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LAPLACIAN ENERGY OF GRAPHS AND DIGRAPHS

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CERTIFICATE

Certified that the thesis entitled "Laplacian energy of graphs and digraphs" being submitted by Hilal Ahmad Ganie, in partial fulfillment of the requirements for the award of Doctor of Philosophy in Mathematics, is his own work carried out by him under my supervision and guidance. The content of this thesis, in full or in parts, has not been submitted to any Institute or University for the award of any degree or diploma.

Professor S. Pirzada.
Supervisor

ABSTRACT

In Chapter 1, we present a brief introduction of spectra of graphs and some definitions. Chapter 2 is a brief review of energy of graphs. We obtain sufficient conditions for the existence of non A-cospectral equienergetic graphs. We also obtain sufficient conditions for the existence of hyperenergetic graphs. In Chapter 3, we study the Laplacian energy of graphs. We obtain bounds for the Laplacian energy of graphs in terms of the number of vertices n, the number of edges m, maximum degree Δ and clique number ω, which improve some previously known bounds. We also construct some new families of non L-cospectral L-equienergetic graphs. In Chapter 4, we study the relation between energy and Laplacian energy of graphs. We give various constructions of the families of graphs G for which energy is greater than the corresponding Laplacian energy. We also give a construction of non bipartite graphs for which energy is less than the corresponding Laplacian energy. In Chapter 5, we study *Laplacian-energy-like invariant* $LEL(G)$ and *Kirchhoff index* $Kf(G)$ of graphs. We obtain a lower bound for $LEL(G)$ and an upper bound for $Kf(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ and a positive real number k. We consider the relation between $LEL(G)$ and $Kf(G)$ and obtain some sufficient conditions for a graph G or its complement $\overline{G}$ to satisfy the inequality $LEL(G) > Kf(G)$. As a consequence, we arrive at a complete comparison of $LEL(G)$ and $Kf(G)$ for the complement of a tree, unicyclic graphs, bicyclic graphs, tricyclic graphs and tetracyclic graphs. In Chapter 6, we study the Laplacian energy of digraphs. We obtain

bounds for the Laplacian energy of digraphs in terms of the number of vertices n, the number of arcs m and numbers M, M_1, K, which improve some previously known bounds.

Dedication

Dedicated to my beloved parents and grand parents

Khazir Mohammad Ganie, Shah Begum and Late Sakhie Mohammad, Azie.

DECLARATION

I, Hilal Ahmad Ganie hereby declare that the thesis entitled "Laplacian energy of graphs and digraphs" being submitted in partial fulfillment of the requirements for the award of Doctor of Philosophy in Mathematics, is my own work carried out by me under the supervision of Prof. S. Pirzada. The content of this thesis, in full or in parts, has not been submitted to any Institute or University for the award of any degree or diploma.

Hilal Ahmad Ganie.

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[**1**] Hilal A. Ganie, S. Pirzada and E. T. Baskoro, On Energy, Laplacian energy and p-fold graphs, *Electronic Journal of Graph Theory and Applications* **3, 1** (2015), 94-107.

[**2**] S. Pirzada and Hilal A. Ganie, Spectra, Energy and Laplacian energy of Strong double graphs, Springer International Publishing Switzerland 2015, D. Mugnolo (ed.), Mathematical Technology of Networks Volume 128 of the series Springer Proceedings in Mathematics and Statistics pp 175-189.

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[**4**] S. Pirzada and Hilal A. Ganie, On Laplacian-energy-like invariant and Incidence energy, *Transactions on Combinatorics*, **4, 3** (2015) 41-51.

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CHAPTER 1

Introduction

1.1 Background

Spectral graph theory (Algebraic graph theory) which emerged in 1950s and 1960s is the study of properties of a graph in relationship to the characteristic polynomial, eigenvalues and eigenvectors of matrices associated to the graph. The major source of research in spectral graph theory has been the study of relationship between the structural and spectral properties of graphs. Another source has research in quantum chemistry. Just as astronomers study stellar spectra to determine the make-up of distant stars, one of the main goals in spectral graph theory is to deduce the principal properties and structure of a graph from its graph spectrum (or from a short list of easily computable invariants). The spectral approach for general graphs is a step in this direction. It has been seen that eigenvalues are closely related to almost all major invariants of a graph, linking one extremal property to another. Evidently, eigenvalues play a central role in our fundamental understanding of graphs. The study of graph eigenvalues realizes increasingly rich connections with many other areas of mathematics. A particularly important development is the interaction between spectral graph theory and differential geometry. There is an interesting analogy between spectral Riemannian geometry and spectral graph theory. The concepts and methods of spectral geometry bring useful tools and crucial insights to the study of graph eigenvalues, which in turn lead to new directions and results in spectral geometry. Algebraic spectral methods are also very useful, especially for extremal examples and constructions. The 1980 monograph 'spectra of graphs' by Cvetković, Doob and Sach [28] summarised nearly all research to date in the area. In 1988 it was updated by the survey 'Recent results in the theory of graph spectra'. The third edition of spectra of graphs (1995) contains a summary of the further contributions to the subject. Since then the theory has been developed to a greater extent and many research papers have been published. It is important to mention that spectral graph theory has a wide range of applications to other areas of mathematics and to other areas of sciences which include Computer Science, Physics, Chemistry, Biology, Statistics etc.

One of the richest theories in spectral graph theory is the energy of graphs.

The concept of energy of a graph is formulated from the pioneering work of Hückel [60, 83] who made certain simplification of Schrodinger's wave equations [28]. Chemists are interested in finding the wave functions and energy levels of a given molecule. The wave functions ϕ are the solutions of Schrodinger's wave equation $(H - E)\phi = 0$, where H is the energy operator and E is the electron energy. In order to solve this equation for molecules, Hückel [83] replaced the Schrodinger's wave function by the speculation equation $\det(H - ES) = 0$, where $H = \alpha I + \beta A$ and $S = I + \sigma A$. Here α (the Coulomb integral for carbon atom), β (the resonance integral for two carbon atoms) and σ are all constants. If we normalize the system so that $\alpha = 0$ (the zero energy reference point) and $\beta = 1$ (the energy unit), then H is the adjacency matrix $A(G)$ of the associated graph G. The wave functions ϕ are then the eigenvalues of $A(G)$. Both wave functions and energy levels can be measured experimentally and accord well with the predictions of Hückel theory.

The spectra of graphs can be used to calculate the energy levels of a conjugated hydrocarbon as calculated with Hückel Molecular Orbital (HMO) method. The details of Hückel theory and how it is related to spectral graph theory can be found in [28].

To study the energy levels of general class of graphs certainly help us in determining the energy levels of various classes of conjugated hydrocarbons in chemistry. Considerable work on this aspect has been done from Hückel [83] till today.

Conjugated hydrocarbons are of great importance for both science and technology. A conjugated hydrocarbon can be characterized as a molecule composed entirely of carbon and hydrogen atoms, every carbon atom having exactly three neighbours (which may be either carbon or hydrogen atoms). For example, benzene is a conjugated hydrocarbon. There are theoretical reasons [60, 130] to associate a graph with a conjugated hydrocarbon according to the following rule:

Every carbon atom is represented by a vertex and every carbon-carbon sigma bond by an edge, hydrogen atoms are ignored, e.g., the molecular graph of benzene is C_6, a cycle on six vertices.

An important quantum-chemical characteristic of a conjugated molecule is its total π-electron energy. Within the Hückel Molecular Orbital (HMO) theory this quantity can be reduced to

$$E = E(G) = \sum_{j=1}^{n} |x_j|,$$

where $x_j,\ j = 1, 2, \ldots, n$, are the eigenvalues of the respective molecular graph.

Gutman [72] in 1978 defined the concept of energy for graphs. This concept became so popular that more than 300 papers have been published in this direction till date. At the beginning some chemical problems were given graph theoretical shape and were solved using spectral graph theory. One such problem can be seen in [74]. Upper and lower bounds for energy were obtained for different classes of graphs which can be used to estimate the total π-electron energy of molecular graphs. Peña and Rada [115] in 2007 extended the concept of energy to digraphs and defined the energy of a digraph as the sum of the absolute values of real parts of eigenvalues of the digraph. They obtained Coulson's integral formula for energy of digraphs and also characterized unicyclic digraphs with minimal and maximal energy.

As one can associate various matrices (like Laplacian matrix, signless Laplacian matrix, distance matrix, normalized Laplacian/signless Laplacian matrix, Randic matrix etc) to a graph. It is natural to define an energy like quantity for these matrices. Since average of the eigenvalues of the matrix $A(G)$ is zero, the energy of a graph G can be viewed as the sum of the absolute deviation of the eigenvalues of the matrix $A(G)$ from their average. Motivated by this, Gutman and Zhou [65] in 2006 considered the sum of the absolute deviations of the eigenvalues of the Laplacian matrix $L(G)$ from their average $\frac{2m}{n}$ and called this quantity as the Laplacian energy $LE(G)$ of graph G, that is,

$$LE(G) = \sum_{j=1}^{n} |\mu_j - \frac{2m}{n}|.$$

It was shown that both energy and Laplacian energy share various properties but there are some differences, as well. In fact, it is shown in [123] that the Laplacian energy has remarkable chemical applications beyond the molecular orbital theory of conjugated molecules. Laplacian graph energy is a broad measure of graph complexity. Song et al. [132] have introduced component-wise Laplacian graph energy, as a complexity measure useful to filter image description hierarchies. Various upper and lower bounds have been established for Laplacian energy for any graph in general and in particular, for different classes of graphs, which connects it with various graph parameters.

From the definition of energy and Laplacian energy, one can observe that both these energies represent the sum of the absolute deviation of corresponding eigenvalues from their average value. Thus, we can define the energy of a given matrix M, and call it as M-energy, as the sum of the absolute deviation of eigenvalues of M from their average value. This way, the energy of a graph is its A-energy and the Laplacian energy of a graph is its L-energy. Other types of energy can be defined in the same way, the difference being only in the matrix under consideration: for example, the energy of a distance matrix is studied in [84]. Among those found in literature, it is the *Laplacian-energy-like invariant* only, defined by Liu and Liu [98], that does not fit this setting (which at the end, may happen to be to its advantage, as a number of extremal problems for Laplacian-energy-like invariant can be solved by considering the coefficients of characteristic polynomial of $L(G)$ and finding transformations which are monotone on these coefficients).

On the other hand, Nikiforov [110] has recently introduced another concept of the energy of a complex matrix M as the sum of the singular values of M, which made possible to determine the energy of random graphs.

Various Laplacian spectrum based graph invariants other than Laplacian energy were considered by different researchers for application point of view, among those the most studied are *Laplacian-energy-like invariant* $LEL(G)$ and *Kirchhoff index* $Kf(G)$ of a graph G. The *Laplacian-energy-like invariant* was put forward by Liu and Liu [98] in 2008 as the sum of the square roots of the Laplacian eigenvalues of G, that is,

$$LEL(G) = \sum_{j=1}^{n} \sqrt{\mu_j}.$$

Stevanoić et al. [134] showed that $LEL(G)$ of a graph G describes well the properties which are accounted by the majority of molecular descriptors: motor octane number, entropy, molar volume, molar refraction, particularly the acentric factor AF parameter, but also more difficult properties like boiling point, melting point and partition coefficient $LogP$. In a set of polycyclic aromatic hydrocarbons, $LEL(G)$ of a graph was proved [134] to be as good as the Randić index (a connectivity index) and better than the Wiener index (a distance based index).

The *Kirchhoff index* $Kf(G)$ of a connected graph G was put forward by Gutman and Mohar [64] and Zhu [161], as the number of vertices times the sum of the reciprocals of positive Laplacian eigenvalues of graph G, that is,

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

This index is also named as total effective resistance [90] or the effective graph resistance [40], and like the Wiener index have found applications in chemistry, electrical network, Markov chains, averaging networks, experiment design, and Euclidean distance embeddings, see [18, 56, 90, 91].

In 2009, Adiga and Smitha [4], motivated by skew energy put forward by Adiga et al. [2] for a digraph $\mathscr{D}$, considered the skew adjacency matrix $S(\mathscr{D}) = (s_{ij})$ of a digraph $\mathscr{D}$, which is defined as, $s_{ij} = 1$, if (v_i, v_j) is an arc, $s_{ij} = -1$, if (v_j, v_i) is an arc and 0, otherwise. Following the definition of Laplacian energy by Lazic [95], they extended the concept of Laplacian energy to digraphs by defining it, as the sum of the absolute values of the eigenvalues of the matrix $D(\mathscr{D}) - S(\mathscr{D})$. Nearly, in the same year, Adiga and Khoshbakht [3] following the definition of Laplacian energy by Gutman et al. defined the Skew Laplacian energy $SLE_g(\mathscr{D})$ of the digraph $\mathscr{D}$ as the sum of the absolute deviations of the eigenvalues of the matrix $D(\mathscr{D}) - S(\mathscr{D})$ from the average degree $\frac{2m}{n}$. Both these definitions of Laplacian energy of a digraph do not get the familiarity among the researchers as the matrix $D(\mathscr{D}) - S(\mathscr{D})$ does not specify the indegree and outdegree of a digraph.

