n-1) - 2m}{k};$$

resulting in

$$Kf(G) \leq \frac{(n+k)(n-1) - 2m}{k}. \tag{2.3}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
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Volume 31, pp. 27-41, January 2016

Suppose inequality (2.1) holds. By direct calculation, it can be transformed into

$$\frac{2m+(n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}} > \frac{(n+k)(n-1)-2m}{k}.$$

Keeping in mind (2.2) and (2.3), it follows that $LEL(G) > Kf(G)$. □

In particular, if $\mu_{n-1} \geq 1$, we have the result stated in Corollary 2.5. In [9], the question was raised whether it is "possible to find a constant c (which may depend on the number of vertices n and maximum vertex degree Δ), such that for any connected graph G with $m \geq c$ edges, $LEL(G) > Kf(G)$ holds". Corollary 2.5 provides a partial answer to this question.

COROLLARY 2.5. *Let G be a connected graph G with algebraic connectivity $\mu_{n-1} \geq 1$. Let m be the number of edges and Δ the maximum degree of G. If*

$$2m > \frac{\sqrt{n}+1}{\sqrt{n}+2}\left(n^2-1-\frac{(n-1)\sqrt{\Delta+1}}{\sqrt{n}+1}\right),$$

then $Kf(G) < LEL(G)$.

COROLLARY 2.6. *Let T be a tree and $\overline{T}$ its complement. If the order of T is $n \geq 7$ and $\Delta(T) \leq n-2$, then $LEL(\overline{T}) > Kf(\overline{T})$.*

Proof. Since any T of order n has minimum degree one and $n-1$ edges, it follows that $\Delta(\overline{T}) = n-2$ and $2m(\overline{T}) = (n-1)(n-2)$. Since $\Delta(T) \leq n-2$, we have $\mu_1(T) \leq n-2$ (as $T \neq K_{n-1,1}$) and so by Lemma 2.3, $\mu_{n-1}(\overline{T}) = n-\mu_1(T) \geq 2$. Therefore,

$$\begin{aligned}
&\frac{2(\sqrt{n}+\sqrt{2})}{\sqrt{n}+2+\sqrt{2}}\left(\frac{(n+2)(n-1)}{2}-\frac{(n-1)\sqrt{2(n-1)}}{\sqrt{n}+\sqrt{2}}\right)\\
&= (n-1)\left(\frac{(n+2)(\sqrt{n}+\sqrt{2})-2\sqrt{2(n-1)}}{\sqrt{n}+2+\sqrt{2}}\right)\\
&< (n-1)(n-2) = 2m(\overline{T})
\end{aligned}$$

if

$$n-2 > \frac{(n+2)(\sqrt{n}+\sqrt{2})-2\sqrt{2(n-1)}}{\sqrt{n}+2+\sqrt{2}},$$

that is, $n+\sqrt{2(n-1)} > 2\sqrt{n}+4.8284$, which is true for $n \geq 7$.

Therefore, by Theorem 2.4, $LEL(G) > Kf(G)$, for $n \geq 7$. □

COROLLARY 2.7. *Let U be a unicyclic graph and $\overline{U}$ its complement. If the order of U is $n \geq 14$ and $\Delta(U) \leq n-2$, then $LEL(\overline{U}) > Kf(\overline{U})$.*

Electronic Journal of Linear Algebra ISSN 1081-3810
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Volume 31, pp. 27-41, January 2016

Proof. Since in a unicyclic graph it is either $\delta(U) = 1$ or $\delta(U) = 2$, and

$$\Delta(\overline{U}) + 1 = \begin{cases} n-1 & \text{if } \delta(U) = 1 \\ n-2 & \text{if } \delta(U) = 2. \end{cases}$$

In addition, $2m(\overline{U}) = n(n-3)$ and $\mu_{n-1}(\overline{U}) = n - \mu_1(U) \geq 1$, as $\mu_1(U) \leq n-1$.

If $\Delta + 1 = n - 1$, then

$$\begin{aligned} \frac{\sqrt{n}+1}{\sqrt{n}+2}\left(n^2 - 1 - \frac{(n-1)\sqrt{\Delta+1}}{\sqrt{n}+1}\right) &= (n-1)\left(\frac{(n+1)(\sqrt{n}+1) - \sqrt{n-1}}{\sqrt{n}+2}\right) \\ &< n(n-3) = 2m(\overline{U}), \end{aligned}$$

provided $n - 3 > \left(\frac{(n+1)(\sqrt{n}+1)-\sqrt{n-1}}{\sqrt{n}+2}\right)$, that is, $n + \sqrt{n-1} > 4\sqrt{n} + 7$, which is true for $n \geq 21$.

