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On Comparison between Laplacian-Energy-Like Invariant and Kirchhoff Index of Graphs

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Abstract

For a connected graph G, the Laplacian-energy-like invariant and Kirchhoff index of G, 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, where μ_i are the Laplacian eigenvalues of G. In this paper, some graphs with $LEL(G) > Kf(G)$ are presented, which extents a result in [1]. The comparison between $LEL(G)$ and $Kf(G)$ of chemical graphs is completely determined. Moreover, the comparisons between the two variants for regular graphs and its line graphs, and graphs with given clique number are studied.

1. Introduction

Let G be a simple graph with n vertices and m edges. The cyclomatic number of G is $c = m - n + 1$. For example, if $c = 0, 1, 2, 3, 4$, then G is called a tree, unicyclic, bicyclic, tricyclic, and tetracyclic graph, respectively. Let d_i be the degree of a vertex v_i in G.

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The maximum and minimum vertex degrees in G are denoted by Δ and δ, respectively. A chemical graph is a connected graph with the maximum vertex degree at most 4. The Laplacian matrix of G is defined as $L = D - A$, where A is the adjacency matrix of G and $D = diag(d_1, d_2, \ldots, d_n)$ the diagonal matrix of vertex degrees. The Laplacian spectrum of G is the spectrum of its Laplacian matrix, and consists of the values $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$.

The Laplacian-energy-like invariant of G, denoted by $LEL(G)$, has recently been defined as [2]

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

There are several works about the graph invariant (see [3] and the references therein).

In 1993, Klein and Randić [4] introduced resistance distance based on the electrical network theory. The Kirchhoff index [5] is defined as $Kf(G) = \sum_{i<j} r_{ij}$, where r_{ij} is the resistance distance between vertices v_i and v_j. For a connected graph G with $n \geq 2$ vertices, it has been proven [6,7] that $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$.

Das et al. [1] established two sufficient conditions under which $LEL(G) < Kf(G)$ and nine graphs with $LEL(G) > Kf(G)$ are shown.

In this paper, some graphs with $LEL(G) > Kf(G)$ are presented, which extents a result in [1]. The comparison between $LEL(G)$ and $Kf(G)$ of chemical graphs is completely determined. Moreover, the comparisons between the two variants of regular graphs and its line graphs, and graphs with given clique number are studied.

2. Some graphs with LEL larger than Kf

Lemma 2.1 [8] *Let $G + e$ be obtained by adding a new edge to the connected graph G. If $LEL(G) > Kf(G)$, then $LEL(G + e) > Kf(G + e)$ holds.*

Denoted by $\overline{G}$ the complement of G. Let $\overline{G^*(n)}$ be the graph depicted in Figure A:

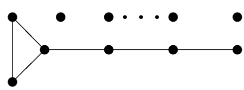


Figure A. The graph $\overline{G^*(n)}$.

Theorem 2.1 *Let G be a connected graph with $n \geq 7$ vertices. If $\overline{G}$ is a spanning subgraph of $\overline{G^*(n)}$, then $LEL(G) > Kf(G)$.*

Proof. Since $\overline{G}$ is a spanning subgraph of $\overline{G^*(n)}$, $G^*(n)$ is a spanning subgraph of G.

The Laplacian spectrum of $\overline{G^*(n)}$ is $Spec_L(\overline{G^*(n)}) = \{4.214, 3, 3, 1.461, 0.325, 0, \ldots, 0\}$. Then the Laplacian spectrum of $G^*(n)$ is $Spec_L(G^*(n)) = \{n, \ldots, n, n - 0.325, n - 1.461, n - 3, n - 3, n - 4.214, 0\}$.

Hence $LEL(G^*(n)) = (n-6)\sqrt{n} + \sqrt{n - 0.325} + \sqrt{n - 1.461} + 2\sqrt{n-3} + \sqrt{n - 4.214}$ and $Kf(G^*(n)) = n(\frac{n-6}{n} + \frac{1}{n - 0.325} + \frac{1}{n - 1.461} + \frac{2}{n-3} + \frac{1}{n - 4.214})$.

Let $f(n) := LEL(G^*(n)) - Kf(G^*(n))$.

Obviously, $f(n)$ is an increasing function on n. Then $f(n) \geq f(7) \doteq 3.92698 > 0$.

By Lemma 2.1, $LEL(G) \geq LEL(G^*(n)) > Kf(G^*(n)) \geq Kf(G)$. $\square$

The union of simple graphs G and H is the graph $G_1 \cup G_2$ with vertex set $V((G) \cup V(H)$ and edge set $E(G) \cup E(H)$. Let $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by connecting all vertices of G_1 by all vertices of G_2.

Let $G_1(n) = K_{n-2} \vee (2K_1)$; $G_2(n) = K_{n-4} \vee C_4$; $G_3(n) = K_{n-3} \vee (K_1 \cup K_2)$; $G_4(n) = K_{n-6} \vee (C_4 \vee 2K_1)$; $G_5(n) = K_{n-5} \vee ((K_2 \cup K_1) \vee 2K_1)$; $G_6(n) = K_{n-4} \vee P_4$; $G_7 = K_{n-3} \vee (3K_1)$; $G_8(n) = K_{n-4} \vee (K_1 \cup K_3)$.

