



## REMARKS ON “COMPARISON BETWEEN THE LAPLACIAN ENERGY-LIKE INVARIANT AND THE KIRCHHOFF INDEX”\*

XIAODAN CHEN<sup>†</sup> AND GUOLIANG HAO<sup>‡</sup>

**Abstract.** The Laplacian-energy-like invariant and the Kirchhoff index of an  $n$ -vertex simple connected graph  $G$  are, respectively, defined to be  $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$  and  $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$ , where  $\mu_1, \mu_2, \dots, \mu_{n-1}, \mu_n = 0$  are the Laplacian eigenvalues of  $G$ . In this paper, some results in the paper [Comparison between the Laplacian-energy-like invariant and the Kirchhoff index. *Electron. J. Linear Algebra* 31:27–41, 2016] are corrected and improved.

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

**AMS subject classifications.** 05C50, 15A18.

**1. Introduction.** All graphs considered in this paper are finite, undirected, and simple. Let  $G$  be a graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ , where  $|E(G)| = m$ . Denote by  $\Delta(G)$  and  $\delta(G)$  the maximum degree and the minimum degree of  $G$ , respectively. A graph  $G$  is  $r$ -regular if  $\Delta(G) = \delta(G) = r$ . The adjacency matrix of  $G$  is  $A(G) = [a_{ij}]_{n \times n}$ , where elements  $a_{ij} = 1$  if the vertices  $v_i$  and  $v_j$  in  $G$  are adjacent, and  $a_{ij} = 0$  otherwise. The Laplacian matrix of  $G$  is defined to be  $L(G) = D(G) - A(G)$ , where  $D(G)$  is the diagonal matrix of vertex degrees of  $G$ . The Laplacian spectrum of  $G$  is  $\text{Spec}_L(G) = \{\mu_1(G), \mu_2(G), \dots, \mu_n(G)\}$ , where  $\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_n(G)$  are the eigenvalues of  $L(G)$  (usually known as the Laplacian eigenvalues of  $G$ ), arranged in nonincreasing order. If the eigenvalue  $\mu_i(G)$  appears  $t_i > 1$  times in  $\text{Spec}_L(G)$ , we write as  $\mu_i(G)^{(t_i)}$  in it for convenience. It is well known [8] that  $\mu_n(G) = 0$  and,  $\mu_{n-1}(G) > 0$  if and only if  $G$  is connected.

The Laplacian-energy-like invariant and the Kirchhoff index of a connected graph  $G$  are defined, respectively, as

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i(G)} \quad \text{and} \quad Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i(G)}.$$

These two Laplacian-spectrum-based invariants, as molecular structure descriptors, have been found noteworthy applications in chemistry [7, 11, 12, 18, 28], and many of their mathematical properties have been established [2, 5, 6, 9, 17, 19, 21, 22, 26, 27, 29, 30, 31, 33, 35, 36].

In [5], Das, Xu and Gutman compared  $LEL(G)$  and  $Kf(G)$  and established several sufficient conditions for  $LEL(G) < Kf(G)$ . They also showed that, if  $m \geq n(n-1)/2 - 4$ , then  $LEL(G) > Kf(G)$ , where  $m$  is the number of edges in  $G$ ; but this condition was far from optimal. Hence, they further posed the following problem:

---

\*Received by the editors on July 17, 2016. Accepted for publication on January 11, 2022. Handling Editor: Bryan Shader. Corresponding Author: Xiaodan Chen.

This work was supported by the National Natural Science Foundation of China (Nos. 11861011 and 12061007) and by the special foundation for Guangxi Ba Gui Scholars.

<sup>†</sup>College of Mathematics and Information Science, Guangxi University, Nanning 530004, P.R. China; Guangxi Center for Mathematical Research, Guangxi University, Nanning 530004, P.R. China ([x.d.chen@live.cn](mailto:x.d.chen@live.cn)).

<sup>‡</sup>College of Science, East China University of Technology, Nanchang 330013, P.R. China ([guoliang-hao@163.com](mailto:guoliang-hao@163.com)).

PROBLEM 1 ([5]). *Is it possible to find a constant  $c$  (which may depend on the number of vertices and maximum vertex degree), such that for any connected graph  $G$  with  $m \geq c$  edges,  $LEL(G) > Kf(G)$ ?*

Motivated by the above problem, the authors of [27] examined sufficient conditions for  $LEL(G) > Kf(G)$ .

THEOREM 2 ([27]). *Let  $G$  be a connected graph with algebraic connectivity  $\mu_{n-1} \geq k$  and let  $m$  be the number of edges and  $\Delta$  the maximum degree of  $G$ . If*

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

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

In particular, if  $\mu_{n-1} \geq 1$ , then the next corollary follows immediately, which can be seen as a partial solution to Problem 1.

COROLLARY 3 ([27]). *Let  $G$  be a connected graph with algebraic connectivity  $\mu_{n-1} \geq 1$ . Let  $m$  be the number of edges and  $\Delta$  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  $LEL(G) > Kf(G)$ .

Furthermore, using Theorem 2, the authors of [27] proved that the inequality  $LEL > Kf$  holds for the complements of trees, unicyclic graphs, bicyclic graphs, tricyclic graphs, and tetracyclic graphs.

