Acta Univ. Sapientiae Informatica **14,** 2 (2022) 185–198

DOI: 10.2478/ausi-2022-0011

Computing Laplacian energy, Laplacian-energy-like invariant and Kirchhoff index of graphs

S. Bhatnagar
Department of Applied Mathematics, Aligarh Muslim University, Aligarh, India
email: sbhatnagar734@gmail.com

Merajuddin
Department of Applied Mathematics, Aligarh Muslim University, Aligarh, India
email: meraj1957@rediffmail.com

S. Pirzada
Department of Mathematics, University of Kashmir, Srinagar, India
email: pirzadasd@kashmiruniversity.ac.in
ORCID:0000-0002-1137-517X

Abstract. Let G be a simple connected graph of order n and size m. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of the graph G, where $D(G)$ and $A(G)$ are the degree diagonal matrix and the adjacency matrix, respectively. Let the vertex degree sequence be $d_1 \geq d_2 \geq \cdots \geq d_n$ and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ be the eigenvalues of the Laplacian matrix of G. The graph invariants, Laplacian energy (LE), the Laplacian-energy-like invariant (LEL) and the Kirchhoff index (Kf), are defined in terms of the Laplacian eigenvalues of graph G, as $LE = \sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right|$, $LEL = \sum_{i=1}^{n-1} \sqrt{\mu_i}$ and $Kf = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}$, respectively. In this paper, we obtain a new bound for the Laplacian-energy-like invariant LEL and establish the relations between Laplacian-energy-like invariant LEL and the Kirchhoff index Kf. Further, we obtain the relations between the Laplacian energy LE and Kirchhoff index Kf.

Computing Classification System 1998: G.2.2
Mathematics Subject Classification 2010: 05C09, 05C12, 05C50, 05C92, 15A18
Key words and phrases: Laplacian matrix; Laplacian energy; Laplacian-energy-like invariant; Kirchhoff index

1 Introduction

Let $G(V(G), E(G))$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$, where order $|V(G)| = n$ and size $|E(G)| = m$. The degree $d(v_i)$ or d_i of a vertex v_i is the number of edges incident on v_i. The set of vertices adjacent to $v \in V(G)$, denoted by $N(v)$, refers to the *neighborhood* of v. Let $max\{d_i : v_i \in V(G)\} = d_1 = \Delta$ and $min\{d_i : v_i \in V(G)\} = d_n = \delta$. More on notations and definitions, we refer to [15].

The adjacency matrix $A(G)$ associated with G is a square matrix defined as $A(G) = (a_{ij})$, where $a_{ij} = 1$, if vertex v_i is adjacent to vertex v_j, and 0 otherwise. The eigenvalues $\lambda_1, \lambda_2 \dots, \lambda_n$ of $A(G)$ forms the adjacency spectrum of G. The well known properties of the adjacency eigenvalues are $\sum_{i=1}^{n} \lambda_i = 0$, $\sum_{i=1}^{n} \lambda_i^2 = 2m$. The Laplacian matrix $L(G)$ of a graph G is defined as $L(G) = D(G) - A(G)$, where $D(G) = diag\{d_1, d_2, \dots, d_n\}$ is the vertex degree diagonal matrix of G and $A(G)$ is the adjacency matrix of G. The eigenvalues $\mu_1, \mu_2, \dots, \mu_n$ of $L(G)$ forms the Laplacian spectrum of G. The Laplacian matrix is a real symmetric and positive semi-definite matrix. The Laplacian eigenvalues can be arranged in the non-increasing order as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$. We note that $\mu_n = 0$ with multiplicity equal to the number of the connected components of G. Also, $\mu_{n-1} > 0$ if and only if the graph G is connected.

Analogous to the adjacency spectrum of a graph, the Laplacian spectrum also satisfies the following relations $\sum_{i=1}^{n} \mu_i = trace(L(G) = D - A) = 2m$, $\sum_{i=1}^{n} \mu_i^2 = trace(L(G) = D - A)^2 = \sum_{i}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m$, where $M_1 = M_1(G)$ is called the first Zagreb index introduced by Gutman and Trinajstic [3]. A modification to the first Zagreb index, called the Forgotten index $F(G)$, see [2, 3], is defined as the sum of the cubes of the vertex degrees of the graph G, that is, $F = F(G) = \sum_{i=1}^{n} d_i^3$.