Then $\overline{G_1(n)} = K_2 \cup (n-2)K_1$; $\overline{G_2(n)} = 2K_2 \cup (n-4)K_1$;$\overline{G_3(n)} = K_{1,2} \cup (n-3)K_1$; $\overline{G_4(n)} = 3K_2 \cup (n-6)K_1$; $\overline{G_5(n)} = K_{1,2} \cup K_2 \cup (n-5)K_1$; $\overline{G_6(n)} = P_4 \cup (n-4)K_1$; $\overline{G_7(n)} = K_3 \cup (n-3)K_1$; $\overline{G_8(n)} = K_{1,3} \cup (n-4)K_1$.

Note that $\overline{G_i(n)}$, $i = 1, \ldots, 8$, are the spanning subgraphs of $\overline{G^*(n)}$.

From Theorem 2.1, we have the following corollary in [1].

Corollary 2.1 [1]. *For any graph $G \in \{K_n, G_1(n), \ldots, G_8(n)\}$, the inequality $LEL(G) > Kf(G)$ holds.*

3. Chemical graphs

Lemma 3.1 [9]. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$Kf(G) \geq -1 + (n-1) \sum_{v_i \in V(G)} \frac{1}{d_i}$$

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

Lemma 3.2 [2]. *Let G be a connected graph with $n \geq 2$ vertices, $m \geq 1$ edges and maximum degree Δ. Then $LEL(G) \leq \sqrt{\Delta+1} + \sqrt{(n-2)(2m-\Delta-1)}$ with equality if and only if $G \cong K_n$ or $G \cong S_n$.*

Lemma 3.3 [1]. *Let G be a connected graph of order n with m edges and minimum degree δ. If $2m \leq (n-1)n^{2/3}$, then $LEL(G) < Kf(G)$.*

Theorem 3.1 *Let G be a chemical graph with $n \geq 10$ vertices. Then $LEL(G) < Kf(G)$.*

Proof. Note that $2m \leq 4n$. Let $f(n) := (n-1)n^{\frac{2}{3}} - 4n$. $f(n)$ is an increasing function for $n \geq 10$. Then $(n-1)n^{\frac{2}{3}} - 2m \geq f(n) \geq f(10) \doteq 1.7743 > 0$. By Lemma 3.3, then $LEL(G) < Kf(G)$ for $n \geq 10$. □

Theorem 3.2 *Let G be a chemical graph with $n = 9$ vertices. Then $LEL(G) < Kf(G)$.*

Proof. There are two cases:

Case 1: $\delta \leq 2$ or $\delta = 3$.

If $\delta \leq 2$, then $2m \leq 4(9-1) + 2 = 34 < (n-1)n^{\frac{2}{3}} = (9-1)9^{\frac{2}{3}} \approx 34.614$.

If $\delta = 3$, and note that there are at least two vertices with degree 3, then $2m \leq 4(9-2) + 3 \cdot 2 = 34 < (9-1)9^{\frac{2}{3}} \approx 34.614$.

By Lemma 3.3, the case holds.

Case 2: $\delta = 4$.

Then G is a connected 4-regular graph. By Lemmas 3.1 and 3.2, $LEL(G) \leq \sqrt{4+1} + \sqrt{(9-2)(36-4-1)} = \sqrt{5} + \sqrt{217} \approx 16.967 < 17 = -1 + (9-1)\sum_{v_i \in V(G)} \frac{1}{4} \leq Kf(G)$.

By all the cases exhausted, the theorem holds. □

Lemma 3.4 *Let G be a chemical graph with $n = 8$ vertices and degree sequence $\pi = (4,4,4,4,4,4,3,3)$. Then $LEL(G) < Kf(G)$.*

Proof. Since G has degree sequence $\pi = (4,4,4,4,4,4,3,3)$, $\overline{G}$ is connected and with degree sequence $\pi' = (4,4,3,3,3,3,3,3)$. Let v_1 and v_2 be the two vertices with degree 4 in $\overline{G}$. There are two cases:

Case 1: $v_1 \sim v_2$ in $\overline{G}$.

$\overline{G}$ is obtained by adding an edge from a graph with degree sequence $\pi^* = (3,3,3,3,3,3,3,3)$. A graph with degree sequence π^* is a cubic graph. From [10] (P.293, 3.4-3.8) and the symmetry of vertices, there are 18 graphs with degree sequence π', and their complement graphs G_i $(i = 1, \ldots, 18)$ with degree sequence π are depicted in Figure B.