COROLLARY 4 ([27]). *Let  $T$  be a tree and  $\bar{T}$  be its complement. If the order of  $T$  is  $n \geq 7$  and  $\Delta(T) \leq n - 2$ , then  $LEL(\bar{T}) > Kf(\bar{T})$ .*

COROLLARY 5 ([27]). *Let  $U$  be a unicyclic graph and  $\bar{U}$  be its complement. If the order of  $U$  is  $n \geq 14$  and  $\Delta(U) \leq n - 2$ , then  $LEL(\bar{U}) > Kf(\bar{U})$ .*

COROLLARY 6 ([27]). *Let  $B$  be a bicyclic graph and  $\bar{B}$  be its complement. If the order of  $B$  is  $n \geq 15$  and  $\Delta(B) \leq n - 2$ , then  $LEL(\bar{B}) > Kf(\bar{B})$ .*

COROLLARY 7 ([27]). *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  $LEL(\overline{TC}) > Kf(\overline{TC})$ .*

COROLLARY 8 ([27]). *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  $LEL(\overline{QC}) > Kf(\overline{QC})$ .*

However, it is unfortunate that Corollary 4 is incorrect. As a counterexample, we consider the tree  $T^*$  with 7 vertices obtained from the star  $K_{5,1}$  by attaching a pendent edge to one of its vertices of degree 1. Clearly, we have  $\Delta(T^*) = 5 = n - 2$ . Now, by the software ‘Mathematica’, we get  $\text{Spec}_L(T^*) = \{6.5341, 6, 6, 6, 4.5173, 0.9486, 0\}$  (up to four decimal places), and thus  $LEL(T^*) \approx 13.0040 < 13.5000 \approx Kf(T^*)$ .

In fact, in the original proof of Corollary 4, the authors of [27] claimed that for any tree  $T$  of order  $n$ , if  $\Delta(T) \leq n - 2$ , then  $\mu_1(T) \leq n - 2$  (as  $T \neq K_{n-1,1}$ ). This is not true. As shown in Lemma 11 below, there are still some other trees  $T$  with  $\mu_1(T) > n - 2$  other than the star  $K_{n-1,1}$ . Similar errors also appear in the original proofs of Corollaries 5, 6, and 7.

In this paper, we first make a slight improvement on Theorem 2. Based on this result, we give a corrected version of Corollary 4 and its proof; we also provide correct proofs for Corollaries 5, 6, and 7. Finally, we present several new sufficient conditions for  $LEL(G) > Kf(G)$ , some of which improve the results in [27]; in particular, we provide a complete (but not the best possible) solution to Problem 1.

**2. Main results.** We first give some known results that will be used later.

PROPOSITION 9.

- (i) ([25]) Let  $G$  be a graph of order  $n$  and  $\bar{G}$  be its complement. Then  $\text{Spec}_L(\bar{G}) = \{n - \mu_{n-1}(G), n - \mu_{n-2}(G), \dots, n - \mu_1(G), 0\}$ .
- (ii) ([1]) For any graph  $G$  of order  $n$ ,  $\mu_1(G) \leq n$  with equality if and only if  $\bar{G}$  is disconnected.
- (iii) ([10]) Let  $G$  be a graph with at least one edge. Then  $\mu_1(G) \geq \Delta(G) + 1$ . Moreover, if  $G$  is connected, then the equality holds if and only if  $\Delta(G) = n - 1$ .
- (iv) ([8]) For any non-complete graph of order  $n$ ,  $\mu_{n-1}(G) \leq \delta(G)$ .
- (v) ([8]) For any graph  $G$  of order  $n$ ,  $\mu_{n-1}(G) \geq 2\delta(G) - n + 2$ .
- (vi) ([3]) If  $G$  is a graph of order  $n \geq 3$  with  $m$  edges, then  $\mu_{n-1}(G) \geq 2m - (n - 2)(\Delta(G) + 1)$ .
- (vii) ([4]) If  $G$  is a graph of order  $n$  with at least one edge, then  $\mu_1(G) = \mu_2(G) = \dots = \mu_{n-1}(G)$  if and only if  $G = K_n$ .

For a square matrix  $M$ , denote by  $\Phi(M, x)$  (or simply,  $\Phi(M)$ ) the characteristic polynomial of  $M$ , i.e.,  $\Phi(M, x) = \det(xI - M)$ . For a vertex  $v \in V(G)$ , let  $L_v(G)$  be the principal sub-matrix of  $L(G)$  obtained by deleting the row and column corresponding to the vertex  $v$ . The following result, due to Guo [14], is usually used to calculate the Laplacian characteristic polynomial of a graph.

LEMMA 10 ([14]). If  $G = G_1u : vG_2$  is the graph obtained by joining the vertex  $u$  of the graph  $G_1$  to the vertex  $v$  of the graph  $G_2$  by an edge, where  $G_1$  and  $G_2$  are vertex-disjoint, then

$$\Phi(L(G)) = \Phi(L(G_1))\Phi(L(G_2)) - \Phi(L(G_1))\Phi(L_v(G_2)) - \Phi(L(G_2))\Phi(L_u(G_1)).$$

Let  $\mathcal{T}(n)$ ,  $\mathcal{U}(n)$ ,  $\mathcal{B}(n)$ , and  $\mathcal{TC}(n)$  denote the sets of all trees, unicyclic graphs, bicyclic graphs, and tricyclic graphs of order  $n$ , respectively.

LEMMA 11 ([34, 13, 32]). For  $n \geq 8$ , if  $T \in \mathcal{T}(n) \setminus \{K_{n-1,1}, T_2, T_3, T_4, T_5\}$ , then  $\mu_1(T) \leq n - 2$ , where  $T_2, T_3, T_4$ , and  $T_5$  are shown in Fig. 1.

LEMMA 12 ([15, 24]). For  $n \geq 10$ , if  $U \in \mathcal{U}(n) \setminus \{U_1, U_2, U_3, U_4\}$ , then  $\mu_1(U) \leq n - 1$ , where  $U_1, U_2, U_3$ , and  $U_4$  are shown in Fig. 2.

LEMMA 13 ([16, 20]). For  $n \geq 11$ , if  $B \in \mathcal{B}(n) \setminus \{B_1, B_2, \dots, B_{11}\}$ , then  $\mu_1(B) \leq n - 1$ , where  $B_1, B_2, \dots, B_{11}$  are shown in Fig. 3.

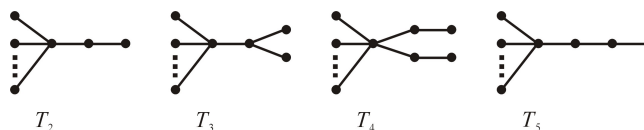


FIGURE 1. The trees  $T_2, T_3, T_4$ , and  $T_5$ .