In Huckel Molecular Orbital (HMO) model, the total π-electron energy E calculated is a quantum-chemical characteristics of large polycyclic conjugated molecules. Gutman [4] defined the energy E of a graph G as the sum of the absolute values of the eigenvalues of the adjacency matrix. That is, $E = \sum_{i=1}^{n} |\lambda_i|$, where λ_i's are the adjacency eigenvalues of the underlying molecular graph. For the adjacency spectrum, the energy $E(G)$ has the following basic properties.

1. $E(G) \geq 0$, equality if and only if $m = 0$,
2. $E(G) = E(G_1) + E(G_2)$, where G_1 and G_2 are the components of G,

3. If one component of the graph G is G_1 and all other components are isolated vertices, then $E(G) = E(G_1)$.

There has been enormous interest on the investigation of graph energy concept and analogous definitions have been formulated for other matrices associated to a graph. Gutman and Zhou [5], put forward the definition of the Laplacian energy $LE(G)$ of a graph G, as the sum of the absolute deviations (that is, the distances from the average) of the Laplacian eigenvalues.

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|,$$

where G is a graph with n vertices and m edges and $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues.

The Laplacian energy has some analogous properties as the energy $E(G)$ but does not possess the basic properties (2) and (3) of $E(G)$. Also, $LE \geq 0$. To overcome this, Liu and Liu [10] introduced the Laplacian-energy-like invariant (LEL) defined as

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

More on LEL can be seen in [11, 12, 13, 14, 17, 18] and in references therein.

The Wiener Index $W(G)$ of a graph G is a topological index and is defined as

$$W(G) = \sum_{i<j} d_{ij},$$

where d_{ij} is the number of edges in the shortest path between the vertices i and j in G. Wiener [21] investigated the Wiener index and found the correlation between the boiling points of paraffin and the structure of the molecules. Analogous to the Wiener index, Klein and Randic [9] defined the Kirchhoff index $Kf(G)$ of a simple connected graph G as

$$Kf(G) = \sum_{i<j} r_{ij},$$

where r_{ij} is the resistance distance between vertices i and j of G. That is, r_{ij} is equal to the resistance between two equivalent points on an associated electronic network, obtained by replacing each edge of G by a unit (1 Ohm) resistor. Gutman and Mohar [6] and Zhu et al. [22] independently proved that the Kirchhoff index can be represented in terms of the Laplacian eigenvalues as

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

In this article, we obtain a bound for the Laplacian-energy-like invariant and establish some relations between the Laplacian-energy-like and the Kirchhoff index. Also, we establish some relations between the Laplacian energy and the Kirchhoff index.

2 Bound on Laplacian-energy-like invariant

Liu and Liu [10] obtained an upper bound for LEL as

$$\mathsf{LEL} \le \sqrt{2m(n-1)}, \tag{1}$$

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

First we have the following lemmas.

Lemma 1 [20] *Let* $a = (a_i)$, $i = 1, 2, \ldots, n$, *be a positive real number sequence with* $0 < r \le a_i \le R < +\infty$. *Then the following inequality holds.*

$$n\sum_{i=1}^{n} a_i^2 - \left(\sum_{i=1}^{n} a_i\right)^2 \ge \frac{n}{2}(R-r)^2, \tag{2}$$

with equality if and only if $a_1 = R, a_n = r$ *and* $a_2 = a_3 = \cdots = a_{n-1} = \frac{r+R}{2}$

Lemma 2 [1] *Let* G *be a simple graph of order* n *with at least one edge. Then* $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$ *if and only if* G *is a complete graph* K_n.

Now, we present a sharp upper bound for the Laplacian-energy-like invariant in terms of the number of vertices n, the number of edges m, the maximum vertex degree Δ and the algebraic connectivity k.

Theorem 3 *Let G be a simple connected graph of order n and size m. Let the maximum vertex degree be Δ and the algebraic connectivity be $\mu_{n-1} \geq k$. Then*

$$\mathsf{LEL}(G) \leq \sqrt{2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{k}\right)^2} \tag{3}$$

with equality if and only if $G \cong K_n$, where K_n is the complete graph of order n.