In 2010, Kissani and Mizoguchi [89] introduced a different way of defining the Laplacian energy for directed graphs, in which only the outdegrees of the vertices are considered rather than both the outdegrees and indegrees. Moreover, Kissani and Mizoguchi [89] established some relation between the Laplacian energy of a graph (as put forward by Lazic [95]) and the Laplacian energy $LE_k(\mathscr{D})$ of the corresponding digraph $\mathscr{D}$ and used the so-called minimization maximum out-degree (MMO) algorithm [10] to determine the digraphs with minimum Laplacian energy. The shortage of this definition is that it does not make use of the inadjacency information of a digraph.

Recently (in 2013) Cai et al. [22] defined a new type of skew Laplacian matrix $\widetilde{SL}(\mathscr{D})$ of a digraph $\mathscr{D}$. Let $D^+(\mathscr{D})$ and $D^-(\mathscr{D})$ be respectively the diagonal matrices of vertex outdegree and vertex indegree and let $A^+(\mathscr{D})$ and $A^-(\mathscr{D})$ be respectively the outadjacency and inadjacency matrix of the digraph $\mathscr{D}$. If $A(G)$

is the adjacency matrix of the underlying graph G of the digraph $\mathscr{D}$, then it is clear that $A(G) = A^+(\mathscr{D}) + A^-(\mathscr{D})$ and $S(\mathscr{D}) = A^+(\mathscr{D}) - A^-(\mathscr{D})$, where $S(\mathscr{D})$ is the skew adjacency matrix of the digraph $\mathscr{D}$. The matrix $\widetilde{SL}(\mathscr{D}) = \widetilde{D}(\mathscr{D}) - S(\mathscr{D})$, where $\widetilde{D}(\mathscr{D}) = D^+(\mathscr{D}) - D^-(\mathscr{D})$ is called, by Cai et al. [22], the skew Laplacian matrix of the digraph $\mathscr{D}$. Following the definition of matrix energy by Nikifrov [110], Cai et al. [22] defined the skew Laplacian energy of a digraph $\mathscr{D}$, as the sum of the absolute values of the eigenvalues of the matrix $\widetilde{SL}(\mathscr{D})$, that is

$$SLE(\mathscr{D}) = \sum_{i=1}^{n} |\nu_i|,$$

where $\nu_1, \nu_2, \ldots, \nu_n$ are the eigenvalues of $\widetilde{SL}(\mathscr{D})$ and obtained various bounds. This definition seems to be well chosen as the matrix $\widetilde{SL}(\mathscr{D})$ specify the inadjacency, outadjacency, indegree and outdegree of a digraph $\mathscr{D}$.

1.2 Basic Definitions

Definition 1.2.1. *Graph.* A graph G is a pair $(V, \mathscr{E})$, where V is a nonempty set of objects called vertices and $\mathscr{E}$ is a subset of $V^{(2)}$, (the set of distinct unordered pairs of distinct elements of V). The elements of $\mathscr{E}$ are called edges of G.

Definition 1.2.2. *Multigraph.* A multigraph G is a pair $(V, \mathscr{E})$, where V is a nonempty set of vertices and $\mathscr{E}$ is a multiset of unordered pairs of distinct elements of V. The number of times an edge occurs in G is called its multiplicity and edges with multiplicity greater than one are called multiple edges.

Definition 1.2.3. *General graph.* A general graph G is a pair $(V, \mathscr{E})$, where V is a non empty set of vertices and $\mathscr{E}$ is a multiset of unordered pairs of elements of V. We denote by (u, v) an edge from vertex u to vertex v. An edge of the form (u, u), where $u \in V$, is called loop of G and edges which are not loops are called proper edges. The number of times a loop occurs is called its multiplicity. A loop with multiplicity greater than one is called a multiple loop.

Definition 1.2.4. *Subgraph of a graph.* Let $G = (V, \mathscr{E})$ be a graph, $H = (U, \mathscr{E}')$ is the subgraph of G whenever $U \subseteq V$ and $\mathscr{E}' \subseteq \mathscr{E}$. If $U = V$ the subgraph is said to be spanning. An induced subgraph $\langle U \rangle$ is the subset of V together with all the edges of G between the vertices in U.

Definition 1.2.5. *Bipartite graph.* A graph $G(V, \mathscr{E})$ is said to be bipartite, if its vertex set V can be partitioned into two parts, say V_1 and V_2 such that each edge has one end in V_1 and other in V_2.

Definition 1.2.6. *Degree.* Degree of a vertex v in a graph $G(V, \mathscr{E})$ is the number of edges incident on v and is denoted by d_v or $d(v)$.

Definition 1.2.7. *k-Regular graph.* A graph $G(V, \mathscr{E})$ is said to be k-regular if for every vertex $v \in V$, $d_v = k$.

Definition 1.2.8. *Path.* A path of length $n-1$ $(n \geq 2)$, denoted by P_n, is a graph with n vertices $v_1, v_2, \ldots, v_n$ and with $n-1$ edges (v_i, v_{i+1}), where $i = 1, 2, \ldots, n-1$.

Definition 1.2.9. *Cycle.* A cycle of length n, denoted by C_n, is the graph with vertex set $v_1, v_2, \ldots, v_n$ having edges (v_i, v_{i+1}), $i = 1, 2, \ldots, n-1$ and (v_n, v_1).

Definition 1.2.10. *Connectedness in graphs.* A graph $G(V, \mathscr{E})$ is said to be connected if for every pair of vertices u and v there is a path from one to other.

Definition 1.2.11. *Matching.* Let $G(V, \mathscr{E})$ be a graph with n vertices and m edges. A k-matching of G is a collection of k independent edges (i.e., edges which do not share a vertex) of G.

Definition 1.2.12. *Clique.* Let $G = (V, \mathscr{E})$ be a graph with n vertices and m edges. A maximal complete subgraph of G is a clique of G. The order of a maximum clique of G is the clique number of G and is denoted by $\omega(G)$.

Definition 1.2.13. *Independent set.* Let $G = (V, \mathscr{E})$ be a graph with n vertices and m edges. A vertex subset U of a graph G is said to be an independent set of G, if the induced subgraph $< U >$ is an empty graph. An independent set of G with maximum number of vertices is called a maximum independent set of G. The number of vertices in a maximum independent set of G is called the independence number of G and is denoted by $\alpha(G)$.

Definition 1.2.14. *Cartesian product.* The Cartesian product of two graphs $G_1(V_1, \mathscr{E}_1)$ and $G_2(V_2, \mathscr{E}_2)$ denoted by $G_1 \times G_2$ is the graph $(V, \mathscr{E})$, where $V = V_1 \times V_2$ and $((x_1, x_2), (y_1, y_2)) \in \mathscr{E}$ if either $x_1 = y_1$ and $(x_2, y_2) \in \mathscr{E}_2$ or $(x_1, y_1) \in \mathscr{E}_1$ and $x_2 = y_2$.

Definition 1.2.15. *Kronecker product.* The Kronecker product of two graphs $G_1(V_1, \mathscr{E}_1)$ and $G_2(V_2, \mathscr{E}_2)$ denoted by $G_1 \otimes G_2$ is the graph $(V, \mathscr{E})$, where $V = V_1 \times V_2$

and $((x_1, x_2), (y_1, y_2)) \in \mathscr{E}$ if $(x_1, y_1) \in \mathscr{E}_1$ and $(x_2, y_2) \in \mathscr{E}_2$.

Definition 1.2.16. (i)*Elementary figure.* We call a graph to be an elementary figure if it is either K_2 or a cycle C_p, $p \geq 3$.
(ii)*Basic figure.* A graph whose components are elementary figures is called a basic figure.

Definition 1.2.17. *Double graph of a graph.* The double graph $D[G]$ of G is a graph obtained by taking two copies of G and joining each vertex in one copy with the neighbours of corresponding vertex in another copy. The k-fold graph $D^k[G]$ of the graph G is obtained by taking k copies of the graph G and joining each vertex in one of the copy with the neighbours of the corresponding vertex in all the other copies. If T_n is the graph obtained from the complete graph K_n by adding a loop at each of the vertex, it is easy to see that $D^k[G] = G \otimes T_k$.

Definition 1.2.18. *Strong double graph of a graph.* The strong double graph of a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the graph $SD(G)$ obtained by taking two copies of the graph G and joining each vertex v_i in one copy with the closed neighbourhood $N[v_i] = N(v_i) \cup \{v_i\}$ of the corresponding vertex in another copy.

For a graph G, let $SD^1(G) = SD(G), SD^2(G) = SD(SD(G)), \cdots SD^t(G) = SD(SD^{t-1}(G))$. Then $SD^t(G)$ is called the t-th iterated strong double graph of the graph G.

Definition 1.2.19. *Extended double cover of a graph.* The extended double cover of a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is a bipartite graph G^* with bipartition (X, Y), $X = \{x_1, x_2, \ldots, x_n\}$ and $Y = \{y_1, y_2, \ldots, y_n\}$, where two vertices x_i and y_j are adjacent if and only if $i = j$ or v_i adjacent v_j in G.

Given a graph G, let $G^{1*} = G^*, G^{2*} = (G^*)^*, \cdots, G^{k*} = (G^{(k-1)*})^*$. Then G^{k*} is called the k-th iterated extended double cover graph of the graph G.

Definition 1.2.20. *Digraph (or directed graph).* A digraph $\mathscr{D}$ is a pair $(V, \mathscr{A})$, where V is a nonempty set of objects called vertices and $\mathscr{A}$ is a subset of $V^{(2)}$, (the set of distinct ordered pairs of distinct elements of V). The elements of $\mathscr{A}$ are called arcs of $\mathscr{D}$.

Definition 1.2.21. *Multidigraph.* A multidigraph $\mathscr{D}$ is a pair $(V, \mathscr{A})$, where V is a nonempty set of vertices and $\mathscr{A}$ is a multiset of ordered pairs of distinct elements of V. The number of times an arc occurs in $\mathscr{D}$ is called its multiplicity and arcs with multiplicity greater than one are called multiple arcs.

Definition 1.2.22. *General digraph.* A general digraph $\mathscr{D}$ is a pair $(V, \mathscr{A})$, where V is a nonempty set of vertices and $\mathscr{A}$ is a multiset of ordered pairs of elements of V. We denote by (u, v) an arc from vertex u to vertex v. An arc of the form (u, u), where $u \in V$, is called loop of $\mathscr{D}$ and arcs which are not loops are called proper arcs. The number of times a loop occurs is called its multiplicity. A loop with multiplicity greater than one is called a multiple loop.

Definition 1.2.23. *Subdigraph of a digraph.* Let $\mathscr{D} = (V, \mathscr{A})$ be a digraph, $H = (U, \mathscr{A}')$ is the subdigraph of $\mathscr{D}$ whenever $U \subseteq V$ and $\mathscr{A}' \subseteq \mathscr{A}$. If $U = V$ the subdigraph is said to be spanning. An induced subdigraph $\langle U \rangle$ is a subset of V together with all the arcs of $\mathscr{D}$ between the vertices of U.

Definition 1.2.24. *Outdegree and indegree.* In a digraph $\mathscr{D} = (V, \mathscr{A})$, the out-degree of a vertex v is the number of vertices to which the vertex v is adjacent, it is denoted by $d^+(v)$ or d_v^+. Similarly the indegree of a vertex v in a digraph $\mathscr{D}$ is the number of vertices from which v is adjacent and it is denoted by $d^-(v)$ or d_v^-. If $d_v^+ = d_v^- = k$, then the digraph is said to be k-regular. A vertex v is said to be isolated if $d_v^+ = d_v^- = 0$.

Definition 1.2.25. Two digraphs $\mathscr{D}_1$ and $\mathscr{D}_2$ are said to be *isomorphic* if their underlying graphs are isomorphic and the direction of arcs are same and we write $\mathscr{D}_1 \cong \mathscr{D}_2$.

Definition 1.2.26. *Complement of a Digraph.* The complement of digraph $\mathscr{D} = (V, \mathscr{A})$ is denoted by $\bar{\mathscr{D}}$. It has a vertex set V and $(u, v) \in \bar{\mathscr{A}}$ if and only if $(u, v) \notin \mathscr{A}$. $\bar{\mathscr{D}}$ is the relative complement of $\mathscr{D}$ in K_n^*, where K_n^* is a complete symmetric digraph, i.e., a digraph in which for every pair of vertices there is a directed arc from one to other.

Definition 1.2.27. *Self complementary digraph.* A digraph $\mathscr{D}$ is said to be self complementary if $\mathscr{D} \cong \bar{\mathscr{D}}$, and $\mathscr{D}$ is said to be self converse if $\mathscr{D} \cong \mathscr{D}'$, where $\mathscr{D}'$ is the digraph obtained from $\mathscr{D}$ by reversing the direction of arcs.

Definition 1.2.28. *Directed Path.* A path of length $n - 1$ $(n \geq 2)$, denoted by P_n, is a digraph with n vertices $v_1, v_2, \ldots, v_n$ and with $n - 1$ arcs (v_i, v_{i+1}), where $i = 1, 2, \ldots, n - 1$.

Definition 1.2.29. *Directed cycle.* A cycle of length n, denoted by C_n, is the digraph with vertex set $v_1, v_2, \ldots, v_n$ having arcs (v_i, v_{i+1}), $i = 1, 2, \ldots, n-1$ and (v_n, v_1). A digraph is acyclic if it has no directed cycles.

Definition 1.2.30. *Strong connectedness.* A digraph $\mathscr{D}$ is called strongly connected if for any two vertices there is a path from one to other. The strong components of a digraph are the maximally strongly connected subdigraphs.

