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On Laplacian–Energy–Like Invariant and Kirchhoff Index

S. Pirzada[1], Hilal A. Ganie[1], Ivan Gutman[2,3]

[1]*Department of Mathematics, University of Kashmir, Srinagar, India*
pirzadasd@kashmiruniversity.ac.in , hilahmad1119kt@gmail.com

[2]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
gutman@kg.ac.rs

[3]*State University of Novi Pazar, Novi Pazar, Serbia*

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Abstract

For a simple connected graph G of order n, the Laplacian–energy–like invariant and the Kirchhoff index are calculated by $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$ and $Kf(G) = n \sum_{i=1}^{n-1} 1/\mu_i$, respectively, where $\mu_1, \mu_2, \ldots, \mu_{n-1}, \mu_n = 0$ are the Laplacian eigenvalues of G. We obtain a sharp upper bound for Kf and a sharp lower bound for LEL. Further, we obtain upper and lower bounds for LEL and Kf for graphs $C(G)$ (the clique–inserted graph or para-line graph), $R(G)$ (obtained by changing each edge of G into a triangle), and $H(G)$ (obtained by inserting a new vertex on each edge of G and by joining two new vertices if they lie on adjacent edges of G), as well as for the line graph of a semiregular graph.

1 Introduction

Let G be a finite, undirected, simple graph with n vertices and m edges, having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix $A(G) = (a_{ij})$ 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 equal to zero otherwise. The eigenvalues of $A(G)$ will be labeled as $\lambda_n \leq \cdots \leq \lambda_2 \leq \lambda_1$.

Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix associated to G, where d_i is the degree of the vertex v_i. Then $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ are called Laplacian and signless Laplacian matrices and their spectra are the Laplacian spectrum (L-spectrum) and the signless Laplacian spectrum of G, respectively. For details of the theory of Laplacian and signless Laplacian spectra see [15,16,30,31,33] and [3–6], respectively.

Since the matrix $L(G)$ is real symmetric, positive semi-definite, we let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1$ be its eigenvalues, forming the Laplacian spectrum of G. For simplicity, we write $\mu_i^{[t_j]}$, to indicate that the eigenvalue μ_i is repeated t_j times in the spectrum. It is well known that μ_n=0 with multiplicity equal to the number of connected components of G and $\mu_{n-1} > 0$ if and only if G is connected [12].

The concept of resistance distance was introduced by Klein and Randić [24]. In a graph G, the resistance distance between vertices v_i and v_j, denoted by r_{ij}, is defined to be the effective resistance between nodes v_i and v_j as computed with Ohms law 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 is defined as $W(G) = \sum\limits_{i<j} d_{ij}$. As an analogue to the Wiener index, the sum $Kf(G) = \sum\limits_{i<j} r_{ij}$ was proposed by Klein [24], later called as the Kirchhoff index of G by Bonchev et al. [2]. Klein and Randić [24] proved that $r_{ij} \leq d_{ij}$ and $Kf(G) \leq W(G)$ with equality if and only if G is a tree.

It can be seen that the Kirchhoff index has a very nice purely mathematical interpretation. It was demonstrated [18] that the Kirchhoff index of a connected graph satisfies the relation

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

The Kirchhoff index has found noteworthy applications in chemistry, as a molecular structure descriptor [2, 8, 11, 34, 36, 50], and many of its mathematical properties have been established [13, 14, 23, 25, 35, 41, 42, 44–46, 48, 49].

A further L–spectrum–based graph invariant was put forward by Liu and Liu [28] as

$$LEL = LEL(G) = \sum_{k=1}^{n-1} \sqrt{\mu_k}$$

and was named Laplacian–energy–like invariant. The motivation for introducing LEL was in its analogy to the earlier studied graph energy [26] and Laplacian energy [20]; for more details we refer to [21] and the references cited therein. Recently, several mathematical investigations of LEL were communicated [9, 17, 19, 29, 38, 43, 51].

Although Kf and LEL both depend on Laplacian eigenvalues, their comparative study started only quite recently [1, 10].

Several lower and upper bounds for LEL have been established [17,39,43]. It is also of interest to study the Kirchhoff index of graphs derived from a particular graph [14,44,46]. Gao, Luo, and Liu [14] obtained formulas and lower bounds for the Kirchhoff index for the line graph, subdivision graph, and total graph of a connected regular graph. The aim of this paper is to establish an upper bound for Kf and a lower bound for LEL. In addition, we obtain lower and upper bounds for LEL and Kf of the graphs $C(G)$, $R(G)$, and $H(G)$, defined in Section 3 (see Fig. 1), as well as for the line graph of a semiregular graph.