FIGURE 2. The unicyclic graphs  $U_1, U_2, U_3$ , and  $U_4$ .

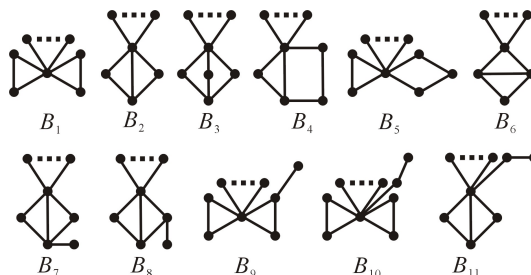


FIGURE 3. The bicyclic graphs  $B_1, B_2, \dots, B_{11}$ .

LEMMA 14 ([23]). For  $n \geq 11$ , if  $H \in \mathcal{TC}(n) \setminus (\mathcal{S}(n, 3) \cup \{H_1, H_2, \dots, H_{27}\})$ , then  $\mu_1(H) \leq n - 1$ , where  $\mathcal{S}(n, 3)$  is the class of graphs obtained from the star  $K_{n-1,1}$  by adding 3 edges among its vertices of degree 1, and  $H_1, H_2, \dots, H_{27}$  are shown in [23], Fig. 2.

Now, we are ready to present the main results of this paper.

THEOREM 15. Let  $G$  be a graph of order  $n$  with  $m$  edges and  $\mu_{n-1}(G) \geq k > 0$ . Then  $LEL(G) > Kf(G)$  provided

$$(2.1) \quad 2m > \frac{k(\sqrt{n} + \sqrt{k})}{k + \sqrt{n} + \sqrt{k}} \left( \frac{(n+k)(n-1)}{k} - \frac{(n-1)\sqrt{nk}}{\sqrt{n} + \sqrt{k}} \right).$$

*Proof.* Our proof follows that given for Theorem 1.2 in [27].

$$(2.2) \quad \begin{aligned} LEL(G) &= \sum_{i=1}^{n-1} \sqrt{\mu_i(G)} = \sum_{i=1}^{n-1} (\sqrt{\mu_i(G)} - \sqrt{\mu_{n-1}(G)}) + (n-1)\mu_{n-1}(G) \\ &= \sum_{i=1}^{n-1} \left( \frac{\mu_i(G) - \mu_{n-1}(G)}{\sqrt{\mu_i(G)} + \sqrt{\mu_{n-1}(G)}} \right) + (n-1)\mu_{n-1}(G) \\ &\geq \sum_{i=1}^{n-1} \left( \frac{\mu_i(G) - \mu_{n-1}(G)}{\sqrt{\mu_1(G)} + \sqrt{\mu_{n-1}(G)}} \right) + (n-1)\mu_{n-1}(G) \\ &= \frac{2m + (n-1)\sqrt{\mu_1(G)\mu_{n-1}(G)}}{\sqrt{\mu_1(G)} + \sqrt{\mu_{n-1}(G)}}. \end{aligned}$$

For  $x > 0$ , consider the following function

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

for which

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

Since  $2m = \sum_{i=1}^{n-1} \mu_i(G) \geq (n-1)\mu_{n-1}(G)$ , we have  $f'(x) \leq 0$ , implying that  $f(x)$  is a decreasing function for  $x > 0$ . Thus, noting that  $\mu_1(G) \leq n$  (by Proposition 9(ii)), from (2.2) we obtain

$$(2.3) \quad LEL(G) \geq f(\mu_1(G)) \geq f(n) = \frac{2m + (n-1)\sqrt{n\mu_{n-1}(G)}}{\sqrt{n} + \sqrt{\mu_{n-1}(G)}}.$$

For  $x > 0$ , again consider the following function

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

for which

$$g'(x) = \frac{n(n-1) - 2m}{2\sqrt{x}(\sqrt{n} + \sqrt{x})^2} \geq 0 \quad (\text{as } n(n-1) \geq 2m).$$

Hence,  $g(x)$  is an increasing function for  $x > 0$ , which, together with (2.3), yields

$$(2.4) \quad LEL(G) \geq g(\mu_{n-1}(G)) \geq g(k) = \frac{2m + (n-1)\sqrt{nk}}{\sqrt{n} + \sqrt{k}} \quad (\text{as } \mu_{n-1}(G) \geq k > 0).$$

On the other hand, we have

$$\begin{aligned} Kf(G) &= n \sum_{i=1}^{n-1} \frac{1}{\mu_i(G)} = n \sum_{i=1}^{n-1} \left( \frac{1}{\mu_i(G)} - \frac{1}{\mu_1(G)} \right) + \frac{n(n-1)}{\mu_1(G)} \\ &= n \sum_{i=1}^{n-1} \left( \frac{\mu_1(G) - \mu_i(G)}{\mu_1(G)\mu_i(G)} \right) + \frac{n(n-1)}{\mu_1(G)} \\ &\leq n \sum_{i=1}^{n-1} \left( \frac{\mu_1(G) - \mu_i(G)}{\mu_1(G)\mu_{n-1}(G)} \right) + \frac{n(n-1)}{\mu_1(G)} \\ (2.5) \quad &= \frac{n[(n-1)(\mu_1(G) + \mu_{n-1}(G)) - 2m]}{\mu_1(G)\mu_{n-1}(G)}. \end{aligned}$$

For  $x > 0$ , consider the following function

$$h(x) = \frac{(n-1)(x + \mu_{n-1}(G)) - 2m}{x\mu_{n-1}(G)},$$

for which

$$h'(x) = \frac{2m - (n-1)\mu_{n-1}(G)}{x^2\mu_{n-1}(G)} \geq 0.$$

Hence,  $h(x)$  is an increasing function for  $x > 0$ , which, together with (2.5), yields

$$(2.6) \quad \begin{aligned} Kf(G) &\leq nh(\mu_1(G)) \leq nh(n) = \frac{n(n-1) - 2m}{\mu_{n-1}(G)} + n - 1 \quad (\text{as } \mu_1(G) \leq n) \\ &\leq \frac{n(n-1) - 2m}{k} + n - 1 \quad (\text{as } \mu_{n-1}(G) \geq k > 0). \end{aligned}$$

Now, from the given condition (2.1), it follows that

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

which, together with (2.4) and (2.6), immediately yields  $LEL(G) > Kf(G)$ .  $\square$

REMARK 16. Noting that  $\Delta(G) + 1 \leq n$  always holds for a graph  $G$  of order  $n$ , one can see that Theorem 15 is indeed an improvement on Theorem 2.