Definition 1.2.31. *Oriented graph.* An oriented graph is a digraph with no symmetric pairs of directed arcs and without loops. An orientation of a graph G is a digraph obtained by giving an arbitrary direction to each edge of G.

CHAPTER 2

On the energy of graphs

In this chapter, we study the energy of graphs and present some well known results on energy of graphs. We obtain lower and upper bounds for the energy of KK_n^j. We consider double graphs, extended double graphs and strong double graphs of a graph. Using these graphs we construct some new families of non A-cospectral equienergetic graphs and bipartite graphs on $n \equiv 0 \pmod 2$. We obtain a sufficient condition for the existence of non A-cospectral equienergetic bipartite graphs on $n \equiv 0 \pmod 4$ and a sufficient condition for the existence of non A-cospectral equienergetic bipartite graphs on $n \equiv 0 \pmod 2$. We give various methods for the construction of new families of non isomorphic A-cospectral graphs. We also obtain sufficient conditions for the existence of hyperenergetic graphs and hyperenergetic bipartite graphs for $n \equiv 0 \pmod 2$.

2.1 Introduction

Let G be a graph with n vertices $v_1, v_2, \ldots, v_n$ and m edges. The adjacency matrix of G is the $n \times n$ matrix $A = A(G) = (a_{ij})$, where

$$a_{ij} = \begin{cases} 1, & \text{if there is an edge from } v_i \text{ to } v_j, \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial $\det(xI - A(G)) = |xI - A(G)|$ of the adjacency matrix $A(G)$ of G is called the adjacency characteristic polynomial of G and is denoted by $\phi(G, x)$. It is clear from the definition that the matrix A is a real symmetric matrix, so all its eigenvalues are real. The eigenvalues of $A(G)$ are called the adjacency eigenvalues (A-eigenvalues) of G. The set of distinct A-eigenvalues of G together with their multiplicities is called the A-spectrum of G. If G has k distinct A-eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ with respective multiplicities $m_1, m_2, \ldots, m_k$, then we write the A-spectrum of G as $Spec_A(G) = \{\lambda_1^{[m_1]}, \lambda_2^{[m_2]}, \ldots, \lambda_k^{[m_k]}\}$.

The following result relates the coefficients of the adjacency characteristic polynomial of a graph with the structure of the graph and is known as Sach's

Theorem [28].

Theorem 2.1.1. *Let G be a graph of order n with adjacency characteristic polynomial*

$$\phi(G, x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + \cdots + a_{n-1} x + a_n,$$

then

$$a_j = \sum_{L \in \pounds_j} (-1)^{p(L)} 2^{|c(L)|},$$

for all $j = 1, 2, \ldots, n$, where $\pounds_j$ is the set of all basic figures L of G of order j, $p(L)$ denotes the number of components of L and $c(L)$ denotes the set of all cycles of L.

A graph is bipartite if and only if it contains no odd cycles. As basic figures of odd order must possess at least one odd cycle, therefore for a bipartite graph $\pounds_{2j+1} = \emptyset$, for all $j \geq 0$ and hence $a_{2j+1} = 0$, for all $j \geq 0$. Consequently, the adjacency characteristic polynomial of a bipartite graph B takes the form

$$\phi(B, x) = \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} a_{2j} x^{n-2j}.$$

The even coefficients of a bipartite graph alternate in sign [28], i.e., $(-1)^j a_{2j} \geq 0$, for all j. Therefore,

$$\phi(B, x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j} x^{n-2j},$$

where $a_{2j} = (-1)^j b_{2j}$ and b_{2j} are non negative integers.

2.2 Energy of graphs

Definition 2.2.1. *Energy of a graph.* Let G be a graph of order n with A-eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. The energy of G is defined as

$$E(G) = \sum_{j=1}^{n} |\lambda_j|.$$

This concept was first introduced in 1978 by Gutman [72]. The following is the integral representation for the energy of a graph (also known as the Coulson's integral formula).

Theorem 2.2.2. *Let G be a graph with n vertices having A-characteristic polynomial $\phi(G, x)$. Then*

$$E(G) = \sum_{j=1}^{n} |\lambda_j| = \frac{1}{\pi} \int_{-\infty}^{\infty} (n - \frac{ix\phi'(G, ix)}{\phi(G, ix)})dx,$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the A-eigenvalues of graph G, $i = \sqrt{-1}$ and $\int_{-\infty}^{\infty} F(x)dx$ denotes the principle value of the respective integral.

The following observations [73] follow from Coulson's integral formula.

Theorem 2.2.3. *If G is a graph of order n, then*

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log |x^n \phi(G, \frac{i}{x})| dx.$$

Theorem 2.2.4. *If G_1 and G_2 are two graphs of the same order, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{\infty} \log |\frac{\phi(G_1, ix)}{\phi(G_2, ix)}| dx.$$

Coulson's integral formula and its various consequences have important chemical applications. Note that the Sach's theorem establishes the explicit dependence of the coefficients of the characteristic polynomial of a graph on the structure of the graph. The Coulson's integral formula establishes the explicit dependence of the energy of a graph on the characteristic polynomial of this graph. By combining Coulson's integral formula with Sach's theorem, we see the dependence of the energy of a graph on the structure of this graph and hence a complete information on the dependence of the total $\pi-$electron energy of molecule (as computed within the HMO model) on the structure of this molecule.

2.3 Bounds for the energy of a graph

Several upper and lower bounds for the energy are known. The following bounds of energy of a graph in terms of order n, size m and the determinant of adjacency matrix is due to McClelland [109].

Theorem 2.3.1. *If G is a graph with n vertices and m edges, then*

$$\sqrt{2m + n(n-1)|\det(A(G))|^{\frac{2}{n}}} \leq E(G) \leq \sqrt{2mn}. \tag{2.1}$$

An immediate consequence of Theorem 2.3.1 is the following observation.

Corollary 2.3.2. *If $\det(A(G)) \neq 0$, then $E(G) \geq \sqrt{2m + n(n-1)} \geq n$.*

The graph energy as a function of the number of edges satisfies the following inequalities [23].

Theorem 2.3.3. *If G is a graph with m edges, then*

$$2\sqrt{m} \leq E(G) \leq 2m$$

with equality on the left if and only if G is a complete bipartite graph plus some isolated vertices and equality on the right if and only if G is a matching of m edges plus some isolated vertices.

The following is a lower bound for the energy of a graph [73] in terms of its number of vertices n.

Theorem 2.3.4. *If G is a graph with n vertices, then*

$$E(G) \geq 2\sqrt{n-1}$$

with equality if and only if $G = K_{1,n-1}$.

Definition 2.3.5 *Strongly regular graph.* A k-regular graph G on n vertices is said to be strongly regular with parameters (n, k, λ, μ) if each pair of adjacent vertices has the same number $\lambda \geq 0$ of common neighbours, and each pair of non adjacent vertices has the same number $\mu \geq 0$ of common neighbours. If $\mu = 0$, then G is a disjoint union of complete graphs, whereas if $\mu \geq 1$ and G is non complete, then A-eigenvalues of G are k, r and s, where r and s are the roots of the quadratic equation

$$x^2 + (\mu - \lambda)x + (\mu - k) = 0.$$

The A-eigenvalue k has the multiplicity one, whereas multiplicities m_r of r and m_s of s can be calculated by solving the simultaneous equations

$$m_r + m_s = n - 1, \quad k + rm_r + sm_s = 0.$$

A strongly regular graph G is said to be primitive if both G and $\bar{G}$ (complement of G) are connected. A strongly regular graph with parameters (n, k, λ, μ) is denoted by $\mathrm{SRG}(n, k, \lambda, \mu)$.

The following result due to Koolen and Moulton [93] improves the McClelland upper bound for the graphs with $\frac{2m}{n} \geq 1$, where n is the number of vertices and m is the number of edges of the graph.

Theorem 2.3.6. *If $2m \geq n$ and G is a graph on n vertices and m edges, then*

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - (\frac{2m}{n})^2]} \tag{2.2}$$

holds. Moreover, equality holds in (2.2) if and only if G is either $\frac{n}{2}K_2$ or K_n or a non-complete connected strongly regular graph with two non trivial A-eigenvalues *both with absolute value* $\sqrt{\frac{(2m-(\frac{2m}{n})^2)}{(n-1)}}$.

Since a graph G with n vertices has at most $\frac{n(n-1)}{2}$ edges, it follows from McClelland's bound (2.1) that

$$E(G) \leq n\sqrt{n-1} \tag{2.3}$$

must hold.

The following result shows that inequality (2.2) allows to improve the bound given by (2.3).

Theorem 2.3.7. *Let G be a graph on n vertices. Then*

$$E(G) \leq \frac{n}{2}(1+\sqrt{n}) \tag{2.4}$$

holds, with equality if and only if G is a strongly regular graph with parameters $(n, \frac{(n+\sqrt{n})}{2}, \frac{(n+2\sqrt{n})}{4}, \frac{(n+2\sqrt{n})}{4})$.

Koolen and Moulton [93] conjectured that for a given $\epsilon > 0$, there exists a graph G of order n such that for almost all $n \geq 1$,

$$E(G) \geq (1-\epsilon)\frac{n}{2}(\sqrt{n}+1),$$

which was later proved by Nikiforov [111]. For energy bounds about bipartite graphs see [94, 122].

Let KK_n^j, $1 \leq j \leq n$, be the graph obtained by taking two copies of the graph K_n and joining a vertex in one copy with the j, $1 \leq j \leq n$, vertices in another copy. The A-spectrum of the graph KK_n^j was discussed in [46] and is given by the following result.

Lemma 2.3.7. *If $1 \leq j \leq n$ and $n \geq 3$, the A-characteristic polynomial of KK_n^j is $(x+1)^{2n-4}h(x)$, where $h(x) = x^4 + (4-2n)x^3 + (n^2-6n+6-j)x^2 + (2n^2-6n+2nj-j^2-3j+4)x + (1+nj^2-2j^2+n^2-2n-2j+3jn-jn^2)$.*

We now find the estimates for the energy of KK_n^j. This family of graphs was introduced in [46], where the spectral properties with respect to different matrices $(A(G), L(G), Q(G))$ were discussed.

Theorem 2.3.8. *For $k \in \mathbb{N} - \{1\}, (k-1)^2 < j \leq k^2$ and $n \geq ((k-1)^2+2)^2 - (k-1)^2$, we have*

$$4n - 8 + 2k < E(KK_n^j) < 4n - 8 + 2(k+1).$$

Proof. By Lemma 2.3.7, the A-characteristic polynomial $\phi(KK_n^j, x)$ of the graph KK_n^j is

$$\phi(KK_n^j, x) = (x+1)^{2n-4}h(x),$$

where $h(x) = x^4 + (4-2n)x^3 + (n^2 - 6n + 6 - j)x^2 + (2n^2 - 6n + 2nj - j^2 - 3j + 4)x + (1 + nj^2 - 2j^2 + n^2 - 2n - 2j + 3jn - jn^2)$.

Let x_1, x_2, x_3, x_4 be the zeros of the polynomial $h(x)$. Then the A-spectrum of the graph KK_n^j is $\{-1^{[2n-4]}, x_1, x_2, x_3, x_4\}$.

For $(k-1)^2 < j \leq k^2$ and $n \geq ((k-1)^2+2)^2 - (k-1)^2$, we have the following.
$h(n) = n^2 + 2n + 1 - 2j^2 - 2j \ > \ 0, \quad h(n-1) = -j^2 \ < \ 0,$
$h(n-2) = (n-1)^2 \ > \ 0, \quad h(0) = 1 - 2j - 2j^2 - 2n + 3nj + nj^2 + n^2 - jn^2 \ < \ 0,$
$h(-k) = k^4 + (2n-4)k^3 + (n^2 - 6n + 6 - j)k^2 - (2n^2 - 6n + 2nj - j^2 - 3j + 4)k + (1 + nj^2 - 2j^2 + n^2 - 2n - 2j + 3jn - jn^2) \ < \ 0,$ *and*
$h(-(k+1)) = k^4 + 2nk^3 + (n^2 - j)k^2 + (j^2 + j - 2nj)k + (jn + nj^2 - jn^2 - j^2) \ > \ 0.$

Therefore, by Intermediate Value Theorem, it follows that $h(x)$ has three positive roots, one in each of the intervals $(0, n-2), (n-2, n-1)$ and $(n-1, n)$, and a single negative root in the interval $(-(k+1), -k)$. Assume that $x_1, x_2, x_3 \ > \ 0$ and $x_4 \ < \ 0$. Since $x_1 + x_2 + x_3 + x_4 = 2(n-2)$. We have

$$\begin{aligned} E(KK_n^j) &= (2n-4)|-1| + |x_1| + |x_2| + |x_3| + |x_4| \\ &= 2n - 4 + x_1 + x_2 + x_3 - x_4 \\ &= 2n - 4 + 2n - 4 - 2x_4 \\ &= 4n - 8 - 2x_4. \end{aligned}$$

The result follows from the fact that $x_4 \in (-(k+1), -k)$ implies $-(k+1) < x_4 < -k$, which implies $k < -x_4 < k+1$. $\square$

Since $(k-1)^2 < j \leq k^2$ implies $k-1 < \sqrt{j} < k$, the following consequence of Theorem 2.3.8, gives the estimates for the energy of KK_n^j in terms of j.