For $n = 14, 15, 16, 17, 18, 19, 20$, it can be checked by direct calculation that

$$\frac{\sqrt{n}+1}{\sqrt{n}+2}\left(n^2 - 1 - \frac{(n-1)\sqrt{\Delta+1}}{\sqrt{n}+1}\right) < n(n-3).$$

Similarly, if $\Delta + 1 = n - 2$, then for $n \geq 14$,

$$\frac{\sqrt{n}+1}{\sqrt{n}+2}\left(n^2 - 1 - \frac{(n-1)\sqrt{n-2}}{\sqrt{n}+1}\right) < n(n-3).$$

Therefore, by Corollary 2.5 it follows that $LEL(\overline{U}) > Kf(\overline{U})$. □

Corollary 2.8. *Let B be a bicyclic graph and $\overline{B}$ be its complement. If the order of B is $n \geq 15$ and $\Delta(B) \leq n-2$, then $LEL(\overline{B}) > Kf(\overline{B})$.*

Proof. Since in a bicyclic graph, either $\delta(B) = 1$ or $\delta(B) = 2$, it follows that

$$\Delta(\overline{B}) + 1 = \begin{cases} n-1 & \text{if } \delta(B) = 1 \\ n-2 & \text{if } \delta(B) = 2. \end{cases}$$

In addition, $2m(\overline{B}) = n(n-3) - 2 = n^2 - 3n - 2$ and $\mu_{n-1}(\overline{B}) = n - \mu_1(B) \geq 1$, as $\mu_1(B) \leq n-1$. Consider the function

$$f(n) = n^2 - 3n - 2 - \frac{(n^2-1)(\sqrt{n}+1) - (n-1)\sqrt{n-2}}{\sqrt{n}+2}$$

for which

$$f'(n) = 2n - 3 - \frac{1}{(\sqrt{n}+2)^2}\left(2n^2 + \frac{13}{2}n^{3/2} - \frac{1}{2\sqrt{n}} - \frac{3n-5}{\sqrt{n-2}} - \frac{n^2-n-1}{\sqrt{n(n-2)}} - 1\right).$$

Electronic Journal of Linear Algebra ISSN 1081-3810
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Volume 31, pp. 27-41, January 2016

It can be seen that $f'(n) > 0$, for all $n \geq 4$, that is $f(n)$ is an increasing function on $[4, \infty)$. So we have $f(n) > f(15) = 0.73565404 > 0$, that is, $f(n) > 0$ for $n \geq 15$, which implies that

$$n^2 - 3n - 2 > \left(\frac{(n^2-1)(\sqrt{n}+1) - (n-1)\sqrt{n-2}}{\sqrt{n}+2} \right).$$

The result follows from Corollary 2.5. □

COROLLARY 2.9. *Let TC be a tricyclic graph and $\overline{TC}$ be its complement. If the order of TC is $n \geq 16$ and $\Delta(TC) \leq n-2$, then $LEL(\overline{TC}) > Kf(\overline{TC})$.*

Proof. Since in a tricyclic graph, either $\delta(TC) = 1$ or $\delta(TC) = 2$ or $\delta(TC) = 3$, it follows that

$$\Delta(\overline{TC}) + 1 = \begin{cases} n-1 & \text{if } \delta(TC) = 1 \\ n-2 & \text{if } \delta(TC) = 2 \\ n-3 & \text{if } \delta(TC) = 3. \end{cases}$$

In addition, $2m(\overline{TC}) = n(n-3) - 4 = n^2 - 3n - 4$ and $\mu_{n-1}(\overline{TC}) = n - \mu_1(TC) \geq 1$, as $\mu_1(TC) \leq n-1$. Proceeding in an analogous manner as in the proof of Corollary 2.8, it can be shown that for $n \geq 16$,

$$n^2 - 3n - 4 > \frac{(n^2-1)(\sqrt{n}+1) - (n-1)\sqrt{n-3}}{\sqrt{n}+2}.$$

The result follows from Corollary 2.5. □

In a fully analogous manner, we also obtain the following.