Proof. From Lemma 1, for $a = (a_i)$, where a_i are all positive real numbers and $0 < r \leq a_i \leq R < +\infty$, we have

$$n\sum_{i=1}^{n} {a_i}^2 - \left(\sum_{i=1}^{n} a_i\right)^2 \geq \frac{n}{2}(R-r)^2.$$

Setting $n := n-1$, $a_i = \sqrt{\mu_i}$, $r = \sqrt{\mu_{n-1}}$ and $R = \sqrt{\mu_1}$, we get

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

Since $\sum_{i=1}^{n-1} \mu_i = \mathsf{trace}(L) = \sum_{i=1}^{n} d_i = 2m$ and $\mathsf{LEL} = \sum_{i=1}^{n-1} \sqrt{\mu_i}$, we have

$$(n-1)2m - (\mathsf{LEL})^2 \geq \left(\frac{n-1}{2}\right)\left(\sqrt{\mu_1} - \sqrt{\mu_{n-1}}\right)^2,$$

$$\text{or}\quad \mathsf{LEL}^2 \leq 2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\mu_1} - \sqrt{\mu_{n-1}}\right)^2,$$

$$\text{or}\quad \mathsf{LEL} \leq \sqrt{2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\mu_1} - \sqrt{\mu_{n-1}}\right)^2}.$$

For $\Delta + 1 \leq x \leq n$, consider the function

$$f(x) = 2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{x} - \sqrt{\mu_{n-1}}\right)^2.$$

Differentiating both sides with respect to x, we have

$$\begin{aligned} f'(x) &= -\left(\frac{n-1}{2}\right) 2\left(\sqrt{x} - \sqrt{\mu_{n-1}}\right)\left(\frac{1}{2\sqrt{x}}\right) \\ &= -\left(\frac{n-1}{2}\right)\left(\frac{\sqrt{x} - \sqrt{\mu_{n-1}}}{\sqrt{x}}\right) \leq 0. \end{aligned}$$

That is, $f(x)$ is a decreasing function of x for $\Delta+1 \leq x$. So

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

Therefore,

$$LEL \leq 2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{\mu_{n-1}}\right)^2.$$

Again, consider the function

$$g(x) = 2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{x}\right)^2 \text{ for } x \geq k.$$

Differentiating both sides with respect to x, we get $g'(x) =$

$$-2\left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{x}\right)\left(\frac{-1}{2\sqrt{x}}\right) = \left(\frac{n-1}{2}\right)\left(\frac{\sqrt{\Delta+1} - \sqrt{x}}{\sqrt{x}}\right).$$

Again, differentiating both sides with respect to x, we get

$$\begin{aligned} g''(x) &= \left(\frac{n-1}{2}\right)\frac{\sqrt{x}\left(-\frac{1}{2\sqrt{x}}\right) - \left(\sqrt{\Delta+1} - \frac{1}{2\sqrt{x}}\right)\sqrt{x}}{x} \\ &= \left(\frac{n-1}{2}\right)\frac{\sqrt{x}\left(-\frac{1}{2\sqrt{x}} - \sqrt{\Delta+1} + \frac{1}{2\sqrt{x}}\right)}{x} \\ &= \left(\frac{n-1}{2}\right)\frac{-\sqrt{\Delta+1}}{\sqrt{x}} = -\left(\frac{n-1}{2}\right)(\frac{\sqrt{\Delta+1}}{\sqrt{x}}) \\ &\leq 0. \end{aligned}$$

This implies that $g(x)$ is an increasing function for $x \geq k$. Therefore,

$$g(x) \leq g(k) = 2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{k}\right)^2.$$

This gives

$$LEL \leq \sqrt{2m(n-1) - \left(\frac{n-1}{2}\right)\left(\sqrt{\Delta+1} - \sqrt{k}\right)^2}.$$

Equality occurs in Inequality (3) if and only if the equality occurs in Lemma 1, that is, if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-1} = \frac{\mu_1+\mu_{n-1}}{2}$, which is possible, if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$, that is, by Lemma 2, if and only if $G \cong K_n$, proving the theorem. □

Remark 4 *It is evident from Inequality (3), that the bound in Theorem 3 is sharper than the bound given in Inequality (1).*

3 Relations between Laplacian-energy-like invariant and Kirchhoff index

In this section, we present two relations between Laplacian-energy-like invariant and Kirchhoff index. First, we have the following observation.