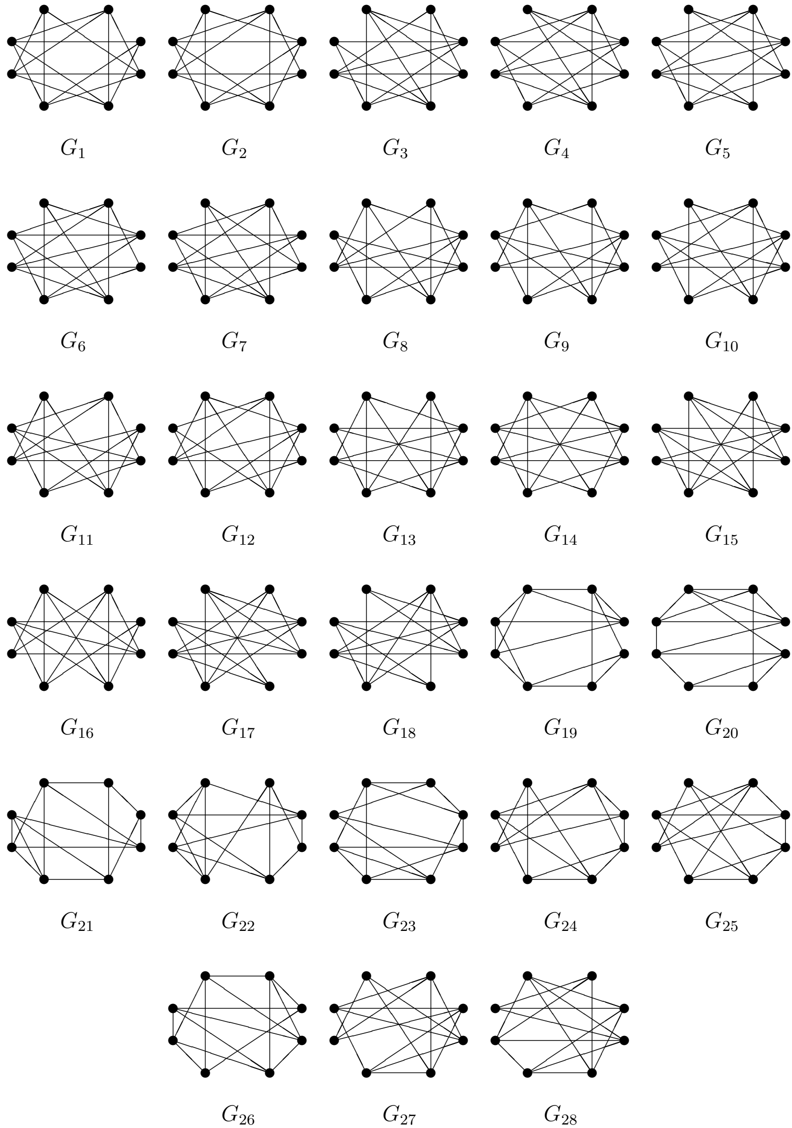


Figure B. Graphs with degree sequence $\pi = (4, 4, 4, 4, 4, 4, 3, 3)$.

Graphs	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8	G_9
LEL	14.2335	14.2511	14.2548	14.2718	14.2412	14.2596	14.2623	14.2607	14.2451
Kf	15.5569	15.1419	15.1719	14.7933	15.4797	15.0283	14.9448	14.9804	15.3419

Table 1. The LEL and Kf of graphs G_i $(i = 1, \ldots, 9)$.

Graphs	G_{10}	G_{11}	G_{12}	G_{13}	G_{14}	G_{15}	G_{16}	G_{17}	G_{18}
LEL	14.2478	14.2737	14.2607	14.2481	14.2003	14.2874	14.2569	14.1011	14.2661
Kf	15.2517	14.7456	14.9804	15.2381	16.6667	14.5714	15.25	15.3983	14.9697

Table 2. The LEL and Kf of graphs G_i $(i = 10, \ldots, 18)$.

By direct calculations, and Tables 1 and 2, $LEL(G) < Kf(G)$.

G_{19}	G_{20}	G_{21}	G_{22}	G_{23}	G_{24}	G_{25}	G_{26}	G_{27}	G_{28}
14.2113	14.228	14.2461	14.2537	14.2669	14.2455	14.2478	14.2613	14.2706	14.2728
16.2	15.7583	15.3112	152079	14.9207	15.3	15.2328	14.9733	14.8261	14.7667

Table 3. The LEL and Kf of graphs G_i $(i = 19, \ldots, 28)$.

Case 2: $v_1 \nsim v_2$ in $\overline{G}$.

Note that $\overline{G}$ has the degree sequence $\pi' = (4, 4, 3, 3, 3, 3, 3, 3)$. By discussing the subcases $|N(v_1) \cap N(v_2)| = 4$, 3 or 2, and adding the edges gradually, we search 10 graphs with degree sequence π' and the complement graphs G_i $(i = 19, \ldots, 28)$ are depicted in Figure B. By direct calculations, from Table 3, $LEL(G) < Kf(G)$.

The result holds. □

Theorem 3.3 *Let G be a chemical graph with $n = 8$ vertices.*

Then $LEL(G) < Kf(G)$ except the graphs depicted in Figure 1.

Proof. There are four cases:

Case 1: $\delta \leq 2$.