The next result is a corrected version of Corollary 4, where the original condition “ $n \geq 7$ ” is revised to “ $n \geq 8$ ”, and the new proof is also given based on Theorem 15.

COROLLARY 17. *Let  $T$  be a tree of order  $n$  and  $\bar{T}$  be its complement. If  $n \geq 8$  and  $\Delta(T) \leq n - 2$ , then  $LEL(\bar{T}) > Kf(\bar{T})$ .*

*Proof.* If  $T \in \mathcal{T}(n) \setminus \{K_{n-1,1}, T_2, T_3, T_4, T_5\}$ , by Lemma 11, we have  $\mu_1(T) \leq n - 2$  and then, by Proposition 9(i), we obtain  $\mu_{n-1}(\bar{T}) = n - \mu_1(T) \geq 2$ . Note that

$$2|E(\bar{T})| = (n-1)(n-2) > \frac{2(\sqrt{n} + \sqrt{2})}{\sqrt{n} + 2 + \sqrt{2}} \left( \frac{(n+2)(n-1)}{2} - \frac{(n-1)\sqrt{2n}}{\sqrt{n} + \sqrt{2}} \right),$$

provided  $n + \sqrt{2n} > 2\sqrt{n} + 2 + 2\sqrt{2}$ , which is true for  $n \geq 8$ . Hence, by Theorem 15,  $LEL(\bar{T}) > Kf(\bar{T})$ .

Otherwise, since  $\Delta(T) \leq n - 2$ , we have  $T \neq K_{n-1,1}$ . It now suffices to show that  $LEL(\bar{T}_i) > Kf(\bar{T}_i)$  for  $i \in \{2, 3, 4, 5\}$ . By Lemma 10 and a direct calculation, we get

$$\begin{aligned} \Phi(L(T_2), x) &= x(x-1)^{n-4} [x^3 - (n+2)x^2 + (3n-2)x - n], \\ \Phi(L(T_3), x) &= x(x-1)^{n-4} [x^3 - (n+2)x^2 + (4n-7)x - n], \\ \Phi(L(T_4), x) &= x(x-1)^{n-6} (x^2 - 3x + 1) [x^3 - (n+1)x^2 + (3n-5)x - n], \\ \Phi(L(T_5), x) &= x(x-1)^{n-5} [x^4 - (n+3)x^3 + (5n-4)x^2 - (6n-10)x + n], \end{aligned}$$

from which we obtain

$$\begin{aligned} \text{Spec}_L(T_2) &= \{\alpha_1, \alpha_2, 1^{(n-4)}, \alpha_3, 0\}, \\ \text{Spec}_L(T_3) &= \{\beta_1, \beta_2, 1^{(n-4)}, \beta_3, 0\}, \\ \text{Spec}_L(T_4) &= \{\gamma_1, \gamma_2, \gamma_3, \gamma_4, 1^{(n-6)}, \gamma_5, 0\}, \\ \text{Spec}_L(T_5) &= \{\theta_1, \theta_2, \theta_3, 1^{(n-5)}, \theta_4, 0\}, \end{aligned}$$

where  $\alpha_1 \geq \alpha_2 \geq \alpha_3$ ,  $\beta_1 \geq \beta_2 \geq \beta_3$ ,  $\gamma_1 \geq \gamma_2 \geq \gamma_3 \geq \gamma_4 \geq \gamma_5$ , and  $\theta_1 \geq \theta_2 \geq \theta_3 \geq \theta_4$  are, respectively, the zeros of the functions

$$\begin{aligned} f_2(x) &= x^3 - (n+2)x^2 + (3n-2)x - n, \\ f_3(x) &= x^3 - (n+2)x^2 + (4n-7)x - n, \\ f_4(x) &= (x^2 - 3x + 1)[x^3 - (n+1)x^2 + (3n-5)x - n], \\ f_5(x) &= x^4 - (n+3)x^3 + (5n-4)x^2 - (6n-10)x + n. \end{aligned}$$

Moreover, we have  $n-1 < \alpha_1 < n$  (by Proposition 9(ii) and (iii)),  $0 < \alpha_3 \leq 1$  (by Proposition 9(iv)), and  $1 < \alpha_2 < 3$  (as  $\alpha_1 + \alpha_2 + \alpha_3 + (n-4) = 2(n-1)$ ); similarly, it is not difficult to verify that  $n-2 < \beta_1 < n$ ,  $0 < \beta_3 \leq 1$ , and  $1 < \beta_2 < 4$ ;  $n-2 < \gamma_1 < n$ ,  $0 < \gamma_5 \leq 1$ , and  $3 < \gamma_4 + \gamma_3 + \gamma_2 < 6$ ;  $n-2 < \theta_1 < n$ ,  $0 < \theta_4 \leq 1$ , and  $2 < \theta_3 + \theta_2 < 5$ .