Corollary 2.3.9. *For $k \in \mathbb{N} - \{1\}, (k-1)^2 < j \leq k^2$ and $n \geq ((k-1)^2+2)^2 - (k-1)^2$, we have*

$$4n - 8 + 2\sqrt{j} < E(KK_n^j) < 4n - 8 + 2(\sqrt{j} + 2).$$

Bapat and Pati [14] proved that the energy of a graph if rational number should be an even integer. Therefore keeping this in mind we have the following consequence of Theorem 2.3.8.

Corollary 2.3.10. *For $k \in \mathbb{N} - \{1\}, (k-1)^2 < j \leq k^2$ and $n \geq ((k-1)^2+2)^2 - (k-1)^2$, the energy of the graph KK_n^j is an irrational number.*

2.4 Equienergetic graphs

Two graphs G_1 and G_2 of the same order are said to be A-cospectral if they have the same A-spectrum and non A-cospectral, otherwise. Since adjacency matrices of isomorphic graphs are permutation similar and similar matrices have same spectrum, it follows that isomorphic graphs are always A-cospectral. However there are non isomorphic graphs, which are A-cospectral [28].

Two graphs G_1 and G_2 of same order are said to be *equienergetic* if they have the same energy. A-cospectral graphs are obviously equienergetic, therefore the problem of equienergetic graphs is considered only for non A-cospectral graphs.

Definition 2.4.1. *Line graph and iterated line graph.* The line graph $L(G)$ of a graph G is the graph whose vertex set is the edge set of G and any two vertices in $L(G)$ are adjacent if and only if the corresponding edges in G share a vertex.

Given a graph G, let $L^1(G) = L(G), L^2(G) = L(L(G)), \cdots, L^k(G) = L(L^{k-1}(G))$. The graph $L^k(G)$ is called k-th iterated line graph of G.

Equienergetic graphs were first constructed by Ramane et al. [124]. The following result shows that for a regular graph, the energy of second iterated line graph depends only on degree and the number of vertices.

Theorem 2.4.2. *If G is an r-regular graph $(r \geq 3)$ of order n, then*

$$E(L^2(G)) = 2nr(r-2).$$

Using Theorem 2.4.2 and noting that iterated line graphs of non A-cospectral regular graphs are non A-cospectral, the following result [124] yields the existence of non A-cospectral equienergetic graphs.

Theorem 2.4.3. *Let G_1 and G_2 be two non A-cospectral regular connected graphs both on n vertices and both of degree $r \geq 3$. Then $L^2(G_1)$ and $L^2(G_2)$ are connected, non A-cospectral and equienergetic.*

An inductive argument shows that k-th iterated line graphs of any two connected, non A-cospectral regular graphs both with same degree and same number of vertices are connected, non A-cospectral and equienergetic.

The following result due to Ramanne et al. [127] gives a method of construction of equienergetic complement graphs.

Theorem 2.4.4. *If G is a regular graph of order n and of degree $r \geq 3$, then*

$$E(\overline{L^2(G)}) = (nr-4)(2r-3) - 2.$$

From Theorem 2.4.4 and noting that complemented iterated line graphs of non A-cospectral regular graphs are non A-cospectral, the following observation [127] shows the existence of equienergetic complement graphs.

Corollary 2.4.5. *Let G_1 and G_2 be two non A-cospectral regular graphs on n vertices and of degree $r \geq 3$. Then $\overline{L^2(G_1)}$ and $\overline{L^2(G_2)}$ are non A-cospectral equienergetic.*

An inductive argument gives the following result [127].

Corollary 2.4.6. *Let G_1 and G_2 be two non A-cospectral regular graphs on n vertices and of degree $r \geq 3$. Then for $k \geq 2$, $\overline{L^k(G_1)}$ and $\overline{L^k(G_2)}$ are non A-cospectral equienergetic.*

Balakrishnan [12] proved that for a non trivial graph Q, if $G = C_4$ and $H = K_2 \otimes K_2$, then $Q \otimes G$ and $Q \otimes H$ are non A-cospectral and equienergetic. Bonifacio et al. [19] have given conditions on an arbitrary pair G and H of equienergetic non A-cospectral graphs to make assertion true for any non trivial connected graph Q. Bonifacio et al. [19] also characterize a graph G for which $G \otimes K_2$ and $G \times K_2$ are non A-cospectral and equienergetic. Indulal and Vijaykumar [86] constructed self complementary equienergetic graphs on p vertices for every $p = 4k$, where $k \geq 2$ and $p = 24t + 1$, where $t \geq 3$.

Let $D^k[G]$ be the k-fold graph of the graph G, the A-spectrum of $D^k[G]$ was considered in [103] and is given by the following result.

Lemma 2.4.9. *If $\lambda_1, \lambda_2, \ldots, \lambda_n$ is the A-spectrum of a graph G, then the A-spectrum of the graph $D^k[G]$ is $k\lambda_1, k\lambda_2, \ldots, k\lambda_n, 0^{[(k-1)n]}$.*

Let G^* be the extended double cover of the graph G. The following result [25] gives the A-spectrum of G^*.

Lemma 2.4.10. *If $\lambda_1, \lambda_2, \ldots, \lambda_n$ is the A-spectrum of a graph G, then the A-spectrum of the graph G^* is $\pm(\lambda_1 + 1), \pm(\lambda_2 + 1), \ldots, \pm(\lambda_n + 1)$.*

The following result gives the A-spectrum (L-spectrum) of the *cartesian product* of graphs [28].

Lemma 2.4.11. If $G_1(n_1, m_1)$ and $G_2(n_2, m_2)$ are two graphs having A-spectrum (L-spectrum) respectively as $\theta_1, \theta_2, \ldots, \theta_{n_1}$ and $\sigma_1, \sigma_2, \ldots, \sigma_{n_2}$, then the A-spectrum (L-spectrum) of $G = G_1 \times G_2$ is $\theta_i + \sigma_j$, where $i = 1, 2, \ldots, n_1$ and $j = 1, 2, \ldots, n_2$.

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the A-spectrum of the graph G, then by Lemma 2.4.11, the

A-spectrum of the graph $G \times K_2$ is $\lambda_i + 1, \lambda_i - 1$, for $i = 1, 2, \ldots, n$. It is clear from Lemma 2.4.10, that the graphs $G \times K_2$ and G^* are non isomorphic A-cospectral if and only if G is bipartite [25]. Further, we have

$$E(G^*) = \sum_{i=1}^{n} |\lambda_i + 1| + \sum_{i=1}^{n} |-\lambda_i - 1| = 2 \sum_{i=1}^{n} |\lambda_i + 1|.$$

Also, by Lemma 2.4.9, the A-spectrum of $D^k[G]$ is $k\lambda_1, k\lambda_2, \ldots, k\lambda_n, 0^{[(k-1)n]}$, so that

$$E(D^k[G]) = \sum_{i=1}^{n} |k\lambda_i| = k \sum_{i=1}^{n} |\lambda_i| = kE(G).$$

The following result gives the A-spectrum (L-spectrum) of the *Kronecker product* of graphs [28].

Lemma 2.4.12. If $G_1(n_1, m_1)$ and $G_2(n_2, m_2)$ are two graphs having A-spectrum (L-spectrum) respectively as $\theta_1, \theta_2, \ldots, \theta_{n_1}$ and $\sigma_1, \sigma_2, \cdots, \sigma_{n_2}$, then the A-spectrum (L-spectrum) of $G = G_1 \otimes G_2$ is $\theta_i \sigma_j$ where $i = 1, 2, \ldots, n_1$ and $j = 1, 2, \ldots, n_2$.

From Lemmas 2.4.11 and 2.4.12, it is clear that the A-spectrum of the graph $(G \otimes K_2) \times K_2$ is $\lambda_i + 1, \lambda_i - 1, -\lambda_i + 1, -\lambda_i - 1,\ i = 1, 2, \ldots, n$. Therefore,

$$\begin{aligned} E((G \otimes K_2) \times K_2) &= 2 \sum_{i=1}^{n} |\lambda_i + 1| + 2 \sum_{i=1}^{n} |\lambda_i - 1| = 2 \left(\sum_{i=1}^{n} |\lambda_i + 1| + \sum_{i=1}^{n} |\lambda_i - 1| \right) \\ &= 2E(G \times K_2) = E(2(G \times K_2)) = E((G \times K_2) \cup (G \times K_2)). \end{aligned}$$

From this, it follows that the graphs $(G \otimes K_2) \times K_2$ and $(G \times K_2) \cup (G \times K_2)$ are equienergetic graphs. Clearly, these graphs are non A-cospectral. In fact, if G is a bipartite graph, then the graphs $(G \otimes K_2) \times K_2$ and $G^* \cup G^*$ are non A-cospectral equienergetic graphs.

As seen above $E(D^k[G]) = k \sum_{i=1}^{n} |\lambda_i| = kE(G) = E(kG) = E(G \cup G \cup \cdots \cup G)$. This shows that the graphs $D^k[G]$ and $(G \cup G \cup \cdots \cup G)$ are non A-cospectral equienergetic. However, we show for any graph G the graphs $D[G]$ and $G \otimes K_2$ are always equienergetic non A-cospectral graphs.

Theorem 2.4.13. *If $D[G]$ is the double graph of the graph G, then the graphs $G \otimes K_2$ and $D[G]$ are non A-cospectral equienergetic graphs.*

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the graph G, then by Lemma 2.4.12, the eigenvalues of the graph $G \otimes K_2$ are $\lambda_i, -\lambda_i,\ i = 1, 2, \ldots, n$ and by Lemma 2.4.9 (for $k = 2$), the eigenvalues of the graph $D[G]$ are $2\lambda_i,\ 0^{[n]},\ i = 1, 2, \ldots, n$. Therefore,

$$E(G \otimes K_2) = \sum_{i=1}^{n} |\lambda_i| + \sum_{i=1}^{n} |-\lambda_i| = 2\sum_{i=1}^{n} |\lambda_i|.$$

Also,

$$E(D[G]) = \sum_{i=1}^{n} |2\lambda_i| = 2\sum_{i=1}^{n} |\lambda_i|.$$

Clearly these graphs are non A-cospectral. $\square$

In general, if $D^k[G]$ is the k-fold graph of the graph G, we have the following observation, the proof of which follows by proceeding similarly as in Theorem 2.4.13.

Theorem 2.4.14. *If $D^k[G]$ is the k-fold graph of the graph G, then the graphs $D^k[G]$ and $G \otimes sK_2$ are non A-cospectral equienergetic graphs if and only if $k = 2^s$.*

Let G be a bipartite graph. It is well known that the spectrum of G is symmetric about the origin (Pairing Theorem), so half of the non-zero eigenvalues of G lies to the left and half lies to the right of origin. Therefore, if γ_+, γ_- and γ_0 are respectively, the number of positive eigenvalues, the number of negative eigenvalues and number of zero eigenvalues of G, then for the bipartite graph G, we have $\gamma_+ = \gamma_-$. Keeping this in mind, we have the following result.

Theorem 2.4.15. *Let G^* be the extended double cover of the bipartite graph G. The graphs G^* and $D[G]$ are non A-cospectral equienergetic if and only if $|\lambda_i| \geq 1$ for all $1 \leq i \leq n$.*

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the graph G. By Lemma 2.4.10, the eigenvalues of the graph G^* are $\lambda_i + 1, -\lambda_i - 1$, for $i = 1, 2, \ldots, n$ and by

Lemma 2.4.9, the eigenvalues of the graph $D[G]$ are $2\lambda_i,\ 0^{[n]}$, for $i = 1, 2, \ldots, n$. Suppose that $|\lambda_i| \geq 1$ for $i = 1, 2, \ldots, n$, then

$$|\lambda_i + 1| = \begin{cases} |\lambda_i| + 1, & \text{if } \lambda_i > 0 \\ |\lambda_i| - 1, & \text{if } \lambda_i < 0. \end{cases}$$

Therefore,

$$\begin{aligned} E(G^*) &= \sum_{i=1}^{n} |\lambda_i + 1| + \sum_{i=1}^{n} |-\lambda_i - 1| = 2\sum_{i=1}^{n} |\lambda_i + 1| \\ &= 2\left(\sum_{\lambda_i > 0} |\lambda_i + 1| + \sum_{\lambda_i < 0} |\lambda_i + 1|\right) = 2\left(\sum_{\lambda_i > 0} (|\lambda_i| + 1) + \sum_{\lambda_i < 0} (|\lambda_i| - 1)\right) \\ &= 2\left((\sum_{\lambda_i > 0} |\lambda_i| + \sum_{\lambda_{<0}} |\lambda_i|) + (\sum_{\lambda_i > 0} 1 - \sum_{\lambda_{<0}} 1) \right) = 2\sum_{i=1}^{n} |\lambda_i| = E(D[G]). \end{aligned}$$

Clearly these graphs are non A-cospectral with same number of vertices.

Conversely, suppose that for the bipartite graph G, the graphs G^* and $D[G]$ are non A-cospectral equienergetic. We will show that $|\lambda_i| \geq 1$ for all $1 \leq i \leq n$.

Assume to the contrary that $|\lambda_i| < 1$ for some i. Then for this i, $|\lambda_i + 1| = \lambda_i + 1$. Without loss of generality, suppose that the eigenvalues of G satisfy $|\lambda_i| \geq 1$, for $i = 1, 2, \ldots, k$ and $|\lambda_i| < 1$, for $i = k+1, k+2, \ldots, n$, as the eigenvalues are real and reordering does not effect the argument. We have the following cases to consider.