Then $2m \leq 4(8-1)+2 = 30$. By Lemmas 3.1 and 3.2, $LEL(G) \leq \sqrt{\Delta+1} + \sqrt{(8-2)(30-\Delta-1)} \leq \sqrt{3+1} + \sqrt{(8-2)(30-3-1)} \approx 14.49 < 14.75 = -1 + (8-1)(\frac{7}{4} + \frac{1}{2}) \leq Kf(G)$.

Case 2: $\delta = 3$ and $\Delta = 3$.

By Lemmas 3.1 and 3.2, $LEL(G) \leq \sqrt{3+1} + \sqrt{(8-2)(24-3-1)} \approx 12.9545 < 17.6667 \approx -1 + (8-1)\frac{8}{3} \leq Kf(G)$.

Case 3: $\delta = 3$ and $\Delta = 4$.

Subcase 3.1: The number of vertices with degree 3 is equal to 2.

By Lemma 3.4, $LEL(G) < Kf(G)$.

Subcase 3.2: The number of vertices with degree 3 is more than 2.

Note that the degrees are 3 or 4, and the number of odd degrees is even. If there are 6 vertices with degree 3, by Lemmas 3.1 and 3.2, then $LEK(G) \leq \sqrt{4+1} + \sqrt{(8-2)(26-4-1)} \approx 13.461 < 16.5 = -1 + (8-1)(\frac{2}{4} + \frac{6}{3}) \leq Kf(G)$. If there are 4 vertices with degree 3, by Lemmas 3.1 and 3.2, $LEL(G) \leq \sqrt{3+1} + \sqrt{(8-2)(28-4-1)} \approx 13.9834 < 15.3333 \approx -1 + (8-1)(\frac{4}{4} + \frac{4}{3}) \leq Kf(G)$.

Case 4: $\delta = 4$ and $\Delta = 4$.

Then G is a connected 4-regular graph and $\overline{G}$ is 3-regular graph. If $\overline{G}$ is disconnected, then $\overline{G} \cong K_4 \cup K_4$, and $G \cong H_1$ (Figure 1). If $\overline{G}$ is connected, then $\overline{G}$ is a cubic graph. By [10], there are 5 cubic graphs with $n = 8$ vertices. The complement graphs (H_2–H_6) of cubic graphs are depicted in Figure 1.

By direct calculations, from Table 4, $LELG > Kf(G)$.

The result holds. $\square$

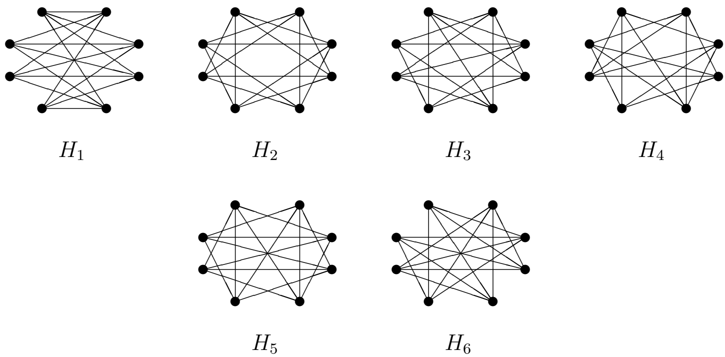


Figure 1. Chemical graphs with $n = 8$ vertices,$\delta = \Delta = 4$ and $LEL > Kf$.

Graphs	H_1	H_2	H_3	H_4	H_5	H_6
LEL	14.8284	14.7687	14.7867	14.7777	14.7627	14.802
Kf	13	13.8095	13.5411	13.6789	14	13.3333

Table 4. The LEL and Kf of chemical graphs with $n = 8$ vertices and $\delta = \Delta = 4$.

Theorem 3.4 *Let G be a chemical graph with $n = 7$ vertices.*

Then $LEL(G) < Kf(G)$ except the graphs depicted in Figures 2 and 3.

Proof. Let t be the number of vertices with degree 4. There are three cases:

Case 1: $t = 0$.

Note that $2m \leq 7 \times 3 = 21 < (7-1)7^{\frac{2}{3}} \approx 21.9958$.

By Lemma 3.3, $LEL(G) < Kf(G)$.

Case 2: $1 \leq t \leq 5$.

There are two subcases.

Subcase 2.1: $\delta \leq 2$.

By Lemma 3.1, $Kf(G) \geq -1 + (7-1)(\frac{5}{4} + \frac{2}{2}) = 12.5$ or $Kf(G) \geq -1 + (7-1)(\frac{5}{4} + \frac{1}{3} + 1) = 14.5$. By Lemma 3.2, $LEL \leq \sqrt{4+1} + \sqrt{(7-2)(25-4-1)} \approx 12.2361$.

This subcase holds.

Subcase 2.2: $\delta \geq 3$.

Note that $1 \leq t \leq 5$, $\delta \geq 3$ and $n = 7$. Then there are three degree sequences: $\pi_1 = (4, 3, 3, 3, 3, 3, 3)$, $\pi_2 = (4, 4, 4, 3, 3, 3, 3)$ and $\pi_3 = (4, 4, 4, 4, 4, 3, 3)$.