Now, from Proposition 9(i), it follows that

$$\begin{aligned} \text{Spec}_L(\overline{T}_2) &= \{n - \alpha_3, n - 1^{(n-4)}, n - \alpha_2, n - \alpha_1, 0\}, \\ \text{Spec}_L(\overline{T}_3) &= \{n - \beta_3, n - 1^{(n-4)}, n - \beta_2, n - \beta_1, 0\}, \\ \text{Spec}_L(\overline{T}_4) &= \{n - \gamma_5, n - 1^{(n-6)}, n - \gamma_4, n - \gamma_3, n - \gamma_2, n - \gamma_1, 0\}, \\ \text{Spec}_L(\overline{T}_5) &= \{n - \theta_4, n - 1^{(n-5)}, n - \theta_3, n - \theta_2, n - \theta_1, 0\}, \end{aligned}$$

and hence, for  $n \geq 8$ ,

$$\begin{aligned} LEL(\overline{T}_2) &= (n-4)\sqrt{n-1} + \sqrt{n-\alpha_3} + \sqrt{n-\alpha_2} + \sqrt{n-\alpha_1} \\ &> (n-3)\sqrt{n-1} + \sqrt{n-3} > 2n - 3/5, \\ Kf(\overline{T}_2) &= n \left( \frac{n-4}{n-1} + \frac{1}{n-\alpha_3} + \frac{1}{n-\alpha_2} + \frac{1}{n-\alpha_1} \right) \\ &= n \left( \frac{n-4}{n-1} + \frac{f'_2(n)}{f_2(n)} \right) = \frac{2n^3 - 9n^2 + 11n + 2}{n^2 - 4n + 3} < 2n - 3/5, \\ LEL(\overline{T}_3) &= (n-4)\sqrt{n-1} + \sqrt{n-\beta_3} + \sqrt{n-\beta_2} + \sqrt{n-\beta_1} \\ &> (n-3)\sqrt{n-1} + \sqrt{n-4} > 2n - 1, \\ Kf(\overline{T}_3) &= n \left( \frac{n-4}{n-1} + \frac{f'_3(n)}{f_3(n)} \right) = \frac{3n^3 - 17n^2 + 25n + 7}{2n^2 - 10n + 8} < 2n - 1, \\ LEL(\overline{T}_4) &= (n-6)\sqrt{n-1} + \sqrt{n-\gamma_5} + \sqrt{n-\gamma_4} + \sqrt{n-\gamma_3} + \sqrt{n-\gamma_2} + \sqrt{n-\gamma_1} \\ &> (n-5)\sqrt{n-1} + \sqrt{n-2} + 2\sqrt{n-6} > 2n - 3, \\ Kf(\overline{T}_4) &= n \left( \frac{n-6}{n-1} + \frac{f'_4(n)}{f_4(n)} \right) = \frac{3n^5 - 23n^4 + 65n^3 - 67n^2 - 3n + 5}{2n^4 - 14n^3 + 32n^2 - 26n + 6} < 2n - 3, \\ LEL(\overline{T}_5) &= (n-5)\sqrt{n-1} + \sqrt{n-\theta_4} + \sqrt{n-\theta_3} + \sqrt{n-\theta_2} + \sqrt{n-\theta_1} \\ &> (n-4)\sqrt{n-1} + \sqrt{n-3} + \sqrt{n-5} > 2n - 2, \\ Kf(\overline{T}_5) &= n \left( \frac{n-5}{n-1} + \frac{f'_5(n)}{f_5(n)} \right) = \frac{3n^4 - 20n^3 + 46n^2 - 31n - 10}{2n^3 - 12n^2 + 21n - 11} < 2n - 2, \end{aligned}$$

which yield  $LEL(\overline{T}_i) > Kf(\overline{T}_i)$  for  $i \in \{2, 3, 4, 5\}$ . □

We next present correct proofs for Corollaries 5, 6 and 7, which are analogous to the proof of Corollary 17.

*Proof of Corollary 5.* If  $U \in \mathcal{U}(n) \setminus \{U_1, U_2, U_3, U_4\}$ , by Lemma 12, we have  $\mu_1(U) \leq n - 1$  and then, by Proposition 9(i), we get  $\mu_{n-1}(\overline{U}) = n - \mu_1(U) \geq 1$ . Note that

$$2|E(\overline{U})| = n(n-3) > \frac{\sqrt{n}+1}{\sqrt{n}+2} \left( n^2 - 1 - \frac{(n-1)\sqrt{n}}{\sqrt{n}+1} \right),$$

provided  $n^2 + 1 > 2n(\sqrt{n} + 3)$ , which is true for  $n \geq 14$ . Hence, by Theorem 15, we obtain  $LEL(\overline{U}) > Kf(\overline{U})$ .

Otherwise, since  $\Delta(U) \leq n - 2$ , we have  $U \neq U_1$ . It now suffices to show that  $LEL(\overline{U}_i) > Kf(\overline{U}_i)$  for  $i \in \{2, 3, 4\}$ . By Lemma 10 and a direct calculation, we get

$$\begin{aligned} \Phi(L(U_2), x) &= x(x-1)^{n-5}(x-2)[x^3 - (n+3)x^2 + (4n-2)x - 2n], \\ \Phi(L(U_3), x) &= x(x-1)^{n-5}[x^4 - (n+5)x^3 + (6n+3)x^2 - (9n-5)x + 3n], \\ \Phi(L(U_4), x) &= x(x-1)^{n-5}(x-3)[x^3 - (n+2)x^2 + (3n-2)x - n]. \end{aligned}$$

Using a fully analogous argument as in the proof of Corollary 17, one can eventually conclude that, for  $n \geq 14$ ,

$$\begin{aligned} LEL(\overline{U}_2) &> (n-4)\sqrt{n-1} > 2n > \frac{2n^4 - 15n^3 + 39n^2 - 34n - 4}{n^3 - 7n^2 + 14n - 8} = Kf(\overline{U}_2), \\ LEL(\overline{U}_3) &> (n-4)\sqrt{n-1} > 2n > \frac{2n^4 - 15n^3 + 38n^2 - 32n - 5}{n^3 - 7n^2 + 14n - 8} = Kf(\overline{U}_3), \\ LEL(\overline{U}_4) &> (n-4)\sqrt{n-1} > 2n > \frac{2n^3 - 9n^2 + 13n + 2}{n^2 - 4n + 3} = Kf(\overline{U}_4), \end{aligned}$$

as desired.