2 Estimates for Kf and LEL

In this section, we obtain a sharp upper bound for the Krichhoff index and a sharp lower bound for the Laplacian–energy–like invariant of a connected graph.

Lemma 2.1. [7] Let G be a graph on $n > 3$ vertices whose distinct Laplacian eigenvalues are $0 < \alpha < \beta$. Then the following holds.
i) The multiplicity of α is $n-2$ if and only if G is one of the graphs $K_{\frac{n}{2},\frac{n}{2}}$ or $K_{n-1,1}$.
ii) The multiplicity of β is $n-2$ if and only if G is the graph $K_n - e$.

Lemma 2.2. [32] Let G be a graph on $n > 5$ vertices whose distinct Laplacian eigenvalues are $0 < \alpha < \beta < \gamma = n$. Then the multiplicity of β is $n-3$ if and only if G is one of the graphs $K_1 \vee (K_{\frac{n-1}{2}} \cup K_{\frac{n-1}{2}})$, $\overline{K_{\frac{n}{3}}} \vee (K_{\frac{n}{3}} \cup K_{\frac{n}{3}})$, $K_1 \vee (K_1 \cup K_{n-2})$.

In the statement of Lemma 2.2 and later throughout this paper, $G_1 \vee G_2$ denotes the join (complete product) of the graphs G_1 and G_2, namely 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.

Theorem 2.3. Let G be a connected graph of order n with m edges having maximum degree Δ and algebraic connectivity $\mu_{n-1} \geq k$. Then

$$Kf(G) \leq \frac{n(\Delta+1) + nk(n-1) + n^2(n-2) - 2mn}{k(\Delta+1)} \tag{1}$$

with equality if and only if $k = n$ and $G \cong K_n$ or $k = 1$ and $G \cong K_{n-1,1}$.

Proof. Since $\Delta + 1 \leq \mu_1 \leq n$, we have

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

Consider the function

$$f(x) = \frac{n(n-1)}{\Delta+1} + \frac{n^2(n-2) - 2mn + n(\Delta+1)}{(\Delta+1)x} \; , \; k \leq x$$

for which

$$f'(x) = \frac{2mn - n^2(n-2) - n(\Delta+1)}{x^2(\Delta+1)} < 0 \;\; \text{for all } k \leq x$$

i.e., $f(x)$ is decreasing for $k \leq x$. Therefore,

$$f(x) \leq \frac{kn(n-1) + n^2(n-2) - 2mn + n(\Delta+1)}{(\Delta+1)k}$$

implying

$$Kf(G) \leq \frac{n(\Delta+1) + kn(n-1) + n^2(n-2) - 2mn}{(\Delta+1)k} \; .$$

Equality in (1) will occur if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-2} = \mu_{n-1} = k$ and $n = \mu_1 = \Delta + 1$. That is, if G is a join of two graphs with $\mu_1 = \Delta + 1$, having two or three distinct Laplacian eigenvalues. If the former is the case, then by a well known fact,

$G \cong K_n$. If G is a join of two graphs having three distinct Laplacian eigenvalues with $\mu_1 = \Delta + 1$, then by Lemma 2.1, $G \cong K_{n-1,1}$.

Conversely if G is K_n or $K_{n-1,1}$, then it is easy to check that equality holds in (1). □

Theorem 2.4. Let G be a connected graph of order n with m edges having maximum degree Δ and algebraic connectivity $\mu_{n-1} \geq k$. Then

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

with equality if and only if $k = n$ and $G \cong K_n$ or $k = n-2$ and $G \cong K_n - e$.

Proof. Since $\Delta + 1 \leq \mu_1 \leq n$, we have

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i} = \sqrt{\mu_1} + (n-2)\sqrt{\mu_{n-1}} + \sum_{i=2}^{n-2} \frac{\mu_i - \mu_{n-1}}{\sqrt{\mu_i} + \sqrt{\mu_{n-1}}}$$

$$\geq \frac{(n-1)\sqrt{\mu_1\, \mu_{n-1}} + 2m}{\sqrt{\mu_1} + \sqrt{\mu_{n-1}}} \geq \frac{(n-1)\sqrt{\mu_1\, k} + 2m}{\sqrt{\mu_1} + \sqrt{k}} .$$