For degree sequence π_1, by Lemmas 3.1 and 3.2, $LEL(G) \leq \sqrt{4+1}+$
$\sqrt{(7-2)(22-4-1)} \approx 11.4556 < 12.5 = -1 + (7-1)(\frac{1}{4} + \frac{6}{3}) \leq Kf(G)$.

For degree sequence π_2, there are 11 chemical graphs, which are No. 489, 490, 491, 492, 495, 496, 497, 498, 514, 515, 516 in [11]. By direct calculations, from Table 5, we have $LEL(G) < Kf(G)$ except the two graphs No. 489 and 490 (H_7, H_8 in Figure 2).

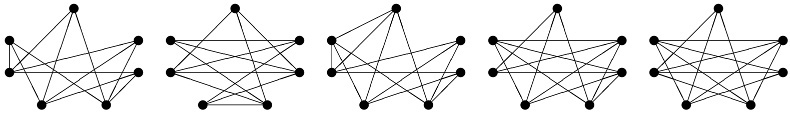
For degree sequence π_3, there are 7 chemical graphs, which are No. 615, 616, 618, 619, 622, 623, and 624 (H_i, $i = 9, \ldots, 15$ in Figure 2) in [11]. By direct calculations, from Table 6, $LEL(G) > Kf(G)$ holds for the graphs in Figure 2.

Graphs	489	490	491	492	495	496	497	498	514
LEL	11.8419	11.8208	11.8122	11.8128	11.8001	11.8047	11.7934	11.7993	11.7729
Kf	11.5	11.8186	11.9348	11.91	12.1243	12	12.3289	12.1403	12.65
Graphs	515	516							
LEL	11.784	11.7788							
Kf	12.4456	12.6316							

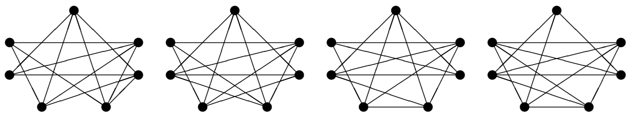
Table 5. The LEL and Kf of chemical graphs with $n = 7$ and $m = 12$.

Graphs	615	616	618	619	622	623	624
LEL	12.3459	12.3373	12.3289	12.3248	12.3152	12.3193	12.162
Kf	10.5667	10.6818	10.7896	10.8853	11.0226	10.9167	11.0015

Table 6. The LEL and Kf of chemical graphs with $n = 7$ and $m = 13$.



H_7 H_8 H_9 H_{10} H_{11}



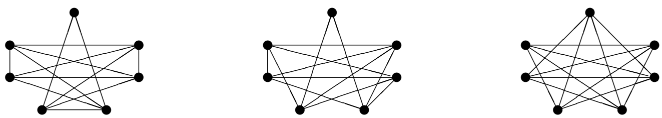
H_{12} H_{13} H_{14} H_{15}

Figure 2. Chemical graphs with degree sequences $(4,4,4,3,3,3,3)$ and $(4,4,4,4,4,3,3)$.

Case 3: $t = 6$ or $t = 7$.

If $t = 6$, then G and $\overline{G}$ have the degree sequences $\pi_4 = (4,4,4,4,4,4,2)$ and $\pi'_4 = (4,2,2,2,2,\ 2,2)$, respectively. From π'_4, the graphs with degree sequence π_4 are depicted in Figure 3. By direct calculations, $LEL(H_{16}) = 12.8439 > 9.69231 = Kf(H_{16})$ and $LEL(H_{17}) = 12.2587 > 11.8435 = Kf(H_{17})$.

If $t = 7$, then G is the 4-regular graphs with $n = 7$ vertices and $G \cong H_{18}$ in Figure 3. Then $LEL(H_{18}) = 12.277 > 11.4408 = Kf(H_{18})$. $\square$



H_{16} H_{17} H_{18}

Figure 3. Chemical graphs with degree sequence $(4,4,4,4,4,4,2)$.

Theorem 3.5 *Let G be a chemical graph with $n = 6$ vertices.*

Then $LEL(G) < Kf(G)$ except the graphs in Figure 4.

Proof. If $m \le 8$, then $2m \le 16 < 16.5096 \approx (6-1)6^{\frac{2}{3}} = (n-1)n^{\frac{2}{3}}$. By Lemma 3.3, $LEL(G) < Kf(G)$. It is only need to consider the cases that $9 \le m \le 12$.

Case 1: $m = 9$.

By [12], there are 14 chemical graphs with degree sequences $\pi_1 = (4,4,4,3,2,1)$, $\pi_2 = (4,4,4,2,2,2)$, $\pi_3 = (4,4,3,3,3,1)$, $\pi_4 = (4,4,3,3,2,2)$, $\pi_5 = (4,3,3,3,3,2)$ and $\pi_6 = (3,3,3,3,3,3)$. For degree sequences π_1, π_2, π_3, and π_4, by Lemma 3.2, $LEL(G(\pi_i)) \le \sqrt{4+1} + \sqrt{(6-2)(18-4-1)} \approx 9.44717$, $i = 1, \ldots 4$. By Lemma 3.1, $Kf(G(\pi_1)) \ge -1 + (6-1)(\frac{3}{4} + \frac{1}{3} + \frac{1}{2} + 1) \approx 11.9167$, $Kf(G(\pi_2)) \ge -1 + (6-1)(\frac{3}{4} + \frac{3}{2} = 10.25$, $Kf(G(\pi_3)) \ge -1 + (6-1)(\frac{2}{4} + \frac{3}{3} + +1) = 11.5$, and $Kf(G(\pi_4)) \ge -1 + (6-1)(\frac{2}{4} + \frac{2}{3} + \frac{2}{2}) \approx 9.83333$. Then $LEL(G(\pi_i)) < Kf(G(\pi_i))$ $(i = 1, \ldots, 4)$.