Case (i). If $\lambda_i > 0$ for $i = 1, 2, \ldots, k$ and $\lambda_i \geq 0$ for $i = k+1, k+2, \ldots, n$, then

$$E(G^*) = 2\left(\sum_{i=1}^{k} |\lambda_i + 1| + \sum_{i=k+1}^{n} |\lambda_i + 1|\right) = 2\left(\sum_{i=1}^{n} |\lambda_i| + n\right).$$

Case (ii). If $\lambda_i > 0$ for $i = 1, 2, \ldots, k$ and $\lambda_i \leq 0$ for $i = k+1, k+2, \ldots, n$, then if γ_0 is the number of zero eigenvalues of G, we have

$$\begin{aligned} E(G^*) &= 2\left(\sum_{i=1}^{k} |\lambda_i + 1| + \sum_{i=k+1}^{n} |\lambda_i + 1|\right) = 2\left(\sum_{i=1}^{k} (|\lambda_i| + 1) + \sum_{i=k+1}^{n} (\lambda_i + 1)\right). \\ &> 2\left(\sum_{i=1}^{k} (|\lambda_i| + 1) + \sum_{i=k+1}^{n} (|\lambda_i| - 1)\right) = 2\left(\sum_{i=1}^{n} |\lambda_i| - \gamma_0\right). \end{aligned}$$

Case (iii). If $\lambda_i < 0$ for $i = 1, 2, \ldots, k$ and $\lambda_i \geq 0$ for $i = k+1, k+2, \ldots, n$, then

$$\begin{aligned}
E(G^*) &= 2\left(\sum_{i=1}^{k} |\lambda_i + 1| + \sum_{i=k+1}^{n} |\lambda_i + 1|\right) = 2\left(\sum_{i=1}^{k}(|\lambda_i| - 1) + \sum_{i=k+1}^{n}(|\lambda_i| + 1)\right). \\
&= 2\left(\sum_{i=1}^{n} |\lambda_i| + \gamma_0\right).
\end{aligned}$$

Case (iv). If $\lambda_i < 0$ for $i = 1, 2, \ldots, k$ and $\lambda_i \leq 0$ for $i = k+1, k+2, \ldots, n$, then

$$\begin{aligned}
E(G^*) &= 2\left(\sum_{i=1}^{k} |\lambda_i + 1| + \sum_{i=k+1}^{n} |\lambda_i + 1|\right) = 2\left(\sum_{i=1}^{k}(|\lambda_i| - 1) + \sum_{i=k+1}^{n}(\lambda_i + 1)\right). \\
&> 2\left(\sum_{i=1}^{k}(|\lambda_i| - 1) + \sum_{i=k+1}^{n}(|\lambda_i| - 1)\right) = 2\left(\sum_{i=1}^{n} |\lambda_i| - n\right).
\end{aligned}$$

Clearly in all these cases, we obtain $E(G^*) \neq E(D[G])$, a contradiction. Therefore the result follows. □

As double graph $D[G]$ of a bipartite graph G is bipartite and extended double cover G^* of the graph G is always bipartite, Theorem 2.4.15 gives a method to construct a pair of non A-cospectral equienergetic connected bipartite graphs from any given connected bipartite graph G for any n.

For any complex square matrices A and B of same order, we have the following observation.

Lemma 2.4.16. *If A and B are complex square matrices of same order, then*

$$\begin{vmatrix} A & B \\ B & A \end{vmatrix} = |A + B||A - B|$$

where the symbol $||$ denotes the determinant of a matrix.

Let $SD(G)$ be the strong double graph of the graph G and let $SD^k(G),\ k \geq 1$ be the k-th iterated strong double graph of the graph G. Using strong double graphs we will construct some new families of non A-cospectral equienergetic graphs from any given graph G. For this, we first obtain the A-spectrum of $SD(G)$

and $SD^k(G)$.

Theorem 2.4.17. *If $\lambda_i,\ i = 1, 2, \ldots, n$ is the A-spectrum of the graph G, then the A-spectrum of the graph $SD(G)$ is $2\lambda_i + 1,\ -1^{[n]},\ i = 1, 2, \ldots, n$.*

Proof. Let A be the adjacency matrix of the graph G and I_n be the Identity matrix of order n. By a suitable relabelling of vertices it can be seen that the adjacency matrix $A(SD(G))$ of the graph $SD(G)$ is

$$A(SD(G) = \begin{pmatrix} A & A(G) + I_n \\ A(G) + I_n & A \end{pmatrix}.$$

Therefore by Lemma 2.4.16, the adjacency characteristic polynomial of $SD(G)$ is

$$\begin{aligned}
\phi(G, \lambda) = |\lambda I_{2n} - A(SD(G))| &= \begin{vmatrix} \lambda I_n - A & -(A + I_n) \\ -(A + I_n) & \lambda I_n - A \end{vmatrix} \\
&= |\lambda I_n - A - (A + I_n)|\,|\lambda I_n - A + (A + I_n)| \\
&= |\lambda - 1)I_n - 2A|\,|(\lambda + 1)I_n| \\
&= (\lambda + 1)^n \phi\left(G, \frac{\lambda - 1}{2}\right),
\end{aligned}$$

and so the result follows. □

Using induction and Theorem 2.4.17, we have the following observation.

Corollary 2.4.18. *If λ_i, $i = 1, 2, \ldots, n$, is the A-spectrum of the graph G, then the A-spectrum of the graph $SD^k(G),\ k \geq 1$ is $2^k\lambda_i + (2^k - 1),\ -1^{[(2^k-1)n]},\ i = 1, 2, \ldots, n$.*

A graph G is said to be A-*integral* if all its adjacency eigenvalues are integers [28]. The following observation is an easy consequence of Corollary 2.4.18, and gives a method to construct new families of A-*integral* graphs from any given A-integral graph G. Also, it gives a method to construct new families of A-cospectral graphs from any given pair of A-cospectral graphs G_1 and G_2.

Corollary 2.4.19. *A graph G is A-integral if and only if the graph $SD^k(G)$ is A-integral. Two graphs $SD^k(G_1)$ and $SD^k(G_2)$ of same order are A-cospectral if and only if the graphs G_1 and G_2 are A-cospectral.*

Indeed, if all the A-eigenvalues of the graph G are integers, then the graph $SD^k(G)$ gives an infinite sequence of graphs having all the A-eigenvalues odd integers in absolute value.

If $\lambda_i,\ i = 1, 2, \ldots, n$, is the A-spectrum of the graph, by Lemmas 2.4.9, 2.4.11 and Theorem 2.4.17, it follows that the A-spectrum of the graphs $SD(G \times K_2)$ and $D[G \times K_2]$ are respectively, as $2\lambda_i + 3, 2\lambda_i - 1, -1^{[2n]}$ and $2\lambda_i + 2, 2\lambda_i - 2, 0^{[2n]}$. So, by Lemma 2.4.12, the A-spectrum of the graph $SD(G \times K_2) \otimes K_2$ is $2\lambda_i + 3, 2\lambda_i - 1, -2\lambda_i - 3, -2\lambda_i + 1, 1^{[2n]}, -1^{[2n]},\ i = 1, 2, \ldots, n$, which by Lemma 2.4.10, is same as the A-spectrum of the graph $(D(G \times K_2))^*$. So it follows that the graphs $SD(G \times K_2) \otimes K_2$ and $(D(G \times K_2))^*$ are A-cospectral for any graph G.

The next result gives the construction of non A-cospectral equienergetic bipartite graphs from any given graph G.

Theorem 2.4.20. *For a bipartite graph G, the graphs $SD(G \otimes K_2)$ and $SD(G) \otimes K_2$ are non A-cospectral equienergetic if $|\lambda_i| \geq \frac{1}{2}$, for all non-zero eigenvalues of G.*

Proof. Let $SD(G)$ be the strong double graph of the graph G. Using Theorem 2.4.17 and Lemma 2.4.12, it is easy to see that the A-spectrum of the graphs $SD(G) \otimes K_2$ and $SD(G) \otimes K_2$ are respectively, $2\lambda_i + 1, -2\lambda_i - 1, -1^{[n]}, 1^{[n]},\ i = 1, 2, \ldots, n$ and $2\lambda_i + 1, -2\lambda_i + 1, -1^{[2n]},\ i = 1, 2, \ldots, n$. Suppose $|\lambda_i| \geq \frac{1}{2}$. Then we have

$$|2\lambda_i + 1| = \begin{cases} 2|\lambda_i| + 1, & \text{if } \lambda_i \geq 0 \\ 2|\lambda_i| - 1, & \text{if } \lambda_i < 0 \end{cases}, \quad |2\lambda_i - 1| = \begin{cases} 2|\lambda_i| - 1, & \text{if } \lambda_i > 0 \\ 2|\lambda_i| + 1, & \text{if } \lambda_i \leq 0. \end{cases}$$

Therefore,

$$
\begin{aligned}
E(SD(G)\otimes K_2) &= 2n + \sum_{i=1}^{n} |2\lambda_i + 1| + \sum_{i=1}^{n} |-2\lambda_i - 1| \\
&= 2n + 2\sum_{i=1}^{n} |2\lambda_i + 1| = 2n + 2\left(\sum_{\lambda_i \geq 0} |2\lambda_i + 1| + \sum_{\lambda_i < 0} |2\lambda_i + 1|\right) \\
&= 2n + 2\left(\sum_{\lambda_i \geq 0} (|2\lambda_i| + 1) + \sum_{\lambda_i < 0} (|2\lambda_i| - 1)\right) \\
&= 2n + 2\sum_{i=1}^{n} 2|\lambda_i| + 2(\gamma_+ + \gamma_0 - \gamma_-) \\
&= 2n + 4E(G) + 2\gamma_0.
\end{aligned}
$$

Also,

$$
\begin{aligned}
&E(SD(G\otimes K_2)) = 2n + \sum_{i=1}^{n} |2\lambda_i + 1| + \sum_{i=1}^{n} |2\lambda_i - 1| \\
&= 2n + \sum_{\lambda_i \geq 0} |2\lambda_i + 1| + \sum_{\lambda_i < 0} |2\lambda_i + 1| + \sum_{\lambda_i > 0} |2\lambda_i - 1| + \sum_{\lambda_i \leq 0} |2\lambda_i - 1| \\
&= 2n + \sum_{\lambda_i \geq 0} (|2\lambda_i| + 1) + \sum_{\lambda_i < 0} (|2\lambda_i| - 1) + \sum_{\lambda_i > 0} (|2\lambda_i| - 1) + \sum_{\lambda_i \leq 0} (|2\lambda_i| + 1) \\
&= 2n + 4E(G) + (\gamma_+ + \gamma_0 - \gamma_-) + (\gamma_- + \gamma_0 - \gamma_+) \\
&= 2n + 4E(G) + 2\gamma_0.
\end{aligned}
$$

Clearly, these graphs are non A-cospectral. $\square$

Theorem 2.4.20 gives sufficient conditions for the existence of non A-cospectral equienergetic bipartite graphs on $n \cong 0(\mod 4)$ vertices.

2.5 Hyperenergetic graphs

From Theorem 2.3.1, a graph G with n vertices and m edges satisfies the upper bound $E(G) \leq \sqrt{2mn}$. This bound depends only on m and n. As among all n-vertex graphs, the complete graph K_n has maximum number of edges which is $\frac{n(n-1)}{2}$. This motivated Gutman to conjecture that among all n-vertex graphs, the complete graph K_n has maximum energy which is equal to $2(n-1)$. Later Godsil [58] in 1980's proved that there exist graphs of order n with energy greater than $2(n-1)$. This motivated the following definition.

Definition 2.5.1. *Hyperenergetic graph.* A graph G of order n is said to be hyperenergetic if $E(G) > 2(n-1)$.

Gutman et al. [76] proved that no Hückel graph (molecular graph) is hyperenergetic. Pirzada [116] proved that Frutch graph is not hyperenergetic. Panigrahi and Mohapatra [114] proved that all primitive strongly regular graphs except $\mathrm{SRG}(5,2,0,1)$, $\mathrm{SRG}(9,4,1,2)$, $\mathrm{SRG}(10,3,0,1)$ and $\mathrm{SRG}(16,5,0,2)$ are hyperenergetic. Balakrishnan posed an open problem in [12] that $K_n - H$ is non-hyperenergetic for $n \geq 4$, where H is a Hamiltonian cycle of K_n. Stevanović and Stanković [133] proved that $K_n - H$ is indeed hyperenergetic, where H is the Hamiltonian cycle of K_n. In fact, they proved the following stronger result.

Theorem 2.5.2. *If $\overline{C_i}(n, k_1, k_2, \ldots, k_m)$, $n \in \mathbb{N}$, $k_1 < k_2 < \cdots < k_m < \frac{n}{2}$, $k_i \in \mathbb{N}$ for $i = 1, 2, \ldots, m$, denotes a circulant graph with vertex set $V = \{0, 1, \cdots, n-1\}$ such that a vertex u is adjacent to all vertices of $V - \{u\}$ except $u \pm k_i \pmod n$, $i = 1, 2, \ldots, m$, then for any given $k_1 < k_2 < \cdots < k_m$ almost all circulant graphs $\overline{C_i}(n, k_1, k_2, \ldots, k_m)$ are hyperenergetic.*

Remark 2.5.3. If H is a Hamiltonian cycle of K_n, then $K_n - H = \overline{C_i}(n, 1)$.