Consider the function

$$f(x) = \frac{(n-1)\sqrt{xk} + 2m}{\sqrt{x} + \sqrt{k}} \ , \quad \Delta + 1 \leq x \leq n$$

for which

$$f'(x) = \frac{k(n-1) - 2m}{2\sqrt{x}(\sqrt{\mu_1} + \sqrt{k})^2} .$$

As $2m > (n-1)k$, $f(x)' < 0$ and thus $f(x)$ is decreasing for $\Delta + 1 \leq x \leq n$. Consequently,

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

implying

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

Equality in (2) will occur if and only if $n = \mu_1 = \mu_2 = \mu_3 = \cdots = \mu_{n-2}$ and $\mu_{n-1} = k$. That is, if G is a join of two graphs having two or three distinct Laplacian eigenvalues. If the former is the case, then, as before, $G \cong K_n$. If G is a join of two graphs having three distinct Laplacian eigenvalues, then by Lemma 2.1, $G \cong K_n - e$.

Conversely if G is K_n or $K_{n-1,1}$, then it is easy to check that equality holds in (2). □

3 LEL and Kf of some derived graphs

In this section several graphs are encountered, derived from a parent graph G. Their definitions and constructions are outlined in later parts of this section. In order to familiarize the readers with them, in Fig. 1 we provide an illustrative example.

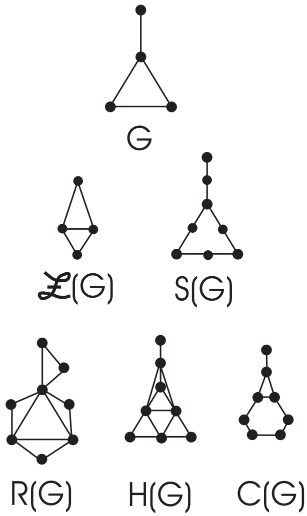

Fig. 1. A (molecular) graph G and some graphs derived from it. $\pounds(G)$ is the line graph of G whereas $S(G)$ is its subdivision graph. Three other, less usual derived graphs are $R(G)$, $H(G)$, and $C(G)$; their definitions are given later in Section 3. As these examples show, all derived graphs preserve the main structural features of the parent graph, often in a one-to-one manner. From the point of view of chemical applications, the structure of a molecule can be represented either by means of the standard molecular graph (in this example, by G) or by any of its derived congeners.

The following results are well known [22, 31].

Lemma 3.1. For a square matrix A, the matrices AA^t and A^tA have the same non-zero eigenvalues.

Lemma 3.2 The spectra of $Q(G)$ and $L(G)$ coincide if and only if G is bipartite.

A bipartite graph G with a bipartition $V(G) = U \cup W$ is said to be (r, s)-semiregular if all vertices in U have degree r and all vertices in W have degree s.

We first investigate the values of LEL and Kf of the line graph $\pounds(G)$ in the case when G is an (r,s)-semiregular graph. Recall that the line graph of a graph G is the graph whose vertex set is in one-to-one correspondence with the set of edges of G where two vertices of the line graph are adjacent if and only if the corresponding edges in G have a vertex in common.

The vertex–edge incidence matrix $I(G) = (b_{ij})$ of a graph G is a $(0,1)$-matrix of order $n \times m$ whose rows and columns are respectively, indexed by the vertices and edges of G, such that $b_{ij} = 1$, if i-th vertex is incident to j-th edge and $b_{ij} = 0$, otherwise.

Denote by $\psi(G,x)$ the Laplacian polynomial $det(xI - L(G))$ of G.

For an (r,s)-semiregular graph G, we can establish the following relationship between $\psi(\pounds(G),x)$ and $\psi(G,x)$.

Lemma 3.3. If G is an (r,s)-regular graph with n vertices and $m = (nrs)/(r+s)$ edges, then

$$\psi(\pounds(G),x) = \big(x-(r+s)\big)^{m-n}\,\psi(G,r+s-x)\ .$$

Proof. Let $I(G)$ be the vertex–edge incidence matrix of the graph G. Then

$$I(G)I(G)^t = Q(G) \qquad \text{and} \qquad I(G)^t\,I(G) = 2I_m + A(\pounds(G)) \tag{3}$$

where I_m is the identity matrix of order m and $Q(G)$ the signless Laplacian matrix.