*Proof of Corollary 6.* Similarly, if  $B \in \mathcal{B}(n) \setminus \{B_1, B_2, \dots, B_{11}\}$ , then by Lemma 13 and Proposition 9(i), we have  $\mu_{n-1}(\overline{B}) = n - \mu_1(B) \geq 1$ . Notice that

$$2|E(\overline{B})| = n(n-3) - 2 > \frac{\sqrt{n}+1}{\sqrt{n}+2} \left( n^2 - 1 - \frac{(n-1)\sqrt{n}}{\sqrt{n}+1} \right),$$

provided  $n^2 + 1 > 2(n+1)\sqrt{n} + 6n + 4$ , which holds for  $n \geq 15$ . So, by Theorem 15, we get  $LEL(\overline{B}) > Kf(\overline{B})$ .

Otherwise, since  $\Delta(B) \leq n - 2$ , we have  $B \notin \{B_1, B_2\}$ . It suffices to show that  $LEL(\overline{B}_i) > Kf(\overline{B}_i)$  for  $i \in \{3, 4, \dots, 11\}$ . By Lemma 10 and a direct calculation, we obtain

$$\begin{aligned} \Phi(L(B_3), x) &= x(x-1)^{n-6}(x-2)^2[x^3 - (n+4)x^2 + (5n-2)x - 3n], \\ \Phi(L(B_4), x) &= x(x-1)^{n-6}[x^5 - (n+8)x^4 + (9n+18)x^3 - (27n+6)x^2 + (31n-10)x - 11n], \\ \Phi(L(B_5), x) &= x(x-1)^{n-6}(x-2)(x-3)[x^3 - (n+3)x^2 + (4n-2)x - 2n], \\ \Phi(L(B_6), x) &= x(x-1)^{n-5}(x-4)[x^3 - (n+3)x^2 + (4n-2)x - 2n], \\ \Phi(L(B_7), x) &= x(x-1)^{n-6}(x-2)[x^4 - (n+6)x^3 + (7n+4)x^2 - (11n-6)x + 4n], \\ \Phi(L(B_8), x) &= x(x-1)^{n-6}[x^5 - (n+8)x^4 + (9n+17)x^3 - (26n+2)x^2 + (27n-13)x - 8n], \\ \Phi(L(B_9), x) &= x(x-1)^{n-6}(x-3)[x^4 - (n+5)x^3 + (6n+3)x^2 - (9n-5)x + 3n], \\ \Phi(L(B_{10}), x) &= x(x-1)^{n-6}(x-2)(x-4)[x^3 - (n+2)x^2 + (3n-2)x - n], \\ \Phi(L(B_{11}), x) &= x(x-1)^{n-6}(x-3)^2[x^3 - (n+2)x^2 + (3n-2)x - n], \end{aligned}$$



from which we can eventually find that, for  $n \geq 15$ ,

$$\begin{aligned} LEL(\overline{B_3}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^4 - 17n^3 + 49n^2 - 50n - 4}{n^3 - 8n^2 + 17n - 10} = Kf(\overline{B_3}), \\ LEL(\overline{B_4}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^5 - 21n^4 + 84n^3 - 152n^2 + 97n + 10}{n^4 - 10n^3 + 34n^2 - 46n + 21} = Kf(\overline{B_4}), \\ LEL(\overline{B_5}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^5 - 21n^4 + 86n^3 - 163n^2 + 114n + 12}{n^4 - 10n^3 + 35n^2 - 50n + 24} = Kf(\overline{B_5}), \\ LEL(\overline{B_6}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^3 - 11n^2 + 19n + 2}{n^2 - 5n + 4} = Kf(\overline{B_6}), \\ LEL(\overline{B_7}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^4 - 17n^3 + 47n^2 - 46n - 6}{n^3 - 8n^2 + 17n - 10} = Kf(\overline{B_7}), \\ LEL(\overline{B_8}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^5 - 21n^4 + 83n^3 - 147n^2 + 90n + 13}{n^4 - 10n^3 + 34n^2 - 46n + 21} = Kf(\overline{B_8}), \\ LEL(\overline{B_9}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^5 - 21n^4 + 85n^3 - 158n^2 + 107n + 15}{n^4 - 10n^3 + 35n^2 - 50n + 24} = Kf(\overline{B_9}), \\ LEL(\overline{B_{10}}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^5 - 21n^4 + 85n^3 - 158n^2 + 106n + 16}{n^4 - 10n^3 + 35n^2 - 50n + 24} = Kf(\overline{B_{10}}), \\ LEL(\overline{B_{11}}) &> (n-5)\sqrt{n-1} > 2n > \frac{2n^3 - 9n^2 + 15n + 2}{n^2 - 4n + 3} = Kf(\overline{B_{11}}), \end{aligned}$$

as desired.

*Proof of Corollary 7.* If  $TC \in \mathcal{TC}(n) \setminus (\mathcal{S}(n, 3) \cup \{H_1, H_2, \dots, H_{27}\})$ , then by Lemma 14 and Proposition 9(i), we have  $\mu_{n-1}(\overline{TC}) = n - \mu_1(TC) \geq 1$ . Note that

$$2|E(\overline{TC})| = n(n-3) - 4 > \frac{\sqrt{n}+1}{\sqrt{n}+2} \left( n^2 - 1 - \frac{(n-1)\sqrt{n}}{\sqrt{n}+1} \right),$$

provided  $n^2 + 1 > 2(n+2)\sqrt{n} + 6n + 8$ , which holds for  $n \geq 16$ . So, by Theorem 15, we obtain  $LEL(\overline{TC}) > Kf(\overline{TC})$ .