If λ_i, $i = 1, 2, \ldots, n$, is the A-spectrum of the graph G, then as seen in Theorem 2.4.17, the A-spectrum of the graph $SD(G)$ is $2\lambda_i + 1, -1^{[n]}$, $i = 1, 2, \ldots, n$. Therefore, the energy of the graph $SD(G)$ is $E(SD(G)) = n + \sum\limits_{i=1}^{n} |2\lambda_i + 1| > 2(2n-1) = E(K_{2n})$ if $\sum\limits_{i=1}^{n} |2\lambda_i + 1| > 3n - 2 = n + 2(n-1) = n + E(K_n)$. Thus, we have the following observation.

Theorem 2.5.4. *Let G be a graph with $|\lambda_i| \geq \frac{1}{2}$, for all non-zero eigenvalues. Then the graph $SD(G)$ is hyperenergetic if $E(G) > n + \gamma_- - 1$, where γ_- is the number of negative eigenvalues of G.*

Proof. Let γ_+, γ_- and γ_0 be the number of positive, number of negative and number of zero eigenvalues of the graph G. Assume that $|\lambda_i| \geq \frac{1}{2}$, for all non-zero eigenvalues of G. Then we have

$$|2\lambda_i + 1| = \begin{cases} 2|\lambda_i| + 1, & \text{if } \lambda_i \geq 0 \\ 2|\lambda_i| - 1, & \text{if } \lambda_i < 0. \end{cases}$$

Therefore, by Theorem 2.4.17, we have

$$\begin{aligned} E(SD(G)) &= n + \sum_{i=1}^{n} |2\lambda_i + 1| \\ &= n + \left(\sum_{\lambda_i \geq 0} |2\lambda_i + 1| + \sum_{\lambda_i < 0} |2\lambda_i + 1| \right) \\ &= n + \left(\sum_{\lambda_i \geq 0} (|2\lambda_i| + 1) + \sum_{\lambda_i < 0} (|2\lambda_i| - 1) \right) \\ &= n + 2E(G) + \gamma_+ + \gamma_0 - \gamma_- \\ &= 2n + 2E(G) - \gamma_-, \quad as \ \ \gamma_+ + \gamma_0 + \gamma_- = n. \end{aligned}$$

For if, $SD(G)$ is hyperenergetic, then $E(SD(G)) > E(K_{2n}) = 2(2n-1)$ implies $2n+2E(G)-\gamma_- > 4n-2$, which gives $E(G) > n+\gamma_- -1$. This proves the result. □

Theorem 2.5.4 gives a sufficient condition for the construction of a hyperenergetic graph from any given graph G of order n.

Theorem 2.5.5. *Let G be a graph with $|\lambda_i| \geq 1$, for all non-zero eigenvalues. Then the graph G^* is hyperenergetic if $E(G) > n+2\gamma_- -1$, where γ_- is the number of negative eigenvalues of G.*

Proof. Let γ_+, γ_- and γ_0 be the number of positive, number of negative and number of zero eigenvalues of the graph G. Assume that $|\lambda_i| \geq 1$, for all non-zero eigenvalues of G. Then we have

$$|\lambda_i + 1| = \begin{cases} |\lambda_i| + 1, & \text{if } \lambda_i \geq 0 \\ |\lambda_i| - 1, & \text{if } \lambda_i < 0. \end{cases}$$

Now using Lemma 2.4.10 and proceeding similarly as in Theorem 2.4.15, the result follows. □

Since extended double cover G^* of the graph G is always bipartite, Theorem 2.5.5 gives a sufficient condition for the construction of a hyperenergetic bipartite graph from any given graph G of order n.

As an immediate consequence of Theorem 2.3.8, we have the following observation gives a sufficient condition for the graph KK_n^j to be hypergenectic.

Corollary 2.5.6. *For $k \in \mathbb{N} - \{1, 2\}, (k-1)^2 < j \leq k^2$ and $n \geq ((k-1)^2 + 2)^2 - (k-1)^2$, the graph KK_n^j is hyperenergetic.*

Proof. Since $k \geq 3$, we have by Theorem 2.3.8, $E(KK_n^j) > 4n - 8 + 2k \geq 4n - 2 = E(K_{2n})$. □

CHAPTER 3

On the Laplacian energy of graphs

In this chapter, we study the Laplacian energy of graphs and present some well known results on Laplacian energy of graphs. We obtain lower and upper bounds for the Laplacian energy of graphs in terms of the number of vertices n, the number of edges m, maximum degree Δ and clique number ω. We consider double graphs, extended double graphs and strong double graphs of a graph and with the help of these graphs, we construct some new families of non L-cospectral L-equienergetic graphs and bipartite graphs on $n \equiv 0 \pmod 2$.

3.1 Introduction

Let G be a graph with n vertices $v_1, v_2, \ldots, v_n$ and m edges and let $d_i = d(v_i)$, $i = 1, 2, \ldots, n$, be the degree of the vertices of G. The (combinatorial) Laplacian matrix of G is the $n \times n$ matrix $L = L(G) = (l_{ij})$, where

$$l_{ij} = \begin{cases} -1, & \text{if there is an edge from } v_i \text{ to } v_j, \\ d_i, & \text{if } i = j \\ 0, & \text{otherwise.} \end{cases}$$

Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex degrees and $A(G)$ be the adjacency matrix of G. It is clear from the definition of Laplacian matrix that $L(G) = D(G) - A(G)$. The matrix $L(G)$ is sometimes called the Kirchhoff matrix of G due to its role in the well known Matrix Tree Theorem (Theorem 3.1.1), which is usually attributed to Kirchhoff. Another name, the matrix of admittance, comes from the theory of electrical networks (admittance=conductivity). For our purpose, we call it the Laplacian matrix of G.

Another way of defining Laplacian matrix is as follows. Orient arbitrarily the edges of a given graph G. That is, for each $e \in \mathscr{E}(G)$, choose one of its ends as the initial vertex, and name the other end the terminal vertex. The oriented incidence matrix of G with respect to the given orientation is the $n \times m$ matrix

$C = C(G) = (c_{ij})$, where

$$c_{ij} = \begin{cases} +1, & \text{if } j\text{th edge is incident to } i\text{th vertex,} \\ -1, & \text{if } j\text{th edge is incident from } i\text{th vertex,} \\ 0, & \text{otherwise.} \end{cases}$$

It is well known [28] that $C(G)C^t(G) = L(G)$. Therefore, if we let μ be any eigenvalue of $L(G)$ and x a corresponding eigenvector, we have:

$$\begin{aligned} \mu||x||^2 &=< \mu x, x >=< L(G)x, x >=< C(G)C^t(G)x, x > \\ &=< C^t(G)x, C^t(G)x >= ||C^t(G)x||^2 \geq 0, \end{aligned}$$

where $<, >$ is the standard inner product. This shows that $L(G)$ is positive semi-definite. Furthermore, as the row sums and column sums of $L(G)$ are all zero, therefore 0 is an eigenvalue of $L(G)$ with all ones vector as corresponding eigenvector. Thus, it follows that $L(G)$ is a real symmetric positive semi-definite with smallest eigenvalue 0 and thus the eigenvalues of $L(G)$ are real and non-negative.

The characteristic polynomial $\det(xI - L(G)) = |xI - L(G)|$ of the Laplacian matrix $L(G)$ of G is called the Laplacian characteristic polynomial of G and is denoted by $\psi(G, x)$. The eigenvalues of $L(G)$ are called the Laplacian eigenvalues (L-eigenvalues) of G. The set of distinct L-eigenvalues of G together with their multiplicities is called the L-spectrum of G. If G has k distinct L-eigenvalues $\mu_1, \mu_2, \ldots, \mu_k$ with respective multiplicities $m_1, m_2, \ldots, m_k$, then we write the L-spectrum of G as $Spec_L(G) = \{\mu_1^{[m_1]}, \mu_2^{[m_2]}, \ldots, \mu_k^{[m_k]}\}$.

In 1847, Kirchhoff [80] proved a result that related the Laplacian matrix of a connected graph G with the number of spanning trees of G, which is popularly known as Kirchhoff's matrix tree theorem.

Theorem 3.1.1. *Let G be a connected graph on n vertices. Then all cofactors of $L(G)$ are equal and the common value is the number of spanning trees in G.*

Since then several authors from different disciplines have enriched the subject. Among the studies of different properties and uses of Laplacian matrices, the study of Laplacian spectrum and its relation with the structural properties of graphs has been one of the most attracting features of the subject.

To know some interesting facts about Laplacian matrix and its eigenvalues, we refer the reader to the survey articles [105, 106, 108]. Let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$ be the eigenvalues of $L(G)$, which are enumerated in non-decreasing order and repeated according to multiplicity. Fiedler [44] was the first to notice that $\mu_{n-1} = 0$ if and only if G is disconnected. More generally, he observed that the multiplicity of the eigenvalue 0 is the same as the number of connected components of G. Viewing μ_{n-1} as an algebraic measure of the connectivity of a graph, Fiedler termed this eigenvalue as the algebraic connectivity of G. Fiedler also proved some remarkable results (see [44]) and showed that further information about the graph structures can be extracted from an eigenvector corresponding to the algebraic connectivity of a connected graph. After these observations, many researchers have studied the relationship of this eigenvector with the graph structure and obtained several interesting results. The eigenvectors corresponding to algebraic connectivity are now popularly known as Fiedler vectors.

The fundamental result, relating the coefficients of $\psi(G, x)$ with the structure of the graph G, is the Kel′mans Theorem (this theorem was first communicated by Kel′mans in 1967 in a booklet entitled Cybernetics in the Service of Communism published in Moscow and Leningrad, in Russian language.)

Theorem 3.1.2. *Let G be a graph of order n with Laplacian characteristic polynomial*

$$\psi(G, x) = x^n + c_1 x^{n-1} + c_2 x^{n-2} + \cdots + c_{n-1} x + c_n.$$

Then

$$c_n = 0, \quad c_j = (-1)^j \sum_{F \in \mathscr{F}_{n-j}} \gamma(F),$$

for all $j = 1, 2, \ldots, n-1$, where $\mathscr{F}_k$ is the set of all spanning forests of G with k components and $\gamma(F)$ is the product of cardinalities of the components of F.

If $\tau(G)$ is the number of spanning trees of the graph G, we have the following observation from Theorem 3.1.2.

Corollary 3.1.3. *Let G be a graph of order n having $\tau(G)$ spanning trees and Laplacian characteristic polynomial*

$$\psi(G, x) = x^n + c_1 x^{n-1} + c_2 x^{n-2} + \cdots + c_{n-1} x + c_n.$$

Then

$$\tau(G) = \frac{1}{n}|c_{n-1}|.$$

This gives the relation between the coefficients of the Laplacian characteristic polynomial with the structure of the graph G.

Using the fact that the coefficients of the characteristic polynomial are symmetric functions of the roots and smallest eigenvalue of $L(G)$ is zero, we have the following observation.

Corollary 3.1.4. *Let G be a graph of order n having $\tau(G)$ spanning trees and Laplacian eigenvalues $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$. Then*

$$\tau(G) = \frac{\mu_1 \mu_2 \mu_3 \cdots \mu_{n-1}}{n} = \frac{1}{n} \prod_{i=1}^{n-1} \mu_i.$$

From this, it is clear that $\tau(G) = 0$ if $\mu_{n-1} = 0$. Since $\tau(G) = 0$ means that the graph is disconnected, therefore this observation also makes it clear that $\mu_{n-1} > 0$ if and only if G is connected.

3.2 Laplacian energy of graphs

Definition 3.2.1. *Laplacian energy of a graph.* Let G be a graph of order n with m edges and having Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$. The Laplacian energy of G is denoted by $LE(G)$ and is defined as

$$LE(G) = \sum_{j=1}^{n} |\mu_j - \frac{2m}{n}|. \tag{3.1}$$

This concept was introduced in 2006 by Gutman and Zhou [65]. The idea of Gutman and Zhou was to conceive a graph energy like quantity that instead of adjacency eigenvalues is defined in terms of Laplacian eigenvalues and that hopefully would preserve the main features of the original graph energy. The definition of $LE(G)$ was therefore so chosen that all the properties possessed by graph energy should be preserved. In fact they were successful, as most of the properties possessed by $E(G)$ are also possessed by $LE(G)$, but there are some dissimilarities.

In analogy to integral representation for $E(G)$, we have the following integral representation for $LE(G)$.

Theorem 3.2.2. *Let G be a graph with n vertices and let $\phi(N,x)$ be the characteristic polynomial of $N = L(G) - \frac{2m}{n}I_n$. Then*

$$LE(G) = \sum_{j=1}^{n} |\mu_j - \frac{2m}{n}| = \frac{1}{\pi}\int_{-\infty}^{\infty} (n - \frac{ix\phi'(N,ix)}{\phi(N,ix)})dx,$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the L-eigenvalues of graph G, $i = \sqrt{-1}$ and $\int_{-\infty}^{\infty} F(x)dx$ denotes the principle value of the respective integral.

The next result [73] follows from Theorem 3.2.2.

Theorem 3.2.3. *If G is a graph of order n, then*

$$LE(G) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{1}{x^2}\log|x^n\phi(N,\frac{i}{x})|dx.$$

The importance of the integral representation for $E(G)$ is that it helps in determination of extremal graphs with respect to energy from any given class of graphs without having the information about the A-spectrum. This property is not possessed by the integral representation for $LE(G)$, as it involves the characteristic polynomial of the matrix $L(G) - \frac{2m}{n}I_n$ and not the matrix $L(G)$.