The line graph $\pounds(G)$ of an (r,s)-semiregular graph G is $(r+s-2)$-regular. Therefore,

$$L(\pounds(G)) = (r+s-2)I_m - A(\pounds(G))\ .$$

Using (3), we have

$$(r+s)I_m - L(\pounds(G)) = I(G)^t\,I(G). \tag{4}$$

It follows from Lemma 3.1 and Eqs. (3) and (4) that $Q(G)$ and $(r+s)I_m - L(\pounds(G))$ have same non-zero eigenvalues. Note that the difference between the dimension of $L(\pounds(G))$ and $Q(G)$ is $m-n$. The proof follows now by Lemma 3.2 and the fact that the leading coefficient of the characteristic polynomial is equal to one. □

By Lemma 3.3, the L-spectrum of an (r,s)-semiregular graph G is

$$\left\{(r+s)^{[m-n]}, r+s-\mu_1, r+s-\mu_2, \ldots, r+s-\mu_n\right\} \tag{5}$$

Theorem 3.4. Let G be an (r,s)-semiregular graph with n vertices. Then

$$LEL(\pounds(G)) \leq \left(\frac{nrs}{r+s} - n + 1\right)\sqrt{r+s} + \sqrt{(n-2)\left[(n-1)(r+s) - \frac{2nrs}{r+s}\right]}$$

with equality if and only if $G \cong K_{n-1,1}$, $n \geq 1$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, n even (≥ 4).

Proof. If m is the number of edges, then $m = nrs/(r+s)$ and $\sum_{i=1}^{n-1} \mu_i = 2m$. Also $\mu_1(G) = r+s$ and $\mu_n(G) = 0$. It follows by (5) and the Cauchy–Schwarz inequality that

$$\begin{aligned}
LEL(\pounds(G)) &= (m-n)\sqrt{r+s} + \sum_{i=1}^{n} \sqrt{r+s-\mu_i} \\
&= (m-n+1)\sqrt{r+s} + \sum_{i=2}^{n-1} \sqrt{r+s-\mu_i} \\
&\leq (m-n+1)\sqrt{r+s} + \sqrt{(n-2)\sum_{i=2}^{n-1}(r+s-\mu_i)} \\
&= (m-n+1)\sqrt{r+s} + \sqrt{(n-2)((n-2)(r+s)-(2m-\mu_1))} \\
&= \left(\frac{nrs}{r+s} - n + 1\right)\sqrt{r+s} + \sqrt{(n-2)\left[(n-1)(r+s) - \frac{2nrs}{r+s}\right]} .
\end{aligned}$$

Equality occurs if and only if $r+s = \mu_1$ and $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$. Since G is (r,s)-semiregular, by Lemma 2.1, G is either $K_{n-1,1}$ or $K_{\frac{n}{2},\frac{n}{2}}$. Conversely it is easy to see that if G is $K_{n-1,1}$ or $K_{\frac{n}{2},\frac{n}{2}}$, then equality holds. □

Since $r+s = \mu_1 \geq \mu_2$ implies $k \geq 1$ for the graph $\pounds(G)$, we have the following observation whose proof follows from Theorem 2.4.

Corollary 3.5. Let G be an (r,s)-semiregular graph with n vertices. Then

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

with equality if and only if $G \cong K_{n-1,1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, n even (≥ 4).

Lemma 3.6. [50] Let G be a connected graph with $n \geq 2$ vertices and vertex degrees $d_i = d(v_i)$, $i = 1, 2, \ldots, n$. Then

$$Kf(G) \geq -1 + (n-1)\sum_{i=1}^{n} \frac{1}{d_i}$$

with equality if and only if $G \cong K_n$ or $G \cong K_{t,n-t}$, $1 \le t \le \lfloor n/2 \rfloor$.

Theorem 3.7. Let G be an (r,s)-semiregular graph with n vertices. Then

$$Kf(\pounds(G)) \ge \frac{m(m+n-1)}{r+s} + \frac{m(n-2)^2}{(n-1)(r+s)-2m}$$

with equality if and only if $G \cong K_{n-1,1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Let $m = nrs/(r+s)$ be the number of edges of G. Since $\mu_1(G) = r+s$ and $\mu_n(G) = 0$, by (5) we get

$$\begin{aligned} Kf(\pounds(G)) &= \frac{m(m-n+1)}{r+s} + m\sum_{i=2}^{n-1} \frac{1}{r+s-\mu_i} \\ &\ge \frac{m(m-n+1)}{r+s} + \frac{m(n-2)^2}{\sum\limits_{i=2}^{n-1}(r+s-\mu_i)} \\ &= \frac{m(m-n+1)}{r+s} + \frac{m(n-2)^2}{(n-1)(r+s)-2m} . \end{aligned}$$