Otherwise, since  $\Delta(TC) \leq n - 2$ , we have  $TC \notin \mathcal{S}(n, 3)$ . Now, we just need to show that  $LEL(\overline{H_i}) > Kf(\overline{H_i})$  for  $i \in \{1, 2, \dots, 27\}$ . Notice that  $\Phi(L(H_i), x), i = 1, 2, \dots, 27$ , have been given in the proof of Lemma 2.5 in [23], from which and with the aid of the software ‘Mathematica’, we can check that, for  $n \geq 16$  and  $i = 1, 2, \dots, 27$ ,  $LEL(\overline{H_i}) > (n-6)\sqrt{n-1} > 2n + 1 > Kf(\overline{H_i})$ .

REMARK 18. We believe that Corollary 8 is true too. However, because of the limitation of the length of this paper, we do not give a complete proof for it. In fact, this proof would be fully analogous to the previous proofs for Corollaries 5, 6, 7 and 17; but the characterization for the tetracyclic graphs  $QC$  with  $\mu_1(QC) > n - 1$ , and a great deal of tedious calculation, would be needed.

We finally provide several new sufficient conditions for  $LEL(G) > Kf(G)$ .

THEOREM 19. *If  $G$  is a graph of order  $n \geq 3$  with  $\mu_{n-1}(G) \geq n^{2/3}$ , then  $LEL(G) > Kf(G)$ .*

*Proof.* Since  $\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_{n-1}(G) > 0$ , we have

$$(2.7) \quad LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i(G)} \geq (n-1)\sqrt{\mu_{n-1}(G)},$$

$$(2.8) \quad Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_{n-1}(G)} \leq \frac{n(n-1)}{\mu_{n-1}(G)},$$

with both equalities in (2.7) and (2.8) holding if and only if  $\mu_1(G) = \mu_2(G) = \dots = \mu_{n-1}(G)$ , which implies  $G = K_n$  (by Proposition 9(vii)).

If  $G = K_n$ , then we have  $LEL(G) = (n-1)\sqrt{n} > n-1 = Kf(G)$ . Otherwise, since  $\mu_{n-1}(G) \geq n^{2/3}$ , from (2.7) and (2.8) it follows that

$$LEL(G) > (n-1)\sqrt{\mu_{n-1}(G)} \geq \frac{n(n-1)}{\mu_{n-1}(G)} > Kf(G),$$

as desired. □

Recall that  $\mu_{n-1}(G) = n - \mu_1(\overline{G})$  (by Proposition 9(i)). This, together with Theorem 19, yields the following result, which can be viewed as a slight improvement of Theorem 2.12 in [27].

**COROLLARY 20.** *If  $G$  is a graph of order  $n \geq 3$  with  $\mu_1(G) \leq n - n^{2/3}$ , then  $LEL(\overline{G}) > Kf(\overline{G})$ .*

Combining Theorem 19 with Proposition 9(v), we obtain the next result.

**THEOREM 21.** *If  $G$  is a graph of order  $n \geq 3$  with  $\delta(G) \geq (n + n^{2/3} - 2)/2$ , then  $LEL(G) > Kf(G)$ .*

**REMARK 22.** In particular, from Theorem 21 one can see that, if  $G$  is an  $r$ -regular graph of order  $n \geq 3$  with  $r \geq (n + n^{2/3} - 2)/2$ , then  $LEL(G) > Kf(G)$ . Therefore, Theorem 21 can be regarded as an extension of Corollary 2.16 in [27].

The next result follows immediately from Theorem 19 and Proposition 9(vi).

**THEOREM 23.** *Let  $G$  be a graph of order  $n \geq 3$  with  $m$  edges. If  $2m \geq (n-2)(\Delta(G) + 1) + n^{2/3}$ , then  $LEL(G) > Kf(G)$ .*

**REMARK 24.** To some extent, Theorem 23 provides a complete (but not the best possible) solution to Problem 1. It would be of interest to find the best possible solution to this problem.

As an application of Theorem 23, we have the following result.

**COROLLARY 25.** *Let  $G$  be an  $r$ -regular graph of order  $n \geq 3$  with  $r \geq (n + n^{2/3} - 2)/2$ . Let  $G^{-k}$  be an edge-deleted subgraph of  $G$  by deleting arbitrary  $k$  edges. If  $0 \leq k \leq r - (n + n^{2/3} - 2)/2$ , then  $LEL(G^{-k}) > Kf(G^{-k})$ .*

*Proof.* Since  $k \leq r - (n + n^{2/3} - 2)/2$  and  $r \geq \Delta(G^{-k})$ , we have

$$2|E(G^{-k})| = 2(|E(G)| - k) = nr - 2k \geq nr - 2r + (n + n^{2/3} - 2) \geq (n-2)(\Delta(G^{-k}) + 1) + n^{2/3}.$$

Thus, by Theorem 23, we obtain the desired result. □

**REMARK 26.** Corollary 25 tells us that not only  $r$ -regular graphs with sufficient large  $r$  but also some of their edge-deleted subgraphs, satisfy  $LEL > Kf$ . So, Corollary 25 can be seen as another extension of Corollary 2.16 in [27].

In particular, taking  $r = n - 1$  in Corollary 25, we have the following result, which can be viewed as an improvement on Corollary 3.5 in [5].

**COROLLARY 27.** *Let  $G$  be a graph of order  $n \geq 14$  with  $m$  edges. If  $m \geq n(n-1)/2 - (n-n^{2/3})/2$ , then  $LEL(G) > Kf(G)$ .*

**Acknowledgements.** The authors are grateful to the anonymous referees for their valuable comments and suggestions, which have considerably improved the presentation of this paper.