By [12], there are three graphs with degree sequence π_5 and two graphs with degree sequence π_6, which are No. 47, 48, 50, 51, 52 graphs in [12]. By direct calculations, from Table 7, $LEL(G) < Kf(G)$ holds except the graph No. 52 (H_{19} in Figure 4).

Graphs	47	48	50	51	52
LEL	9.29787	9.2897	9.31319	9.35045	9.37769
Kf	9.98485	10.25	9.73913	9.4	9

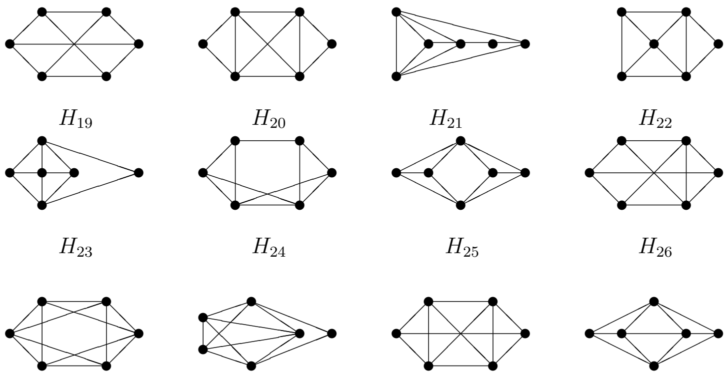
Table 7. The LEL and Kf of chemical graphs with degree sequences $(4,3,3,3,3,2)$ and $(3,3,3,3,3,3)$.

Case 2: $m = 10$.

By [12], there are 8 chemical graphs. By direct calculations, from Table 8, $LEL(G) > Kf(G)$ holds for the graphs No. 23, 26, 27, 29, 30, 31, and 32 (H_{20}–H_{26} in Figure 4) in [12].

Graphs	20	23	26	27	29	30	31	32
LEL	9.66629	9.76183	9.8172	9.8148	9.83182	9.86826	9.8637	9.88171
Kf	11.7333	9.64999	8.93913	9.00878	8.7	8.39231	8.5	8.2

Table 8. The LEL and Kf of chemical graphs with $n = 6$ vertices and $m = 10$ edges.



H_{19} H_{20} H_{21} H_{22}

H_{23} H_{24} H_{25} H_{26}

H_{27} H_{28} H_{29} H_{30}

Figure 4. Chemical graphs with $n = 6$ vertices and $LEL > Kf$.

Case 3: $m = 11$ or 12.

By [12], there are 4 chemical graphs H_{27}–H_{30}, which are depicted in Figure 4. By direct calculations, $LEL(H_{27}) \approx 10.899 > 6.5 = Kf(H_{27})$, $LEL(H_{28}) \approx 10.3358 > 7.4 = Kf(H_{28})$, $LEL(H_{29}) \approx 10.3857 > 7.42857 \approx Kf(H_{29})$, and $LEL(H_{30}) \approx 9.66629 > 7.42857 \approx Kf(H_{30})$.

The result holds. $\square$

Lemma 3.5 [1]. *Let T be a tree of order n. Then $LEL(T) > Kf(T)$ for $n = 2$ and $LEL(T) < Kf(T)$ for $n > 2$.*

Lemma 3.6 [1]. *Let G be a unicyclic graph of order n. Then $LEL(G) > Kf(G)$ for $n = 3$ and $LEL(G) < Kf(G)$ for $n \geq 4$.*

Lemma 3.7 [1]. *Let G be a bicyclic graph of order n. Then $LEL(G) > Kf(G)$ for $n = 4$ and $LEL(G) < Kf(G)$ for $n \geq 5$.*

Lemma 3.8 [8]. *The only connected tricyclic graphs with order $n \leq 5$ for which $LEL(G) > Kf(G)$ holds are $G \cong H_{34}, H_{35}, H_{36}, H_{37}$, depicted in Figure 5.*

Lemma 3.9 [8]. *The only connected tetracyclic graphs with order $n \leq 5$ for which $LEL(G) > Kf(G)$ holds are $G \cong H_{38}, H_{39}$, depicted in Figure 5.*

Theorem 3.6 *Let G be a chemical graph with $n \leq 5$ vertices.*

Then $LEL(G) < Kf(G)$ except the graphs in Figure 5.