COROLLARY 2.10. *Let QC be a tetracyclic graph and $\overline{QC}$ be its complement. If the order of QC is $n \geq 17$ and $\Delta(QC) \leq n-2$, then $LEL(\overline{QC}) > Kf(\overline{QC})$.*

The line graph of the graph G is denoted by $\pounds(G)$. We need the following result by Anderson and Morley [1]:

LEMMA 2.11. *Let $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_1$ be the Laplacian eigenvalues of the graph G and let $t_1 \geq t_2 \geq \cdots \geq t_n$ be the degree sequence of its line graph $\pounds(G)$. Then $\mu_1 \leq t_1 + 2$, with equality if and only if G is a regular or a semiregular bipartite graph.*

THEOREM 2.12. *If G is a graph for which $\mu_1 < n - n^{2/3}$, then $LEL(\overline{G}) > Kf(\overline{G})$.*

Proof. By applying Lemma 2.3, we have

$$LEL(\overline{G}) - Kf(\overline{G}) = \sum_{i=1}^{n-1} \sqrt{n-\mu_i} - \sum_{i=1}^{n-1} \frac{n}{n-\mu_i} = \sum_{i=1}^{n-1} \frac{(n-\mu_i)^{3/2} - n}{n-\mu_i}.$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

For $\mu_{n-1} \leq x \leq \mu_1$, consider the function $f(x) = [(n-x)^{3/2} - n]/(n-x)$, for which

$$f'(x) = -\frac{[\frac{1}{2}(n-x)^{3/2} + n]}{(n-x)^2} < 0,$$

for all $\mu_{n-1} \leq x \leq \mu_1$. Thus, $f(x)$ is decreasing for $\mu_{n-1} \leq x \leq \mu_1$, implying

$$f(x) \geq f(\mu_1) = \frac{(n-\mu_1)^{3/2} - n}{n-\mu_1},$$

that is,

$$LEL(\overline{G}) - Kf(\overline{G}) \geq \frac{(n-1)((n-\mu_1)^{3/2} - n)}{n-\mu_1} > 0,$$

if $(n-\mu_1)^{3/2} - n > 0$, i.e., $\mu_1 < n - n^{2/3}$. □

Remark 2.13. By Lemma 2.11, $\mu_1 \leq t_1 + 2$, where t_1 is the maximum vertex degree of the line graph $\pounds(G)$. From Theorem 2.12, it follows that $f(x) \geq f(t_1+2) = \frac{(n-t_1-2)^{3/2}-n}{n-t_1-2}$, which gives $LEL(\overline{G}) > Kf(\overline{G})$ if $t_1 < n - n^{2/3} - 2$.

The kite $Ki_{n,\omega}$ is the graph of order n, obtained by attaching a pendent path on $n-\omega$ vertices to a vertex of the complete graph of order ω. Let $\Gamma_{n,k}$ be the class of graphs of order n obtained by attaching a pendent path on $n-k$ vertices to a vertex of a connected graph of order k. In particular, $Ki_{n,k} \in \Gamma_{n,k}$. The following result can be found in [18, 19].

Lemma 2.14. *Let $G' = G + e$ be the graph obtained from G by inserting into it a new edge e. Then the Laplacian eigenvalues of G interlace the Laplacian eigenvalues of G', that is,*

$$\mu_1(G') \geq \mu_1(G) \leq \mu_2(G') \geq \mu_2(G) \geq \cdots \geq \mu_n(G') \geq \mu_n(G) = 0.$$

Corollary 2.15. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n - k \geq n^{2/3} + 2$. Then $LEL(\overline{G}) > Kf(\overline{G})$.*

Proof. Since $G \in \Gamma_{n,k}$, G is an edge-deleted subgraph of $Ki_{n,k}$. By Lemma 2.14, for $j = 1, 2, \ldots, n$, we have $\mu_j(G) \leq \mu_j(Ki_{n,k})$. There exists an edge e in $E(Ki_{n,k})$ such that $Ki_{n,k} - e = K_k \cup P_{n-k}$. Since $k \geq 4$, by Lemma 2.14, and in view of $\sum_{i=1}^{n} (\mu_i(G+e) - \mu_i(G)) = 2$, it follows that $k+1 \leq \mu_1(Ki_{n,k}) \leq k+2$. So

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

$\mu_1(G) \leq \mu_1(Ki_{n,k}) \leq k+2$. If $\mu_1(G) < n - n^{2/3}$, then $k+2 < n - n^{2/3}$, that is $n - k > n^{2/3} + 2$. □

COROLLARY 2.16. *Let $G \ncong K_n$ be an r-regular graph with n vertices. If $r < (n - n^{2/3})/2$, then $LEL(\overline{G}) > Kf(\overline{G})$. If $r > (n + n^{2/3} - 2)/2$, then $LEL(G) > Kf(G)$.*

Proof. Since G is r-regular, its line graph $\pounds(G)$ is $t_1 = (2r-2)$-regular. Assume that $r < (n - n^{2/3})/2$. Then $t_1 = 2r - 2 < n - n^{2/3} - 2$. By Remark 2.13, $LEL(\overline{G}) > Kf(\overline{G})$.