Lemma 5 [8] *Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \dots, n$, be two sequences of positive real numbers such that $p_1+p_2+\cdots+p_n = 1$ and $0 < r \le a_i \le R <= \infty$. Then the following inequality holds.*

$$\sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} \frac{p_i}{a_i} \le \frac{1}{4}\left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}}\right)^2.$$

Lemma 6 [7] *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a positive real number sequence and let $a = (a_i), b = (b_i), \dots, c = (c_i), i = 1, 2, \dots, n$, be r sequences of non-negative real numbers of similar monotonicity. Then the following inequality holds.*

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i b_i \dots c_i \ge \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \cdots \sum_{i=1}^{n} p_i c_i,$$

with equality if and only if $r-1$ sequences are constant.

Theorem 7 *Let G be a simple connected graph of order n and size m. Let the maximum vertex degree be Δ, first Zagreb index M_1 and the algebraic connectivity be $\mu_{n-1} \ge k$. Then,*

$$LEL \ge \sqrt{\frac{4k(M_1+2m)(Kf)}{(n+k)^2}}. \tag{4}$$

with equality if and only if $G \cong K_n$, where K_n is the complete graph of order n.

Proof. From Lemma 5, for real numbers p_i, $a_i > 0$ and $\sum_{i=1}^{n} p_i = 1$, $0 < r \leq a_i \leq R < +\infty$, we have

$$\sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} \frac{p_i}{a_i} \leq \frac{1}{4}\left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}}\right)^2.$$

Setting $p_i = \frac{\sqrt{\mu_i}}{LEL}$, $a_i = (\mu_i)^{\frac{3}{2}}$ $\quad i = 1, 2, \ldots, n-1$, where $LEL = \sum_{i=1}^{n-1} \sqrt{\mu_i}$, we get

$$\sum_{i=1}^{n-1}\left(\frac{\mu_i^2}{LEL}\right)\sum_{i=1}^{n-1}\left(\frac{\frac{1}{\mu_i}}{LEL}\right) \leq \frac{1}{4}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2$$

$$\text{or} \quad \frac{\sum_{i=1}^{n-1}\mu_i^2 \sum_{i=1}^{n-1}\frac{1}{\mu_i}}{LEL^2} \leq \frac{1}{4}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2$$

$$\text{or} \quad \frac{(M_1 + 2m)(\frac{Kf}{n})}{LEL^2} \leq \frac{1}{4}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2.$$

This gives

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

For $\Delta + 1 \leq x \leq n$, consider the function, $f(x) = \frac{x}{(x+\mu_{n-1})^2}$. Differentiating both sides with respect to x, we get

$$\begin{aligned} f'(x) &= \frac{(x + \mu_{n-1})^2(1) - 2x(x + \mu_{n-1})}{(x + \mu_{n-1})^4} \\ &= \frac{x + \mu_{n-1} - 2x}{(x + \mu_{n-1})^3} = \frac{\mu_{n-1} - x}{(x + \mu_{n-1})^3} \leq 0. \end{aligned}$$

This implies that $f(x)$ is a decreasing function. Thus,

$$f(x) \geq f(n) = \frac{n}{(n + \mu_{n-1})^2}.$$

Therefore,

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

Now, for $x \geq k$, consider the function $g(x) = \frac{x}{(n+x)^2}$.
As it is an increasing function of x, so we have $g(x) \geq g(k) = \frac{k}{(n+k)^2}$. Therefore,

$$LEL \geq \sqrt{\frac{4(M_1 + 2m)(Kf)k}{(n+k)^2}},$$

Equality occurs in Theorem 7 if and only if the sequence a_i in Lemma 5 is a constant, that is all a_i's are equal. Therefore $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$. Then, by Lemma 2, $G \cong K_n$ and the proof is complete. □

4 Relation between Laplacian energy and Kirchhoff index

In this section, we obtain two relations between the Laplacian energy and the Kirchhoff index. We begin with the following.