Proof. Let G be a chemical graph with $n \leq 5$ vertices. Then $m \leq 10$ holds. By [10], there are 30 graphs with $n \leq 5$. By Lemmas 3.5–3.9, we only need to compare LEL and Kf for K_5 and $K_5 - e$ (H_{40}, H_{41} in Figure 5). By direct calculations, $LEL(K_5) = 4\sqrt{5} > Kf(K_5) = 4$ and $LEL(K_5 - e) \approx 8.44025 > 4.66667 \approx Kf(K_5 - e)$. $\square$

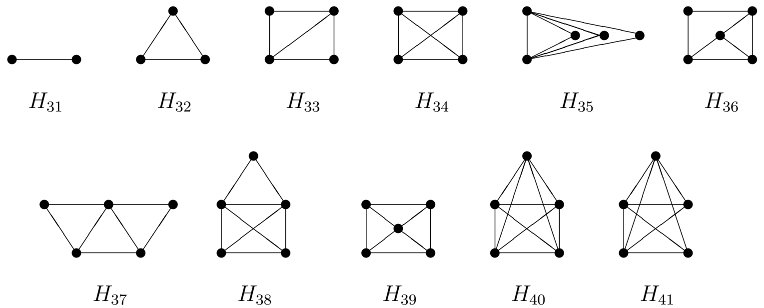


Figure 5. Chemical graphs with $n \leq 5$ vertices and $LEL > Kf$.

By Theorems 3.1–3.6, the following holds:

Theorem 3.7 *Let G be a chemical graph with n vertices. Then $LEL(G) < Kf(G)$ except the graphs H_i $(i = 1, \ldots, 41)$ in Figures 1-5.*

4. Regular graphs and line graphs

Theorem 4.1 *Let G be a connected r-regular graph with n vertices. If $r \leq (\frac{n-1}{n})n^{2/3}$, then $LEL(G) < Kf(G)$.*

Proof. Note that $2m = nr$. If $nr \leq (n-1)n^{2/3}$, i.e., $r \leq (\frac{n-1}{n})n^{2/3}$, by Lemma 3.1, then $LEL(G) < Kf(G)$. $\square$

Remark 4.1 For a r-regular graphs with $r = n^{\frac{2}{3}}$, let $r = 4 = 8^{\frac{2}{3}} = n^{\frac{2}{3}}$, by the proof of Theorem 3.3, then there exit graphs with $LEL(G) > Kf(G)$.

The line graph of G, denoted by $l(G)$, is the graph whose vertices correspond to the edges of G, with two vertices of $l(G)$ being adjacent if and only if the corresponding edges of G share a common vertex.

Lemma 4.1 [13]. *Let G be a r-regular graph with n vertices, m edges. Then $P_{l(G)} = (x - 2r)^{m-n} P_G(x)$.*

Theorem 4.2 *Let G be a r-regular graph with $r \leq (\frac{n-1}{n})n^{2/3}$.*

Then $LEL(l(G)) < Kf(l(G))$, where $l(G)$ is the line graph of G.

Proof. By Lemma 4.1, the Laplacian spectrum of $l(G)$ is

$Spec_L(l(G)) = \{(2r)^{m-n}, \mu_1, \ldots, \mu_{n-1}, 0\}$.

Then $LEL(l(G)) - Kf(l(G)) = (m-n)\sqrt{2r} + \sum_{i=1}^{n-1}\sqrt{\mu_i} - m[\sum_{i=1}^{n-1}\frac{1}{\mu_i} + (m-n)\frac{1}{2r}]$

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

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

$$= LEL(G) - Kf(G) + (m-n)(\sqrt{2r} - \frac{n-1}{2r} - \frac{n}{4}).$$

Let $f(r) = \sqrt{2r} - \frac{n-1}{2r} - \frac{n}{4}$. Obviously, $f(r)$ is an increasing function on r.

$$\begin{aligned} \text{Then } f(r) \leq f(\frac{n-1}{n}n^{\frac{2}{3}}) &= \sqrt{2\frac{n-1}{n}n^{\frac{2}{3}}} - \frac{1}{2}n^{\frac{1}{3}} - \frac{n}{4} \\ &< \sqrt{2n^{\frac{2}{3}}} - \frac{1}{2}n^{\frac{1}{3}} - \frac{n}{4} \\ &= \sqrt{2}n^{\frac{1}{3}} - \frac{1}{2}n^{\frac{1}{3}} - \frac{n}{4} = n^{\frac{1}{3}}(\sqrt{2} - \frac{1}{2} - \frac{1}{4}n^{\frac{2}{3}}) < 0 \text{ for } n \geq 3. \end{aligned}$$

Additionally, by Theorem 4.1, $LEL(G) < Kf(G)$.

Then $LEL(l(G)) < Kf(l(G))$. □

5. Graphs with given vertices and clique number

The independent number of a graphs G, denoted by α, is the number of vertices in the largest independent set of G.

Let $\overline{CS}(n, n-\alpha) := K_\alpha \cup (n-\alpha)K_1$. It is easy to see that the Laplacian spectrum of the complete split graph $CS(n, n-\alpha)$ is $Spec_L(CS(n, n-\alpha)) = \{n^{(n-\alpha)}, (n-\alpha)^{(\alpha-1)}, 0\}$.