Equality occurs if and only if $r+s = \mu_1$ and $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$. By Lemma 2.1, then G is either $K_{n-1,1}$ or $K_{\frac{n}{2},\frac{n}{2}}$. □

Since for the graph $\pounds(G)$ we have $k \ge 1$, we arrive at:

Corollary 3.8.

$$Kf(\pounds(G)) \le n + \frac{n^3 - n^2 - n - 2mn}{r+1}$$

with equality if and only if $G \cong K_{n-1,1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

For a graph G, the para-line graph, denoted by $C(G)$, is defined as the line graph of the subdivision graph $S(G)$. (Recall that the subdivision graph $S(G)$ of a graph G is obtained by inserting a vertex to every edge of G.) The concept of the para-line graph (or clique-inserted graph [47]) was first introduced by Shirai [37], who obtained the spectrum of the para-line graph of a regular graph G with infinite number of vertices in terms of the spectrum of G. Since the subdivision graph of an r-regular graph is $(r,2)$-semiregular, the para-line graph of an r-regular graph is the line graph of an $(r,2)$-semiregular graph. It is clear that the para-line graph of an r-regular graph is an r-regular graph.

Lemma 3.9. If G is an r-regular with n vertices, then

$$\psi(C(G),x) = (-1)^m \left(x-(r+2)\right)^{m-n} (x-r)^{m-n}\, \psi(G, x(r+2-x)) .$$

Proof. The subdivision graph $S(G)$ is an $(r,2)$-semiregular graph with $n+\frac{nr}{2}$ vertices and nr edges. By Lemma 3.3,

$$\psi(C(G),x)=\big(x-(r+2)\big)^{m-n}\,\psi(S(G),r+2-x). \tag{6}$$

It is known [24] that

$$\psi(S(G),x)=(-1)^m\,(2-x)^{m-n}\,\psi(G,x(r+2-x))\ .$$

Therefore

$$\psi(S(G),r+2-x)=(-1)^m\,(x-r)^{m-n}\,\psi(G,x(r+2-x))$$

which combined with Eq. (6) yields

$$\psi(C(G),x)=(-1)^m\,(x-(r+2))^{m-n}\,(x-r)^{m-n}\,\psi(G,x(r+2-x))\ .$$

□

By Lemma 3.9, the L-spectrum of $C(G)$ is

$$\left\{(r+2)^{[m-n]}\,,\ r^{[m-n]}\,,\ \frac{(r+2)\pm\sqrt{(r+2)^2-4\mu_i}}{2}\,,\ i=1,2,\cdots,n\right\}. \tag{7}$$

Theorem 3.10. Let G be a connected r-regular graph with n vertices. Then

$$(m-n)\sqrt{r}+m\sqrt{r+2}<LEL(C(G))\leq(m-1)\sqrt{r}+(m-n+1)\sqrt{r+2}+(n-1)\sqrt{2}$$

with equality on the right if and only if $G\cong K_2$.

Proof. By (7) and the fact that $\mu_i=r-\lambda_{n+i-1}\,,\ i=1,2,\ldots,n$, and that $\lambda_1=r$, we get

$$\begin{aligned}LEL(C(G)) &= (m-n)\sqrt{r}+(m-n+1)\sqrt{r+2}\\ &+\sum_{i=2}^{n}\left(\sqrt{\frac{1}{2}\left[(r{+}2){+}\sqrt{r^2{+}4\lambda_i{+}4}\right]}+\sqrt{\frac{1}{2}\left[(r{+}2){-}\sqrt{r^2{+}4\lambda_i{+}4}\right]}\right).\end{aligned}$$

By the Perron–Frobenius theorem, $-r\leq\lambda_i<r$, for $i=2,3,\ldots,n$. For $-r\leq x<r$, consider the function

$$f(x)=\sqrt{\frac{1}{2}\left[(r+2)+\sqrt{r^2+4x+4}\right]}+\sqrt{\frac{1}{2}\left[(r+2)-\sqrt{r^2+4x+4}\right]}\ .$$