#### REFERENCES

- [1] W.N. Anderson and T.D. Morley. Eigenvalues of Laplacian of a graph. *Linear Multilinear Algebra*, 18:141–145, 1985.
- [2] B. Arsić, I. Gutman, K.C. Das, and K. Xu. Relations between Kirchhoff index and Laplacian-energy-like invariant. *Bull. Cl. Sci. Math. Nat. Sci. Math.*, 37:59–70, 2012.
- [3] X. Chen and K.C. Das. Characterization of extremal graphs from Laplacian eigenvalues and the sum of powers of the Laplacian eigenvalues of graphs. *Discrete Math.*, 338:1252–1263, 2015.
- [4] K.C. Das. A sharp upper bound for the number of spanning trees of a graph. *Graph. Combinator.*, 23:625–632, 2007.
- [5] K.C. Das, K. Xu, and I. Gutman. Comparison between Kirchhoff index and the Laplacian-energy-like invariant. *Linear Algebra Appl.*, 436:3661–3671, 2012.
- [6] K.C. Das, I. Gutman, and A.S. Çevik. On the Laplacian-energy-like invariant. *Linear Algebra Appl.*, 442:58–68, 2014.
- [7] E. Estrada and N. Hatano. Topological atomic displacements, Kirchhoff and Wiener indices of molecules. *Chem. Phys. Lett.*, 486:166–170, 2010.
- [8] M. Fiedler. Algebraic connectivity of graphs. *Czech. Math. J.*, 23:298–305, 1973.
- [9] X. Gao, Y. Luo, and W. Liu. Resistance distances and the Kirchhoff index in Cayley graphs. *Discrete Appl. Math.*, 159:2050–2057, 2011.
- [10] R. Grone and R. Merris. The Laplacian spectrum of a graph II. *SIAM J. Discrete Math.*, 7:221–229, 1994.
- [11] I. Gutman and B. Mohar. The quasi-Wiener and the Kirchhoff indices coincide. *J. Chem. Inf. Comput. Sci.*, 36:982–985, 1996.
- [12] I. Gutman, B. Zhou, and B. Furtula. The Laplacian-energy like invariant is an energy like invariant. *MATCH Commun. Math. Comput. Chem.*, 64:85–96, 2010.
- [13] J. Guo. On the Laplacian spectral radius of a tree. *Linear Algebra Appl.*, 368:379–385, 2003.
- [14] J. Guo. On the second largest Laplacian eigenvalue of trees. *Linear Algebra Appl.*, 404:251–261, 2005.
- [15] S. Guo. The largest eigenvalues of Laplacian matrices of unicyclic graphs (in Chinese). *Appl. Math. J. Chinese Univ. Ser. A*, 16(2):131–135, 2001.
- [16] C. He, J. Shao, and J. He. On the Laplacian spectral radii of bicyclic graphs. *Discrete Math.*, 308:5981–5995, 2008.
- [17] A. Ilić, D. Krtinić, and M. Ilić. On Laplacian like energy of trees. *MATCH Commun. Math. Comput. Chem.*, 64:111–122, 2010.
- [18] D.J. Klein and M. Randić. Resistance distance. *J. Math. Chem.*, 12:81–95, 1993.
- [19] R. Li. Lower bounds for the Kirchhoff index. *MATCH Commun. Math. Comput. Chem.*, 70:163–174, 2013.
- [20] S. Li, S.K. Simić, D.V. Tošić, and Q. Zhao. On ordering bicyclic graphs with respect to the Laplacian spectral radius. *Appl. Math. Lett.*, 24:2186–2192, 2011.
- [21] B. Liu, Y. Huang, and Z. You. A survey on the Laplacian-energy-like invariant. *MATCH Commun. Math. Comput. Chem.*, 66:713–730, 2011.
- [22] J. Liu and B. Liu. A Laplacian-energy-like invariant of a graph. *MATCH Commun. Math. Comput. Chem.*, 59:355–372, 2008.
- [23] M. Liu, F. Wei, and B. Liu. On the Laplacian spectral radii of tricyclic graphs. *Ars. Comb.*, 114:129–143, 2014.
- [24] Y. Liu, J. Shao, and X. Yuan. Some results on the ordering of the Laplacian spectral radii of unicyclic graphs. *Discrete Appl. Math.*, 156:2679–2697, 2008.
- [25] B. Mohar. The Laplacian spectrum of graphs. In: Y. Alavi, G. Chartrand, O.R. Oellermann, and A.J. Schwenk (Eds.). *Graph Theory, Combinatorics, and Applications*, Vol. 2. Wiley, New York, 1991, pp. 871–898.
- [26] S. Pirzada, H.A. Ganie, and I. Gutman. On Laplacian-energy-like invariant and Kirchhoff index. *MATCH Commun. Math. Comput. Chem.*, 73:41–59, 2015.
- [27] S. Pirzada, H.A. Ganie, and I. Gutman. Comparison between the Laplacian-energy-like invariant and the Kirchhoff index. *Electron. J. Linear Algebra*, 31:27–41, 2016.

- [28] D. Stevanović, A. Ilić, C. Onișor, and M.V. Diudea. LEL-a newly designed molecular descriptor. *Acta Chim. Slov.*, 56:410–417, 2009.
- [29] W. Wang, D. Yang, and Y. Luo. The Laplacian polynomial and Kirchhoff index of graphs derived from regular graphs. *Discrete Appl. Math.*, 161:3063–3071, 2013.
- [30] K. Xu and K.C. Das. Extremal Laplacian-energy-like invariant of graphs with given matching number. *Electron. J. Linear Algebra*, 26:131–140, 2013.
- [31] Y. Yang and D.J. Klein. Comparison theorems on resistance distances and Kirchhoff indices of S, T-isomers. *Discrete Appl. Math.*, 175:87–93, 2014.
- [32] A. Yu, M. Lu, and F. Tian. Ordering trees by their Laplacian spectral radii. *Linear Algebra Appl.*, 405:45–59, 2005.
- [33] H. Zhang, Y. Yang, and C. Li. Kirchhoff index of composite graphs. *Discrete Appl. Math.*, 157:2918–2927, 2009.
- [34] X. Zhang and J. Li. The two largest eigenvalues of Laplacian matrices of trees (in Chinese). *J. China Univ. Sci. Technol.*, 28:513–518, 1998.
- [35] B. Zhou and N. Trinajstić. The Kirchhoff index and the matching number. *Int. J. Quantum Chem.*, 109:2978–2981, 2009.
- [36] B. Zhu. The Laplacian-energy-like of graphs. *Appl. Math. Lett.*, 24:1604–1607, 2011.