For an r-regular graph, we have $D(G) = rI_n$ and so $L(G) = D(G) - A(G) =$

$rI_n - A(G)$, that is, $L(G) - rI_n = -A(G)$. Therefore, we have the following observation.

Theorem 3.2.4. *If G is an r-regular graph, then*

$$LE(G) = E(G).$$

This shows that the concept of energy and Laplacian energy of a graph are same for regular graphs, so Laplacian energy will be of interest mainly for non-regular graphs.

3.3 Bounds for Laplacian energy

Various lower and upper bounds for the Laplacian energy $LE(G)$ are known, which give its connection with the different parameters of a graph. Here, we list some of the well known bounds.

For a graph with n vertices and m edges having vertex degrees d_i, $i = 1, 2, \ldots, n$, let

$$M = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i - \frac{2m}{n}\right)^2.$$

It is clear that $M \geq m$ for all graphs G, and that $M = m$ holds if and only if G is a regular graph.

The following bounds are obtained in the basic paper [65] on Laplacian energy $LE(G)$, which are analogues to the corresponding bounds on energy $E(G)$.

Theorem 3.3.1. *Let G be a graph with n vertices and m edges and let M be defined above. Then*

$$LE(G) \leq \sqrt{2Mn},$$

with equality if and only if G is either regular of degree 0 or consists of α copies of complete graphs of order k and $(k-2)\alpha$ isolated vertices, $\alpha \geq 1$, $k \geq 2$.

Theorem 3.3.2. *If G is a graph with n vertices and m edges having no isolated vertex, then*

$$2\sqrt{M} \leq LE(G) \leq 2M,$$

with equality on the left if and only if G is a complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ and equality on the right if and only if G is a matching of $m = \frac{n}{2}$ edges.

Since $M \geq m$, from Theorem 3.3.2, it follows that $LE(G) \geq 2\sqrt{M} \geq 2\sqrt{m}$.

Theorem 3.3.3. *If G is a graph on n vertices and m edges having $p \geq 1$ components, then*

$$LE(G) \leq \frac{2m}{n}p + \sqrt{(n-p)\left[2M - p(\frac{2m}{n})^2\right]}. \tag{3.2}$$

For $p = 1$, equality in (3.2) is attained if and only if G is either $\frac{n}{2}K_2$ or K_n or a non-complete connected strongly regular graph with two non trivial L-eigenvalues both with absolute value $\sqrt{\frac{(2m-(\frac{2m}{n})^2)}{(n-1)}}$. For $p = n$, $G \cong \overline{K_n}$ and equality holds trivially. For any p, $2 \leq p \leq n-1$, equality in (3.2) holds for the graphs consisting of $\alpha \geq 1$ copies of complete graphs on k vertices and $(k-2)\alpha$, $k \geq 2$ isolated vertices, provided $(k-1)\alpha = p$.

Using the fact that arithmetic mean is greater than or equal to the geometric mean, it can be seen that the upper bound given by Theorem 3.3.3 improves the upper bound given by Theorem 3.3.1.

The following [156] is the bound for Laplacian energy $LE(G)$ as a function of the determinant of the matrix $N = L(G) - \frac{2m}{n}I_n$.

Theorem 3.3.4. *Let G be a graph with n vertices and m edges and let N be the matrix defined above, then*

$$\sqrt{2M + n(n-1)|det(N)|^{\frac{2}{n}}} \leq LE(G) \leq \sqrt{2M(n-1) + n|det(N)|^{\frac{2}{n}}}.$$

The following [128] is an upper bound for Laplacian energy $LE(G)$ in terms of the number of vertices n and the number of edges m.

Theorem 3.3.5. *Let G be a graph of order n with $m > 0$ edges. Then*

$$LE(G) \leq 4m\left(1 - \frac{1}{n}\right),$$

with equality if and only if $G \cong K_2 \cup K_{n-2}$.

The following [154] is a lower bound for Laplacian energy $LE(G)$ in terms of the number of vertices n and the number of edges m.

Theorem 3.3.6. *Let G be a graph with $n \geq 3$ vertices. Then*

$$LE(G) \geq \frac{4m}{n},$$

with equality if and only if G is a regular complete k-partite graph, for $1 \leq k \leq n$.

Let σ, $1 \leq \sigma \leq n-1$, be the number of Laplacian eigenvalues greater than or equal to average vertex degree $\overline{d} = \frac{2m}{n}$ and let

$$S_\sigma(G) = \sum_{j=1}^{\sigma} \mu_j.$$

Using equation (3.1) and the fact that $\sum_{j=1}^{n} \mu_j = 2m$, we have

$$\begin{aligned}
LE(G) &= \sum_{j=1}^{n} |\mu_j - \frac{2m}{n}| = \sum_{j=1}^{\sigma}\left(\mu_j - \frac{2m}{n}\right) + \sum_{j=\sigma+1}^{n}\left(\frac{2m}{n} - \mu_j\right) \\
&= \sum_{j=1}^{\sigma} \mu_j - \frac{2m}{n}\sigma + \frac{2m}{n}(n-\sigma) - \sum_{j=\sigma+1}^{n} \mu_j \\
&= 2S_\sigma(G) - \frac{4m\sigma}{n}.
\end{aligned}$$

This shows that,

$$LE(G) = 2S_\sigma(G) - \frac{4m\sigma}{n}. \tag{3.3}$$

In fact in [35], it can be seen that

$$LE(G) = 2\max_{1 \leq j \leq n-1}\{S_j(G) - \frac{2mj}{n}\}. \tag{3.4}$$

Das et al. [35] obtained the following lower bound for Laplacian energy $LE(G)$ in terms of the number of vertices n, the number of edges m and maximum degree Δ.

Theorem 3.3.7. *Let G be a graph with n vertices and m edges having maximum degree Δ, then*

$$LE(G) \geq 2\left(\Delta + 1 - \frac{2m}{n}\right), \tag{3.5}$$

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

In [35], it is shown that the lower bound (3.5) is better than the lower bound given by Theorem 3.3.2, for a tree T, $(T \neq P_n)$ of order n. Also the lower bound (3.5) is better than the lower bound given by Theorem 3.3.6, for a tree T of order n with maximum degree $\Delta \geq \frac{n}{\sqrt{2}} + 1$.

Remark 3.3.8. For a connected graph having vertex degrees $d_n \leq d_{n-1} \leq \cdots \leq d_1$, Grone [61] proved that

$$S_k(G) = \sum_{j=1}^{k} \mu_j \geq \sum_{j=1}^{k} d_j + 1,$$

for all k, $1 \leq k \leq n-1$. Therefore, one can always improve the lower bound (3.5) as follows,

$$LE(G) = 2S_\sigma(G) - \frac{4m\sigma}{n} \geq 2\left(\sum_{j=1}^{\sigma} d_j + 1 - \frac{2m\sigma}{n}\right).$$

The following upper bound for Laplacian energy $LE(G)$ is in terms of the number of vertices, the number of edges m and maximum degree Δ, and can be found in [35].

Theorem 3.3.9. *Let G be a graph with n vertices and $m \geq \frac{n}{2}$ edges having maximum degree Δ. Then*

$$LE(G) \leq 2\left(2m - \Delta - \frac{2m}{n} + 1\right), \tag{3.6}$$

with equality if and only if $G \cong K_{1,n-1}$ *or* $G \cong K_{1,\Delta} \cup \overline{K}_{n-\Delta-1}$ $\left(\frac{n}{2} \leq \Delta \leq n-2\right)$.

In [35] it is shown that the upper bound (3.6) is better than the upper bound (3.2) for trees with maximum degree $\Delta \geq \frac{n}{2}$, $n \geq 37$.

The following result gives a lower bound for the largest Laplacian eigenvalue μ_1 in terms of maximum degree Δ and an upper bound in terms of number of vertices n of the graph G [28, 44, 62].

Lemma 3.3.10. *Let* G *be a connected graph of order* n *and let* Δ *be its maximum degree. Then* $\Delta + 1 \leq \mu_1 \leq n$. *Equality holds on the left if* $\Delta = n-1$ *and on the right if and only if* G *is the join of two graphs.*

If $G+e$ is the graph obtained from G by adding the edge e, then the Laplacian eigenvalues of $G+e$ and G interlace as can be seen in [21].

Lemma 3.3.11. *Let* $G' = G + e$ *be the graph obtained from* G *by adding a new edge* e. *Then the Laplacian eigenvalues of* G *interlace the Laplacian eigenvalues of* G', *that is,*

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

Let K_ω be a complete graph with ω vertices. From K_ω, we construct a new graph, denoted by $KS_{n,\omega}$, by adding $n-\omega$ pendant edges to any one vertex of K_ω. The graph $KS_{n,\omega}$ is of order n and with clique number ω. Also from K_ω, we construct another graph, denoted by $Ki_{n,\omega}$, by attaching a path of length $n-\omega-1$ to any one vertex of K_ω. We note that $KS_{n,n-1} = Ki_{n,n-1}$ and $KS_{n,n} = Ki_{n,n} = K_n$.

We now obtain a lower bound for the Laplacian energy $LE(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ and clique number ω of the graph G.

Theorem 3.3.12. *Let* G *be a connected graph of order* $n \geq 2$ *with* m *edges,* *maximum degree* Δ *and clique number* ω. *Then*

$$LE(G) \geq 2\left(\Delta + 1 + \omega^2 - (\frac{2m}{n} + 2)\omega + \frac{2m}{n}\right), \tag{3.7}$$

with equality if and only if $G \cong KS_{n,\omega}$ *or* $G \cong K_n$.

Proof. Let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$ be the Laplacian eigenvalues of G and let σ, $(1 \leq \sigma \leq n-1)$ be the number of Laplacian eigenvalues greater than or equal to average degree $\overline{d} = \frac{2m}{n}$. Using equation (3.4), we have

$$\begin{aligned} LE(G) &= 2S_\sigma(G) - \frac{4m\sigma}{n} = \max_{1\leq i\leq n-1}\left\{2S_i(G) - \frac{4mi}{n}\right\} \\ &\geq 2\left(S_{\omega-1}(G) - \frac{2m}{n}(\omega-1)\right), \end{aligned}$$

as $2 \leq \omega \leq n$, with equality if and only if $\sigma = \omega - 1$.

In order to obtain inequality (3.7), we need to show that $S_{\omega-1}(G) \geq \Delta + 1 + \omega(\omega-2)$. Since clique number of G is ω, therefore K_ω is a subgraph of G.

If $\omega = n$, then $G = K_n$ and $\sigma = n - 1 = \omega - 1$ with $S_{\omega-1}(G) = S_{n-1}(K_n) = n(n-1) = n + n(n-2) = \Delta + 1 + \omega(\omega-2)$. Therefore, equality occurs in (3.7) for this case.

So assume that $\omega \leq n-1$. Let v_1 be the vertex of maximum degree in G, that is $\deg(v_1) = \Delta$ and $N_G(v_1)$ be the set of neighbours of v_1 in G. Since G is connected, so $\Delta \geq \omega$. Therefore, we have two possibilities (1) $\Delta = n-1$ or (2) $\Delta \leq n-2$.

Case (1). Let $\Delta = n-1$. Then $KS_{n,\omega}$ is the subgraph of G, that is, $KS_{n,\omega} \subseteq G$. The Laplacian spectrum of $KS_{n,\omega}$ is $\{n, \omega^{[\omega-2]}, 1^{[n-\omega]}, 0\}$. If $G \cong KS_{n,\omega}$, then since $n = \mu_1(KS_{n,\omega}) = \Delta + 1$ and $\sigma = \omega - 1$ in $KS_{n,\omega}$, equality occurs in (3.7). If $G \neq KS_{n,\omega}$, then by Lemmas 3.3.10 and 3.3.11, we have $\mu_1(G) \geq \Delta + 1$ and $\mu_i(G) \geq \mu_i(KS_{n,\omega}) = \omega$, for all $i = 2, 3, \ldots, \omega - 1$, where at least one inequality is strict.

Therefore,

$$\begin{aligned} S_{\omega-1}(G) &= \sum_{i=1}^{\omega-1}\mu_i(G) = \mu_1(G) + \sum_{i=2}^{\omega-1}\mu_i(G) \\ &> \Delta + 1 + \sum_{i=2}^{\omega-1}\mu_i(KS_{n,\omega}) = \Delta + 1 + \omega(\omega-2). \end{aligned}$$

Thus the result is true in this case.

Case (2). Let $\Delta \le n-2$. Since $\omega \le \Delta \le n-2$, we have two subcases to consider. Either (2.1) $\Delta = \omega$ or (2.2) $\Delta \ge \omega + 1$.

Subcase (2.1). If $\Delta = \omega$, then we can assume that the maximum degree vertex v_1 is in $V(K_\omega)$ in G. In this case $Ki_{\omega+1,\omega}$ is a subgraph of G. The Laplacian spectrum of $Ki_{\omega+1,\omega}$ is $\{\omega+1, \omega^{[\omega-2]}, 1, 0\}$. So, by Lemmas 3.3.10 and 3.3.11, we have $\mu_1(G) \ge \Delta + 1$, and $\mu_i(G) \ge \mu_i(Ki_{\omega+1,\omega}) = \omega$, for all $i = 2, 3, \ldots, \omega - 1$, where at least one inequality is strict.

Therefore,

$$\begin{aligned} S_{\omega-1}(G) &= \sum_{i=1}^{\omega-1} \mu_i(G) = \mu_1(G) + \sum_{i=2}^{\omega-1} \mu_i(G) \\ &> \Delta + 1 + \sum_{i=2}^{\omega-1} \mu_i(Ki_{\omega+1,\omega}) = \Delta + 1 + \omega(\omega-2). \end{aligned}$$

Thus, the result in true in this case as well.