It can be seen that $f'(x) < 0$ for all $-r \leq x < r$. That is, $f(x)$ is decreasing for $-r \leq x < r$. Therefore $f(r) < f(x) \leq f(-r)$, that is, $\sqrt{r+2} < f(x) \leq \sqrt{r} + \sqrt{2}$. This gives

$$LEL(C(G)) > (m-n)\sqrt{r} + (m-n+1)\sqrt{r+2} + \sum_{i=2}^{n} \sqrt{r+2}$$
$$= (m-n)\sqrt{r} + m\sqrt{r+2}$$

and

$$LEL(C(G)) \leq (m-n)\sqrt{r} + (m-n+1)\sqrt{r+2} + \sum_{i=2}^{n} \sqrt{r} + \sqrt{2}$$
$$= (m-1)\sqrt{r} + (m-n+1)\sqrt{r+2} + (n-1)\sqrt{2}\,.$$

Equality will occur on the right if and only if G is a regular graph and $\lambda_1 = r, \lambda_2 = \lambda_3 = \cdots = \lambda_n = -r$. That is, if and only if G is a regular graph with two distinct adjacency eigenvalues r and $-r$ with multiplicities 1 and $n-1$, respectively. Therefore, G must be a complete graph. Note that the sum of the adjacency eigenvalues of G is equal to zero; that is, $r + (n-1)(-r) = 0$. This implies that G is a complete graph with two vertices, i.e., $G \cong K_2$. □

Theorem 3.11. If G is a connected r-regular graph with n vertices, then

$$Kf(C(G)) = n\left(\frac{nr}{2} - n\right) + \frac{nr(\frac{nr}{2} - n)}{r+2} + r(r+2)Kf(G)\,.$$

Proof. Let $C(G)$ be the para-line graph of the r-regular graph G having n vertices and $m = nr/2$ edges. Then the number of vertices of $C(G)$ is nr. Therefore by (7),

$$Kf(C(G)) = nr\frac{m-n}{r} + nr\frac{m-n}{r+2} + nr\sum_{i=1}^{n-1} \frac{2}{(r+2) + \sqrt{(r+2)^2 - 4\mu_i}}$$
$$+ nr\sum_{i=1}^{n-1} \frac{2}{(r+2) - \sqrt{(r+2)^2 - 4\mu_i}}$$
$$= n(m-n) + \frac{nr(m-n+1)}{r+2} + nr\sum_{i=1}^{n-1} \frac{r+2}{\mu_i}$$
$$= n\left(\frac{nr}{2} - n\right) + \frac{nr(\frac{nr}{2} - n + 1)}{r+2} + r(r+2)Kf(G).$$

□

The following is an immediate consequence of Theorem 3.11 and Lemma 3.6.

Corollary 3.12. Let G be a connected r-regular graph with n vertices. Then

$$Kf(C(G)) \geq n(m-n) + \frac{nr(m-n)}{r+2} + (n^2-n-r)(r+2)$$

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

For a graph G with vertex set $V(G)$ and edge set $E(G)$, let $R(G)$ be the graph obtained by adding a vertex e' corresponding to the edge $e = uv$ of the graph G and by joining each new vertex e' to the end vertices u and v of the corresponding edge $e = uv$. That is, $R(G)$ is obtained from G by replacing each edge $e = uv$ of G by a triangle uev.

Lemma 3.13. [40] If G is an r-regular graph ($r \neq 2$) with n vertices and m-edges, then

$$\psi(R(G),x) = (x-2)^{m-n}\,(x-3)^n\,\psi\left(G, \frac{x(x-r-2)}{x-3}\right).$$

By Lemma 3.13, the L-spectrum of $R(G)$ is

$$\left\{ 2^{[m-n]}, \frac{(\mu_i+r+2)+\sqrt{(\mu_i+r+2)^2-12\mu_i}}{2}, \frac{(\mu_i+r+2)-\sqrt{(\mu_i+r+2)^2-12\mu_i}}{2} \right\} \tag{8}$$

where $i = 1,2,\ldots,n$.

Theorem 3.14. Let G be an r-regular graph ($r \neq 2$) with n vertices and $m = nr/2$ edges. Then

$$n\sqrt{r+2} + \frac{n(r-2)}{\sqrt{2}} < LEL(R(G)) \leq (n-1)(\sqrt{3r}+\sqrt{2}) + \sqrt{r+2} + \frac{n(r-2)}{\sqrt{2}}$$

with equality on the right if and only if $G \cong K_2$.