Since $\overline{G}$ is $(n-1-r)$-regular, its line graph $\pounds(\overline{G})$ is $t_1 = (2n-2r-4)$-regular. Assume that $r > (n + n^{2/3} - 2)/2$. Then $t_1 = (2n - 2r - 4) < n - n^{2/3} - 2$. By Remark 2.13, $LEL(G) > Kf(G)$. □

The following result has been proven in [3].

LEMMA 2.17. *Let $G + e$ be the graph obtained by adding a new edge to the connected graph G. If $Kf(G) < LEL(G)$, then $Kf(G+e) < LEL(G+e)$.*

Let KK_n^j be the graph obtained from two copies of complete graphs K_n, by joining a vertex of one copy with j, $1 \leq j \leq n$, vertices of the other copy. The Laplacian spectrum of KK_n^j was obtained in [13] and is given by

$$Sp_L(KK_n^j) = \left\{ n^{2n-j-2}, (n+1)^{j-1}, \frac{(n+j+1) \pm \sqrt{(n+j+1)^2 - 8j}}{2}, 0 \right\}.$$

Therefore,

$$\begin{aligned} LEL(KK_n^j) &= (2n-j-2)\sqrt{n} + (j-1)\sqrt{n+1} \\ &\quad + \sqrt{\frac{(n+j+1) + \sqrt{(n+j+1)^2 - 8j}}{2}} \\ &\quad + \sqrt{\frac{(n+j+1) - \sqrt{(n+j+1)^2 - 8j}}{2}} \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} Kf(KK_n^j) &= \frac{2n(2n-j-2)}{n} + \frac{2n(j-1)}{n+1} + \frac{2n}{\frac{(n+j+1)+\sqrt{(n+j+1)^2-8j}}{2}} \\ &\quad + \frac{2n}{\frac{(n+j+1)+\sqrt{(n+j+1)^2-8j}}{2}} \\ &= 4n - 2j - 4 + \frac{2n(j-1)}{n+1} + \frac{n(n+j+1)}{j}. \end{aligned} \tag{2.5}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

For $j \geq \frac{n}{4}$ and $n \geq 22$, it is easy to see that

$$(2n-j-2)\sqrt{n}+(j-1)\sqrt{n+1} > 4n-2j-3+\frac{n(n+j+1)}{j}.$$

Therefore, from (2.4) and (2.5), we have $LEL(KK_n^j) > Kf(KK_n^j)$. Thus, using Lemma 2.17, we arrive at the following result.

THEOREM 2.18. *For $j \geq n/4$, let KK_n^j be a spanning subgraph of the graph G. Then for $n \geq 22$ we have $LEL(G) > Kf(G)$.*

From Theorem 2.18, we observe the following. If G is a graph of order n, ($n \equiv 0 \pmod 8$) having two cliques of order $n/2$ each, such that there are at least $n/8$ edges between a vertex in one of the cliques and $n/8$ vertices of the other clique, then for $n \geq 44$, $LEL(G) > Kf(G)$.

It is clear from above that $\mu_1(KK_n^j) = n+1 < 2n-(2n)^{2/3}$, for $n \geq 7$. For the complement of the graph KK_n^j, from Theorem 2.12, it follows that $LEL\left(\overline{KK_n^j}\right) > Kf\left(\overline{KK_n^j}\right)$ holds for all $n \geq 7$ and $1 \leq j \leq n-1$. Thus, using Lemma 2.17, we arrive at the following result.

THEOREM 2.19. *If $\overline{KK_n^j}$ is a spanning subgraph of a graph G with $2n$ vertices, then $LEL(G) > Kf(G)$ for $n \geq 7$.*

The *join (complete product)* $G_1 \vee G_2$ of the graphs G_1 and G_2 is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set consisting of all the edges of G_1 and G_2 together with the edges joining each vertex of G_1 with every vertex of G_2. The Laplacian spectrum of the join is given by the the following result [18, 19].