Lemma 8 [19] (Radon Inequality). *If $a_i, x_i > 0$, $n > 0$, $i \in 1, 2, \ldots, n$, then*

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \frac{(\sum_{i=1}^{n} x_i)^{r+1}}{(\sum_{i=1}^{n} a_i)^r}$$

where r is an arbitrary real number such that $r \leq 1$ or $r \geq 0$. Equality holds if and only if either $r = -1$, or $r = 0$ or $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

Lemma 9 [1] *Let G be a graph of order $n \geq 3$ vertices and maximum degree Δ. Then $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$ if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\Delta,\Delta}$.*

Theorem 10 *Let G be a graph on n vertices and m edges with maximum degree Δ. Then,*

$$(2m - \Delta - 1)\left[(2m - \Delta - 1) - \frac{4m}{n}(n-2) + \frac{4m^2}{n^3}(Kf - 1)\right] \geq (LE - \Delta - 1)^2$$

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

Proof. In Lemma 8 (Radon inequality), setting

$$r = 1, \quad x_i = \left|\mu_i - \frac{2m}{n}\right|, \quad a_i = \mu_i, \quad i = 2, 3, \ldots, n-1,$$

we obtain

$$\sum_{i=2}^{n-1} \frac{(\mu_i - \frac{2m}{n})^2}{\mu_i} \geq \frac{(\sum_{i=2}^{n-1} |\mu_i - \frac{2m}{n}|)^2}{\sum_{i=2}^{n-1} \mu_i}.$$

We have, $(\mu_i - \frac{2m}{n})^2 = (\mu_i)^2 + \frac{4m^2}{n^2} - \frac{4m}{n}\mu_i$. Therefore,

$$\begin{aligned}
\sum_{i=2}^{n-1} \frac{(\mu_i - \frac{2m}{n})^2}{\mu_i} &= \sum_{i=2}^{n-1} \mu_i + \frac{4m^2}{n^2} \sum_{i=2}^{n-1} \frac{1}{\mu_i} - \frac{4m}{n} \sum_{i=2}^{n-1} 1 \\
&= (2m - \mu_1) + \frac{4m^2}{n^2}\left(\frac{Kf}{n} - \frac{1}{\mu_1}\right) - \frac{4m}{n}(n-2) \\
&= (2m - \mu_1) + \frac{4m^2}{n^3}\left(Kf - \frac{n}{\mu_1}\right) - \frac{4m}{n}(n-2)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\left(\sum_{i=2}^{n-1} |\mu_i - \frac{2m}{n}|\right)^2}{\sum_{i=2}^{n-1} \mu_i} &= \frac{\left(\sum_{i=1}^{n} |\mu_i - \frac{2m}{n}| - (\mu_1 - \frac{2m}{n}) - (\frac{2m}{n} - 0)\right)^2}{\sum_{i=1}^{n} \mu_i - \mu_1 - 0} \\
&= \frac{(LE - \mu_1)^2}{2m - \mu_1},
\end{aligned}$$

since $\mu_n = 0$. Thus,

$$(2m - \mu_1) + \frac{4m^2}{n^3}\left(Kf - \frac{n}{\mu_1}\right) - \frac{4m}{n}(n-2) \geq \frac{(LE - \mu_1)^2}{2m - \mu_1}$$

$$\text{or } (2m - \mu_1)\left((2m - \mu_1) + \frac{4m^2}{n^3}\left(Kf - \frac{n}{\mu_1}\right) - \frac{4m}{n}(n-2)\right) \geq (LE - \mu_1)^2.$$

Since $\Delta + 1 \leq \mu_1 \leq n$, so

$$\big(2m-(\Delta+1)\big)\left[(2m-(\Delta+1)) + \frac{4m^2}{n^3}(Kf - 1) - \frac{4m}{n}(n-2)\right] \geq (LE - n)^2,$$

For equality in Theorem 10, all the above inequalities must be equalities. Therefore, we have $\mu_2 = \mu_3 = \mu_{n-1}$. Since $\mu_1 = \Delta + 1$, so by Lemma 9, $G \cong K_n$, or $G \cong K_{1,n-1}$, completing the proof. □