Proof. By (8) and the fact that $\mu_i = r - \lambda_{n+i-1}$, $i = 1,2,\ldots,n$, and $\lambda_1 = r$,

$$\begin{aligned} LEL(R(G)) &= (m-n)\sqrt{2} + \sqrt{r+2} \\ &+ \sum_{i=2}^{n} \sqrt{\frac{1}{2}\left[(2r+2-\lambda_i) + \sqrt{\lambda_i^2 - 4(r-2)\lambda_i + 4(r^2-r+1)}\right]} \\ &+ \sum_{i=2}^{n} \sqrt{\frac{1}{2}\left[(2r+2-\lambda_i) - \sqrt{\lambda_i^2 - 4(r-2)\lambda_i + 4(r^2-r+1)}\right]}\,. \end{aligned}$$

By the Perron–Frobenius Theorem, $-r \le \lambda_i < r$, for $i = 2, 3, \ldots, n$. Now, for $-r \le x < r$, consider the function

$$\begin{aligned} f(x) &= \sqrt{\frac{1}{2}\left[(2r+2-x) + \sqrt{x^2 - 4(r-2)x + 4(r^2-r+1)}\right]} \\ &+ \sqrt{\frac{1}{2}\left[(2r+2-x) - \sqrt{x^2 - 4(r-2)x + 4(r^2-r+1)}\right]}\,. \end{aligned}$$

It is easy to see that $f'(x) < 0$ for all $-r \le x < r$. That is, the function $f(x)$ is decreasing for $-r \le x < r$. Therefore $f(r) < f(x) \le f(-r)$, that is, $\sqrt{r+2} < f(x) \le \sqrt{3r} + \sqrt{2}$. This gives

$$LEL(R(G)) > (m-n)\sqrt{2} + \sqrt{r+2} + \sum_{i=2}^{n} \sqrt{r+2} = n\sqrt{r+2} + \frac{n(r-2)}{\sqrt{2}}$$

and

$$\begin{aligned} LEL(R(G)) &\le (m-n)\sqrt{2} + \sqrt{r+2} + \sum_{i=2}^{n} (\sqrt{3r} + \sqrt{2}) \\ &= (n-1)(\sqrt{3r} + \sqrt{2}) + \sqrt{r+2} + \frac{n(r-2)}{\sqrt{2}}\,. \end{aligned}$$

Proceeding similarly as in Theorem 3.10, it can be seen that equality occurs if and only if $G \cong K_2$. □

Wang, Yang, and Luo [40] considered the Kirchhoff index of the graph $R(G)$ and found a lower bound (Theorem 3.14, in [40]). We now obtain the same lower bound by a new and simpler proof.

Theorem 3.15. Let G be a connected r-regular ($r \ne 2$) graph with n vertices. Then

$$Kf(R(G)) \ge \frac{(n^2-n)(r+2)^2}{6r} + \frac{(n^2-n-r-2)(r+2)}{6} + \frac{n^2(r^2-4)}{8} + \frac{n}{2}$$

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

Proof. Let m' and n' be, respectively, the number of edges and vertices of $R(G)$. Then $m' = 3m = \frac{3nr}{2}$ and $n' = m + n = \frac{n(r+2)}{2}$, where n and m are the number of vertices and number of edges of the parent graph G. We then have

$$\begin{aligned} Kf(R(G)) &= (m+n)\frac{1}{r+2} + (m+n)\frac{m-n}{2} \\ &+ (m+n)\sum_{i=1}^{n-1} \frac{2}{(\mu_i + r + 2) + \sqrt{(\mu_i + r + 2)^2 - 12\mu_i}} \end{aligned}$$

$$\begin{aligned}
&+ \quad (m+n)\sum_{i=1}^{n-1}\frac{2}{(\mu_i+r+2)-\sqrt{(\mu_i+r+2)^2-12\mu_i}}\\
&= \quad (m+n)\frac{1}{r+2}+(m+n)\frac{m-n}{2}+(m+n)\sum_{i=1}^{n-1}\frac{\mu_i+r+2}{3\mu_i}\\
&= \quad (m+n)\frac{1}{r+2}+(m+n)\frac{m-n}{2}+(m+n)\frac{n-1}{3}+(m+n)\frac{r+2}{3n}Kf(G)\\
&= \quad \frac{(r+2)^2}{6}Kf(G)+\frac{(n^2-n)(r+2)}{6}+\frac{n^2(r^2-4)}{8}+\frac{n}{2}\,.
\end{aligned}$$

Using Lemma 3.6, the result follows. □

Theorem 3.16. Let G be a connected r-regular graph with n vertices and with second smallest Laplacian eigenvalue $\mu_{n-1} \leq [k^2 - k(r+2)]/(k-3)$. Then

$$Kf(R(G)) \leq \frac{2nr + nk(n-1) + n^2(n-2) - 2mn}{2kr}$$

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

Proof. Theorem 3.16 follows from Theorem 2.3 and the fact that $\Delta(R(G)) = 2r$. □

For a graph G with vertex set $V(G)$ and edge set $E(G)$, let $H(G)$ be the graph obtained by inserting a new vertex e' onto each edge $e = uv$ of G and joining two new vertices if they lie on adjacent edges of G.