Lemma 5.1 [14]. *Let G be a graph of order n with independent number α. Then $LEL(G) \leq (n-\alpha)\sqrt{n} + (\alpha-1)\sqrt{n-\alpha}$.*

Lemma 5.2 [15]. *Let G be a non-complete connected graph. If $G+e$ is obtained from G by adding and edge, then $Kf(G+e) < Kf(G)$.*

Lemma 5.3 *Let G be a connected graph with n vertices and independent number α. Then $Kf(G) \geq (n-\alpha) + \frac{n(\alpha-1)}{n-\alpha}$.*

Proof. Note that G is a graph with the independent number α. Then the most edges of

G is from $K_{n-\alpha}$ and αK_1 by connecting each vertex of αK_1 and each vertex of $K_{n-\alpha}$. By Lemma 5.2, $Kf(G) \geq Kf(CS(n, n-\alpha)) = (n-\alpha) + \dfrac{n(\alpha-1)}{n-\alpha}$. $\square$

Theorem 5.1 *Let G be a connected graph with n vertices and independent number α. If $\alpha > n - \sqrt{n}$, then $LEL(G) < Kf(G)$ holds except the graphs in Figure 6.*

Proof. It is discussed on n.

Case 1: $n \geq 9$.

Let $f(\alpha) = (n-\alpha) + \dfrac{n(\alpha-1)}{n-\alpha} - [(n-\alpha)\sqrt{n} + (\alpha-1)\sqrt{n-\alpha}]$. Consider the first derivative of $f(\alpha)$,

$f'(\alpha) = -1 + \dfrac{n(n-1)}{(n-\alpha)^2} + \sqrt{n} - \sqrt{n-\alpha} + \dfrac{\alpha-1}{2\sqrt{n-\alpha}} > 0$. Then $f(\alpha)$ is an increasing function on α. For $\alpha \geq n - n^{\frac{1}{2}}$ and $n \geq 9$,

$f(\alpha) \geq f(n - n^{\frac{1}{2}}) = n(n^{\frac{1}{2}} - n^{\frac{1}{4}} - 2) + n^{\frac{3}{4}} + n^{\frac{1}{4}} := g(n) \geq g(9) \approx 0.339746 > 0.$

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

Case 2: $n = 8, 7$ or 6.

When $n = 8$, noting that $\alpha \geq n - \sqrt{n} = 8 - \sqrt{8} \approx 5.57$, we have $\alpha = 6$ or 7. If $\alpha = 6$, by Lemmas 5.1 and 5.3, then $LEL(G) \leq (8-6)\sqrt{8} + (6-1)\sqrt{2} = 9\sqrt{2} < (8-6) + \dfrac{8(6-1)}{8-6} = 22 \leq Kf(G)$. If $\alpha = 7$, then $G \cong S_8$. By Lemma 3.5, $LEL(G) < Kf(G)$.

When $n = 7$ or 6, similar to $n = 8$ and by direct calculations, $LEL(G) < Kf(G)$.

Case 3: $n = 5$.

Note that $\alpha \geq n - \sqrt{n} = 5 - \sqrt{5} \approx 2.76$. Then $\alpha = 3$ or 4. If $\alpha = 3$ and $G \cong CS(5,2)$, by direct calculation, $LEL(G) = (5-3)\sqrt{5} + (3-1)\sqrt{2} \approx 7.3 > 7 = (5-3) + \dfrac{5(3-1)}{5-3} = Kf(CS(5,2))$. Let $CS(5,2) - e$ be a graph with independent number 3 by deleting an edge e from $CS(5,2)$. If $G \ncong CS(5,2)$, by Lemmas 5.1 and 5.3, then $LEL(G) \leq LEL(CS(5,2) - e) \leq 6.65028 < 7.667 \leq Kf(CS(5,2) - e) < Kf(G)$.

If $\alpha = 4$, then $G \cong S_5$. By Lemma 3.5, $LEL(G) < Kf(G)$.

Case 4: $n = 4$.

This case is similar to Case 3. By direct calculations, $LEL(G) < Kf(G)$ except $LEL(CS(4,2)) = (4-2)\sqrt{4} + (2-1)\sqrt{2} = 4 + \sqrt{2} > 4 = (4-2) + \dfrac{4(2-1)}{4-2} = Kf(CS(4,2))$.

Case 5: $n = 3$ or 2.

If $n = 3$ and $\alpha \geq 3 - 3^{\frac{1}{3}} \approx 1.26795$, then $G \cong S_3$. By Lemma 3.5, $LEL(G) < Kf(G)$. If $n = 2$ and $\alpha \geq 2 - 2^{\frac{1}{3}}$, then $G \cong S_2$. By Lemma 3.5, $LEL(G) > Kf(G)$.

The result holds. □

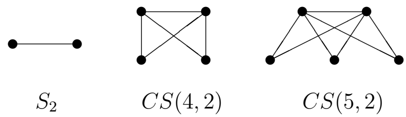


Figure 6. Graphs with independent number $\alpha \geq n - n^{\frac{1}{2}}$ and $LEL > Kf$.

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