LEMMA 2.20. *If $G_1(n_1, m_1)$ and $G_2(n_2, m_2)$ are two graphs having Laplacian spectra $Sp_L(G_1) = \{\mu_1, \mu_2, \ldots, \mu_{n_1-1}, \mu_{n_1} = 0\}$ and $Sp_L(G_2) = \{\sigma_1, \sigma_2, \ldots, \sigma_{n_2-1}, \sigma_{n_2} = 0\}$, then $Sp_L(G_1 \vee G_2) = \{n_1+n_2, n_1+\sigma_1, n_1+\sigma_2, \ldots, n_1+\sigma_{n_2-1}, n_2+\mu_1, n_2+\mu_2, \ldots, n_2+\mu_{n_1-1}, 0\}$.*

THEOREM 2.21. *For $p \geq 4$, let $K_p \vee \overline{K_r}$, $1 \leq r \leq p$, be a spanning subgraph of a graph G of order $n = p+r$. Then $LEL(G) > Kf(G)$.*

Proof. The Laplacian spectra of K_p and $\overline{K_r}$ are $\{p^{p-1}, 0\}$ and $\{0^r\}$, respectively. Therefore, by Lemma 2.20, $Sp_L(K_p \vee \overline{K_r}) = \{(p+r)^p, p^{r-1}, 0\}$. This implies

$$\begin{aligned} Kf(K_p \vee \overline{K_r}) &= \frac{np}{p+r} + \frac{n(r-1)}{p} \\ &\leq (p+r-1)+(p-1) \leq 2(p+r-2) \end{aligned}$$

and

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

$$\begin{aligned} LEL(K_p \vee \overline{K_r}) &= p\sqrt{p+r} + (r-1)\sqrt{p} \\ &\geq (p+r-1)\sqrt{p} \geq 2(p+r-2) \end{aligned}$$

resulting in $LEL(K_p \vee \overline{K_r}) \geq Kf(K_p \vee \overline{K_r})$. Theorem 2.21 now follows from Lemma 2.17. □

The Laplacian spectrum of the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ is $\left\{n, (\frac{n}{2})^{n-2}, 0\right\}$. For $n \geq 5$, this yields $Kf(K_{\frac{n}{2},\frac{n}{2}}) = 2n-3 < \sqrt{n} + (n-2)\sqrt{\frac{n}{2}} = LEL(K_{\frac{n}{2},\frac{n}{2}})$. Then Lemma 2.17 leads to the following result.

THEOREM 2.22. *If $K_{\frac{n}{2},\frac{n}{2}}$ is a spanning subgraph of a graph G of order n, then $Kf(G) < LEL(G)$, for all $n \geq 5$.*

The sufficient condition given by Theorem 2.4, seems to be useful for graphs with large number of edges and large number of vertices. We now state an analogous condition pertaining to the graph complement.

THEOREM 2.23. *Let G be a connected graph with n vertices with largest Laplacian eigenvalue $\mu_1 \leq \frac{n}{2}$ and algebraic connectivity $\mu_{n-1} \geq k$. If*

$$2m < \frac{(\Delta+1)(n-\Delta-1)\left(n(n-1) + (n-1)\sqrt{k(n-k)}\right)}{n(\sqrt{n-k}+\sqrt{k}) + (\Delta+1)(n-\Delta-1)} \tag{2.6}$$

then $LEL(\overline{G}) > Kf(\overline{G})$.

Proof. Using Lemma 2.3, since $\Delta + 1 \leq \mu_1 \leq \frac{n}{2}$, we have

$$\begin{aligned} Kf(\overline{G}) &= n\sum_{i=1}^{n-1} \frac{1}{n-\mu_i} = n\sum_{i=1}^{n-1}\left(\frac{1}{n-\mu_i} - \frac{1}{\mu_1}\right) + \frac{n(n-1)}{\mu_1} \\ &= n\sum_{i=1}^{n-1}\left(\frac{\mu_1+\mu_i-n}{\mu_1(n-\mu_i)}\right) + \frac{n(n-1)}{\mu_1} \\ &\leq n\sum_{i=1}^{n-1}\left(\frac{\mu_1+\mu_i-n}{\mu_1(n-\mu_1)}\right) + \frac{n(n-1)}{\mu_1} \\ &= \frac{2mn}{\mu_1(n-\mu_1)} \leq \frac{2mn}{(\Delta+1)(n-\Delta-1)} \end{aligned} \tag{2.7}$$