Lemma 3.17. [40] Let G be an r-regular graph with n vertices and $m = nr/2$ edges. Then

$$\psi(H(G),x) = (-1)^m\,(r+1-x)^n\left(\frac{x^2-(3r+2)x+2r(r+1)}{r-x}\right)^{m-n}\psi\left(G,\frac{x(r+2-x)}{r+i-x}\right)\,.$$

By Lemma 3.17, the L-spectrum of $H(G)$ is

$$\left\{(2r+2)^{m-n}\ ,\ \frac{1}{2}\left[(\mu_i+r+2)+\sqrt{(\mu_i+r+2)^2-4\mu_i(r+1)}\right]\ ,\right.$$

$$\left.\frac{1}{2}\left[(\mu_i+r+2)-\sqrt{(\mu_i+r+2)^2-4\mu_i(r+2)}\right]\right\} \tag{9}$$

where $i = 1, 2, \ldots, n$.

Theorem 3.18. Let G be a connected r-regular graph with n vertices and $m = nr/2$ edges. Then

$$n\sqrt{r+2}+\frac{n(r-2)\sqrt{2r+2}}{2} < LEL(H(G)) \leq (n-1)\sqrt{r}+\sqrt{r+2}+\frac{(nr-2)\sqrt{2r+2}}{2}$$

with equality on the right if and only if $G \cong K_2$.

Proof. By (9) and the fact that $\mu_i = r - \lambda_{n+i-1}$, $i = 1, 2, \ldots, n$, and $\lambda_1 = r$,

$$
\begin{aligned}
LEL(H(G)) &= (m-n)\sqrt{2r+2} + \sqrt{r+2} + \sum_{i=2}^{n} \sqrt{\frac{1}{2}\left[(2r+2-\lambda_i)+\sqrt{\lambda_i^2+4r+4}\right]} \\
&+ \sum_{i=2}^{n} \sqrt{\frac{1}{2}\left[(2r+2-\lambda_i)+\sqrt{\lambda_i^2+4r+4}\right]}.
\end{aligned}
$$

The result is now obtained by proceeding similarly as in Theorem 3.10. □

The Kirchhoff index of the graph $H(G)$ was examined in [40] and the following lower bound was obtained (Theorem 3.4. in [40]). Here we provide a simpler proof.

Theorem 3.19. [40] Let G be a connected r-regular graph with n vertices and $m = nr/2$ edges. Then

$$
Kf(H(G)) \geq \frac{(r+2)^2\,(n^2-n)}{2r(r+1)} + \frac{(r+2)^2\,(n^2-4)-4n}{8(r+1)}
$$

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

Proof. Let n' and m' be respectively, the number of vertices and edges of $H(G)$. Then $n' = m + n = n(r+2)/2$ and $m' = nr^2/2$. Using (9) we get

$$
\begin{aligned}
Kf(H(G)) &= (m+n)\,\frac{m-n}{2r+2} + (m+n)\,\frac{1}{r+2} + (m+n) \\
&+ (m+n)\sum_{i=1}^{n-1} \frac{2}{(\mu_i+r+2)+\sqrt{(\mu_i+r+2)^2-4\mu_i(r+1)}} \\
&+ (m+n)\sum_{i=1}^{n-1} \frac{2}{(\mu_i+r+2)-\sqrt{(\mu_i+r+2)^2-4\mu_i(r+1)}} \\
&= (m+n)\frac{1}{r+2} + (m+n)\frac{m-n}{2} + (m+n)\sum_{i=1}^{n-1}\frac{\mu_i+r+2}{\mu_i(r+1)} \\
&= (m+n)\frac{1}{r+2} + (m+n)\frac{m-n}{2} + (m+n)\frac{n-1}{r+1} \\
&+ (m+n)\frac{r+2}{n(r+1)}Kf(G) = \frac{(r+2)^2}{2(r+1)}Kf(G) + \frac{n^2(r+2)^2-4n}{8(r+1)}\ .
\end{aligned}
$$

The result follows by using Lemma 3.6. □

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