Theorem 11 *If G is a connected graph on n vertices and m edges with maximum vertex degree Δ, then*

$$\left(F + 3M_1 - 6C_3 - (\Delta+1)^3\right) + \frac{4m^2}{n^2}\left(2m - (\Delta+1)\right) - \frac{4m}{n}\left(M_1 + 2m - (\Delta+1)^2\right) \geq \frac{n\left(LE - (\Delta+1)\right)^2}{(Kf - 1)},$$

where F, M_1 and C_3 are the Forgotten index, first Zagreb index and the number of the triangles, respectively. And equality occurs if and only if $G \cong K_n$ or $\mu_1 = \mu_2 = \cdots = \mu_p$, $\mu_{p+1} = \mu_{p+2} = \cdots = \mu_{n-1}$, $(1 \leq p \leq n-2)$ with $n(\mu_1^2 + \mu_{n-1}^2) = 2m(\mu_1 + \mu_{n-1})$.

Proof. In Radon inequality, set $r = 1$, $x_i = \left|\mu_i - \frac{2m}{n}\right|$, $a_i = \frac{1}{\mu_i}$, $i = 2, 3, \ldots, n-1$, we get

$$\sum_{i=2}^{n-1}\left(\mu_i - \frac{2m}{n}\right)^2 \mu_i \geq \frac{\left(\sum_{i=2}^{n-1}\left|\mu_i - \frac{2m}{n}\right|\right)^2}{\sum_{i=2}^{n-1}\frac{1}{\mu_i}}.$$

Now,

$$\begin{aligned}
\sum_{i=2}^{n-1}\left(\mu_i - \frac{2m}{n}\right)^2 \mu_i &= \sum_{i=2}^{n-1}\left(\mu_i^3 + \frac{4m^2}{n^2}\mu_i - \frac{4m}{n}\mu_i^2\right) \\
&= \sum_{i=2}^{n-1}\mu_i^3 + \frac{4m^2}{n^2}\sum_{i=2}^{n-1}\mu_i - \frac{4m}{n}\sum_{i=2}^{n-1}\mu_i^2 \\
&= \left(\sum_{i=1}^{n-1}\mu_i^3 - \mu_1^3\right) + \frac{4m^2}{n^2}\left(\sum_{i=1}^{n-1}\mu_i - \mu_1\right) - \frac{4m}{n}\left(\sum_{i=1}^{n-1}\mu_i^2 - \mu_1^2\right) \\
&= (F + 3M_1 - 6C_3 - \mu_1^3) + \frac{4m^2}{n^2}(2m - \mu_1) - \frac{4m}{n}(M_1 + 2m - \mu_1^2).
\end{aligned}$$

For the Laplacian, we have

$$\sum_{i=1}^{n-1} \mu_i = \mathrm{trace}(D-A) = \sum_{i=1}^{n} d_i = 2m,$$
$$\sum_{i=1}^{n-1} \mu_i^2 = \mathrm{trace}(D-A)^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m,$$
$$\sum_{i=1}^{n-1} \mu_i^3 = \mathrm{trace}(D-A)^3 = \mathrm{trace}(D^3 - 3D^2A + 3DA^2 - A^3) = F + 3M_1 - 6C_3,$$

and

$$\frac{\left(\sum_{i=2}^{n-1} \left|\mu_i - \frac{2m}{n}\right|\right)^2}{\sum_{i=2}^{n-1} \frac{1}{\mu_i}} = \frac{\left(\sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right| - (\mu_1 - \frac{2m}{n}) - (\frac{2m}{n} - \mu_n)\right)^2}{\sum_{i=1}^{n-1} \frac{1}{\mu_i} - \frac{1}{\mu_1}}$$
$$= \frac{(LE - \mu_1)^2}{\frac{Kf}{n} - \frac{1}{\mu_1}} = \frac{n(LE - \mu_1)^2}{Kf - \frac{n}{\mu_1}}.$$

Therefore,

$$\left(F + 3M_1 - 6C_3 - \mu_1^3\right) + \frac{4m^2}{n^2}(2m - \mu_1) - \frac{4m}{n}(M_1 + 2m - \mu_1^2)$$
$$\geq \frac{n(LE - \mu_1)^2}{Kf - \frac{n}{\mu_1}}.$$

For, $\Delta + 1 \leq \mu_1 \leq n$, this becomes

$$\left(F + 3M_1 - 6C_3 - (\Delta+1)^3\right) + \frac{4m^2}{n^2}\left(2m - (\Delta+1)\right)$$
$$- \frac{4m}{n}\left(M_1 + 2m - (\Delta+1)^2\right) \geq \frac{n\left(LE - (\Delta+1)\right)^2}{Kf - 1}.$$

Equality case can be proved as the equality shown in Theorem 3.1 in [14]. This completes the proof. □

Acknowledgements

The research of Sandeep Bhatnagar is supported by CSIR, India as a Senior Research Fellowship, file No.09/112(0642)/2019-EMR-I. The research of S.