and

$$\begin{aligned} LEL(\overline{G}) &= \sum_{i=1}^{n-1}\sqrt{n-\mu_i} = \sum_{i=1}^{n-1}\left(\sqrt{n-\mu_i} - \sqrt{\mu_{n-1}}\right) + (n-1)\sqrt{\mu_{n-1}} \\ &= \sum_{i=1}^{n-1}\left(\frac{n-\mu_i-\mu_{n-1}}{\sqrt{n-\mu_i}+\sqrt{\mu_{n-1}}}\right) + (n-1)\sqrt{\mu_{n-1}} \end{aligned}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

$$\geq \sum_{i=1}^{n-1} \left(\frac{n-\mu_i-\mu_{n-1}}{\sqrt{n-\mu_{n-1}}+\sqrt{\mu_{n-1}}} \right) + (n-1)\sqrt{\mu_{n-1}}$$

$$= \frac{n(n-1)-2m+(n-1)\sqrt{\mu_{n-1}(n-\mu_{n-1})}}{\sqrt{n-\mu_{n-1}}+\sqrt{\mu_{n-1}}}. \tag{2.8}$$

For $k \leq x \leq \delta$, consider the function

$$f(x) = \frac{n(n-1)-2m+(n-1)\sqrt{nx-x^2}}{\sqrt{n-x}+\sqrt{x}}$$

for which

$$f'(x) = \frac{1}{\left(\sqrt{n-x}+\sqrt{x}\right)^2} \left[\left(\sqrt{n-x}+\sqrt{x}\right) \frac{(n-1)(n-2x)}{2\sqrt{nx-x^2}} \right.$$
$$\left. - \left(n(n-1)-2m+(n-1)\sqrt{nx-x^2}\right) \left(\frac{1}{2\sqrt{x}} - \frac{1}{2\sqrt{n-x}} \right) \right] > 0,$$

for all $k \leq x \leq \delta$. Therefore, the function $f(x)$ is increasing for $k \leq x \leq \delta$. Therefore,

$$f(x) \geq f(k) = \frac{n(n-1)-2m+(n-1)\sqrt{nk-k^2}}{\sqrt{n-k}+\sqrt{k}}$$

from which it follows that

$$LEL(\overline{G}) \geq \frac{n(n-1)-2m+(n-1)\sqrt{nk-k^2}}{\sqrt{n-k}+\sqrt{k}}.$$

Keeping in mind the relations (2.7) and (2.8), inequality (2.6) can be transformed into

$$\frac{2mn}{(\Delta+1)(n-\Delta-1)} < \frac{n(n-1)-2m+(n-1)\sqrt{nk-k^2}}{\sqrt{n-k}+\sqrt{k}},$$

whose direct consequence is $Kf(\overline{G}) < LEL(\overline{G})$. □

The importance of the Theorem 2.23 is that it is directly applicable to the complement $\overline{G}$ of the graph G and, under the conditions stated in the theorem, is an improvement of the Theorem 2.12, for all $n \geq 9$. The condition $\mu_1(G) \leq \frac{n}{2}$, in Theorem 2.23, by Lemma 2.3, gives $\mu_{n-1}(\overline{G}) \geq \frac{n}{2}$. That is, this theorem is applicable to the graphs whose complements have a higher value of algebraic connectivity. As an instance, we have the following corollary.

COROLLARY 2.24. *Let T be a tree on $n \geq 41$ vertices with largest Laplacian eigenvalue $\mu_1 \leq \frac{n}{2}$ and algebraic connectivity $\mu_{n-1} \geq 0.1$. Then $LEL(\overline{T}) > Kf(\overline{T})$.*

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 27-41, January 2016

Proof. For all $\mu_1 \leq \frac{n}{2}$ and $n \geq 41$, by Theorem 2.23, we have

$$2(n-1) < \frac{(\Delta+1)(n-\Delta-1)(n-1)(n+\sqrt{0.1(n-0.1)})}{n(\sqrt{n-0.1})+\sqrt{0.1}+(\Delta+1)(n-\Delta-1)}.$$

which is clearly true, as for a tree T of order n has $n-1$ edges and $\Delta+1 \leq \mu_1 \leq \frac{n}{2}$ gives $\Delta+1 \leq \frac{n}{2}$ and $n-\Delta-1 \geq \frac{n}{2}$. □

We have partially solved the problem in [9] to find a constant c (which may depend on the number of vertices n and maximum vertex degree Δ), such that for any connected graph G with $m \geq c$ edges, $LEL(G) > Kf(G)$. It will be of interest in future to find more sufficient conditions for the inequality $LEL(G) > Kf(G)$.

Acknowledgement. The authors would like to thank the anonymous referee for his/her helpful suggestions.

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