Pirzada is supported by SERB-DST, New Delhi under the research project number CRG/2020/000109.

References

[1] K.C. Das, A sharp upper bound for the number of spanning trees of a graph, *Graphs Comb.* **23** (2007) 625–632. ⇒188, 193

[2] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190. ⇒186

[3] I. Gutman, N. Trinajstic, Graph Theory and Molecular Orbitals, Total π-electron energy of alternate hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538. ⇒186

[4] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sekt. Forschungszenturm Graz* **103** (1978) 1–22. ⇒186

[5] I. Gutman, B. Zhou, Laplacian energy of a graph, *Linear Algebra Appl.* **414** (2006) 29–37. ⇒187

[6] I. Gutman, B. Mohar, The quasi-Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985. ⇒188

[7] T. Hayashi, On some inequalities, *Rend. Circ. Mat. Palermo* **44** (1920) 336–340. ⇒191

[8] P. Henrici, Two remarks on Kantorovich inequality, *Amer. Math. Monthly* **68(9)** (1961) 904–906. ⇒191

[9] D.J. Klein, M. Randic, Resistence distance, *J. Math. Chem.* **12** (1993) 81–95. ⇒187

[10] J. Liu, B.A. Liu, A Laplacian-Energy-like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 355–372. ⇒187, 188

[11] B. Liu, Z.Y. Liu, A Survey on the Laplacian-energy-like invariant, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 713–730. ⇒187

[12] E.I. Milovanovic, I. Z. Milovanovic, M. M. Matejic, On relation between Kirchhoff index and Laplacian-energy-like invariant of graphs, *Math. Int. Res.* **2** (2017) 141–154. ⇒187

[13] I. Milovanovic, E. Milovanovic, E. Glogic, M. Matejic, On Kirchhoff index, Laplacian energy and their relation, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 405–418. ⇒187

[14] P. Milosevic, E. Milovanovic, M. Matejic, I. Milovanovic, On relations between Kirchhoff index, Laplacian energy, Laplacian–energy–like invariant and degree deviation of graphs, *Filomat* **34**(2020) 1025—1033. ⇒187, 196

[15] S. Pirzada, *An Introduction to Graph Theory*, Universities Press, Hyderabad, India, 2012. ⇒186

[16] S. Pirzada, H.A. Ganie, On Laplacian-Energy-like invariant and Incidence energy, *Trans. Comb.* **4(3)** (2015) 25–35. ⇒

[17] S. Pirzada, H.A. Ganie, I. Gutman, On Laplacian-Energy-like invariant and Kirchhoff Index, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 41–60. ⇒187

[18] S. Pirzada, H. A. Ganie, I. Gutman, Comparison between Laplacian-energy-like invariant and the Kirchhoff index, *Elec. J. Lin. Algebra* **31** (2016) 27–41. ⇒187

[19] J. Radon, Theorie und Anwendungen der absolut Additiven Mengenfunktionnem, *Sitzungsber Acad. Wissen, Wien* **122** (1913) 1295–1438. ⇒193

[20] J. Szőkefalvi Nagy, Uber algebraische Gleichungenmit lauter reellen Wurzeln, *Jahresbericht der deutschen Mathematiker Vereingung* **27** (1918) 37–43. ⇒188

[21] H. Wiener, Structural determination of paraffin boilling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20. ⇒187

[22] H.Y. Zhu, D.J. Klein, I. Lukovits, Extensions of the Wiener numbers, *J. Chem. Inform. Comput. Sci.* **36(3)** (1996) 420–428. ⇒188

Received: October 1, 2022 • Revised: November 6, 2022