Subcase (2.2). Let $\omega + 1 \le \Delta \le n-2$. Assume $S = V(K_\omega) = \{u_1, u_2, \ldots, u_\omega\}$ is the vertex set of K_ω in G. We have either $v_1 \in S$ or $v_1 \notin S$.

If $v_1 \in S$, then $KS_{\Delta+1,\omega}$ is a subgraph of G. The Laplacian spectrum of $KS_{\Delta+1,\omega}$ is $\{\Delta+1, \omega^{[\omega-2]}, 1^{[\Delta-\omega+1]}\}$. Again by Lemmas 3.3.10 and 3.3.11, we have $\mu_1(G) \ge \Delta + 1$, and $\mu_i(G) \ge \mu_i(KS_{\Delta+1,\omega}) = \omega$, for all $i = 2, 3, \ldots, \omega - 1$, where at least one inequality is strict.

Therefore,

$$\begin{aligned} S_{\omega-1}(G) &= \sum_{i=1}^{\omega-1} \mu_i(G) = \mu_1(G) + \sum_{i=2}^{\omega-1} \mu_i(G) \\ &> \Delta + 1 + \sum_{i=2}^{\omega-1} \mu_i(KS_{\Delta+1,\omega}) = \Delta + 1 + \omega(\omega-2). \end{aligned}$$

Thus, the result is true in this case as well.

Now, let $v_1 \notin S$. In this case, suppose that $S \cap N_G(v_1) = \{u_1, u_2, \ldots, u_p\}$. Since ω is the clique number of the connected graph G, we have $0 \le p \le \omega - 1$ (if $p = \omega$, then the clique number of G is $\omega + 1$, a contradiction). Since $\omega + 1 \le \Delta \le n-2$, we have $\Delta - p - 1 \ge \Delta - \omega \ge 1$ and G is connected. In this case $Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}$ is a subgraph of G. The Laplacian spectrum of $Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}$

is $\{\omega+1, \omega^{[\omega-2]}, \Delta-p+1, 1^{[\Delta-p]}, 0, 0\}$. Proceeding similarly as above, the result follows in this case as well. It is clear from the above discussion that the equality holds if $G \cong K_n$ or $G \cong KS_{n,\omega}$.

Conversely, if G is isomorphic to one of the graphs K_n or $KS_{n,\omega}$, then it is easy to see that equality holds in (3.7). $\square$

Remark 3.3.13. If $\omega = 2$, (that is, for bipartite graphs G), the lower bound (3.7) is same as the lower bound (3.5). For $\omega \geq 3$, we note that the lower bound (3.7) is better than the lower bound (3.5), if $\omega \geq \frac{2m}{n}$. This is true, since

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

implies that $\omega \geq \dfrac{2m}{n}$. In particular, if $\omega = 3$ and G is unicyclic graph or bicyclic graph or tricyclic graph, then $3 = \omega \geq \dfrac{2m}{n}$, for $n \geq 4$.

Remark 3.3.14. For $\omega = 2$, the lower bounds (3.7) and (3.5) are same. For $\omega \geq 3$, we observe that the lower bound (3.7) is better than the lower bound given in Theorem 3.3.6, if $\omega \geq \Delta - 1$, $\Delta \geq 8$. This can be seen as follows. We have

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

which implies that $\dfrac{2m}{n} \leq \omega + \dfrac{\Delta+1}{\omega-2}$. Since $\dfrac{2m}{n} \leq \Delta$, therefore $\Delta \leq \omega + \dfrac{\Delta+1}{\omega-2}$, which implies that $\omega^2 - \omega(\Delta+2) + 3\Delta + 1 \geq 0$, further implies that $\omega \geq \dfrac{\Delta+2+\sqrt{\Delta^2-8\Delta}}{2}$.

Clearly,

$$\Delta - 1 = \frac{\Delta+2+\sqrt{(\Delta-4)^2}}{2} \geq \frac{\Delta+2+\sqrt{\Delta^2-8\Delta}}{2},$$

and hence the observation.

In the graph G, let d_i be the degree of the vertex v_i, for all $i = 1, 2, \ldots, n$. The first Zagreb index $M_1(G)$ is defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2.$$

and was introduced in [68] and elaborated in [67]. The main properties of $M_1(G)$ were summarized in [112]. Some recent results on the first Zagreb index are reported in [30].

Remark 3.3.15. For $\omega = 2$, we note that the lower bound (3.7) and (3.5) are same. For $\omega \geq 3$, we observe that the lower bound (3.7) is better than the lower bound given by Theorem 3.3.2, for almost all connected graphs. This can be seen as follows. We have

$$\begin{aligned}
& 2\left(\Delta+1+\omega^2-(\frac{2m}{n}+2)\omega+\frac{2m}{n}\right) \geq 2\sqrt{m+\frac{1}{2}\sum_{i=1}^{n}\left(d_i-\frac{2m}{n}\right)^2} \\
\implies & \left(\Delta+1+\omega^2-(\frac{2m}{n}+2)\omega+\frac{2m}{n}\right)^2 \geq m+\frac{1}{2}\left(\sum_{i=1}^{n}d_i^2+\frac{4m^2}{n}-8m^2\right) \\
\implies & M_1(G) \leq 2\left(\Delta+1+\omega(\omega-2)-(\omega-1)\frac{2m}{n}\right)^2+2m(8m-\frac{4m}{n}-1).
\end{aligned}$$

Since the clique number of G is ω, it follows that G is $K_{\omega+1}$-free. Therefore from [153],

$$M_1(G) \leq \frac{2\omega-2}{\omega}mn,$$

and we have

$$(1-\frac{1}{\omega})2mn \leq 2\left(\Delta+1+\omega(\omega-2)-(\omega-1)\frac{2m}{n}\right)^2+2m(8m-\frac{4m}{n}-1),$$

which gives, $n \leq 8m-\frac{4m}{n}-1$, that is, $m \geq \frac{n+1}{8-\frac{4}{n}}$.

Since G is connected, $m \geq n-1$, and so $n \geq \frac{n+1}{8-\frac{4}{n}}+1$, which is true for all $n \geq 2$. This shows that the lower bound (3.7) is better than the lower bound given by Theorem 3.3.2, for almost all connected graphs.

For k, $1 \leq k \leq n$, let $S_k(G)=\sum_{i=1}^{k}\mu_i$, be the sum of k largest Laplacian eigenvalues of the graph G. Brouwer [21] conjectured that

$$S_k(G) \leq m+\frac{k(k+1)}{2},$$

for all $1 \leq k \leq n$. Haemers et al. [79] showed that the Conjecture is true for all graphs when $k=2$ and is true for trees. Du et al. [39] obtained various upper bounds for $S_k(G)$ and proved that the conjecture is also true for unicyclic and bicyclic graphs. For the progress on this conjecture see [21, 79].

Du et al. [39] obtained the following upper bound for $S_k(G)$ in terms of clique number ω.

Theorem 3.3.16. *Let G be a graph with n vertices and m edges having clique number $\omega \geq 3$. Then*

$$S_k(G) \leq \sigma\omega + 2m - \omega(\omega - 1), \tag{3.8}$$

for $1 \leq k \leq \omega - 2$.

The following observation due to Fulton [50] gives the relation between the sum of k largest eigenvalues of the sum of two real symmetric matrices and the sum of the k largest eigenvalues of the individual matrices.

Lemma 3.3.17. *Let A and B be two real symmetric matrices of order n. Then for any $1 \leq k \leq n$,*

$$\sum_{i=1}^{k} \lambda_i(A+B) \leq \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_i(B),$$

where $\lambda_i(X)$ is the i^{th} eigenvalue of X.

First we obtain an upper bound for $S_\sigma(G)$ in terms of the number of edges m, maximum degree Δ and the clique number ω.

Theorem 3.3.18. *Let G be a connected graph of order $n \geq 2$ with m edges, maximum degree Δ and the clique number ω. Let σ, $(1 \leq \sigma \leq n-1)$ be the number of Laplacian eigenvalues greater than or equal to $\frac{2m}{n}$. Then*

$$S_\sigma(G) \leq (\sigma - 1)\omega + 2m - (\Delta + 1) - \omega^2 + 3\omega, \tag{3.9}$$

with equality if and only if $G \cong KS_{n,\omega}$ or $G \cong K_n$.

Proof. As the clique number of G is ω, with $2 \leq \omega \leq n$, we have two possibilities, case (1) $\omega = n$, or case (2) $\omega \leq n - 1$.

Case (1). If $\omega = n$, then $G \cong K_n$ and so, for $1 \leq \sigma \leq n-1$, we have

$$\begin{aligned} S_\sigma(G) &= S_\sigma(K_n) = \sigma n = (\sigma-1)n + n \\ &= (\sigma-1)n + n(n-1) - n - n^2 + 3n \\ &= (\sigma-1)\omega + 2m - (\Delta+1) - \omega^2 + 3\omega. \end{aligned}$$

As $2m = n(n-1)$, $\Delta = n-1$ and $\omega = n$, therefore equality occurs in (3.9) in this case.

Case (2). Now assume that $\omega \leq n-1$. Let H be a subgraph of G, having clique number ω. Let $|E(G)| = m(G)$ and $|E(H)| = m(H)$ respectively, be the number of edges in G and H. Since $\omega \leq n-1$, we consider two possibilities, subcase (2.1) $\Delta = n-1$, or subcase (2.2) $\Delta \leq n-2$.

Subcase (2.1). Let $\Delta = n-1$. Then $H = KS_{n,\omega}$. The Laplacian spectrum of $KS_{n,\omega}$ is $\{n, \omega^{[\omega-2]}, 1^{[n-\omega]}, 0\}$. Therefore, for $1 \leq \sigma \leq n-1$, by Lemma 3.3.17, we have

$$\begin{aligned} S_\sigma(G) &= \sum_{i=1}^{\sigma} \mu_i(G) \leq \sum_{i=1}^{\sigma} \mu_i(H) + \sum_{i=1}^{\sigma} \mu_i(G \setminus H) \\ &= S_\sigma(KS_{n,\omega}) + S_\sigma(G \setminus KS_{n,\omega}) \\ &\leq n + (\sigma-1)\omega + 2(m(G) - m(KS_{n,\omega})) \\ &= (\sigma-1)\omega + 2m - (\Delta+1) - \omega^2 + 3\omega, \end{aligned}$$

as $S_\sigma(G \setminus KS_{n,\omega}) \leq S_{n-1}(G \setminus KS_{n,\omega}) = 2m(G) - (\omega^2 - 3\omega + 2n)$ and $2m(KS_{n,\omega}) = \omega^2 - 3\omega + 2n$. Clearly, the equality occurs if and only if $\sigma - 1 = \omega - 2$ and $2m = \omega^2 - 3\omega + 2n$, that is, if and only if $G \cong KS_{n,\omega}$.

Subcase (2.2). Assume that $\Delta \leq n-2$. Since G is connected, we have two possibilities (2.2.1) $\omega = \Delta$, or (2.2.2) $\omega + 1 \leq \Delta \leq n-2$.

Subcase (2.2.1). Let $\omega = \Delta$. Then $H = Ki_{\omega+1,\omega}$. The Laplacian spectrum of $Ki_{\omega+1,\omega}$ is $\{\omega+1, \omega^{[\omega-2]}, 1, 0\}$. Therefore, for $1 \leq \sigma \leq n-1$, by Lemma 3.3.17, we have

$$
\begin{aligned}
S_\sigma(G) &= \sum_{i=1}^{\sigma}\mu_i(G) \le \sum_{i=1}^{\sigma}\mu_i(H) + \sum_{i=1}^{\sigma}\mu_i(G\setminus H)\\
&= S_\sigma(Ki_{\omega+1,\omega}) + S_\sigma(G\setminus Ki_{\omega,\omega})\\
&\le \omega+1+(\sigma-1)\omega+2(m(G)-m(Ki_{\omega+1,\omega}))\\
&= (\sigma-1)\omega+2m(G)+\omega+1-(\omega^2-\omega+2)\\
&= (\sigma-1)\omega+2m-(\omega+1)-\omega^2+3\omega\\
&= (\sigma-1)\omega+2m-(\Delta+1)-\omega^2+3\omega,
\end{aligned}
$$

as $m(Ki_{\omega+1,\omega}) = \frac{\omega^2-\omega+2}{2}$. Since G is connected, equality does not occur in this case. For, if equality occurs, then $G \cong Ki_{\omega+1,\omega}$ and so $n = |G| = |Ki_{\omega+1,\omega}| = \omega+1 \le n-1 < n$, a contradiction.

Subcase (2.2.2). Now, assume that $\omega+1 \le \Delta \le n-2$. Let v_1 be the vertex of maximum degree in G and let $N_G(v_1)$ be the neighbour set of v_1 in G. Let $S = V(K_\omega) = \{u_1, u_2, \ldots, u_\omega\}$ be the vertex set of K_ω in G. We have $v_1 \in S$ or $v_1 \notin S$.

If $v_1 \in S$, then $H = KS_{\Delta+1,\omega}$ is a subgraph of G. The Laplacian spectrum of $KS_{\Delta+1,\omega}$ is $\{\Delta+1, \omega^{[\omega-2]}, 1^{[\Delta-\omega+1]}\}$. Therefore, for $1 \le \sigma \le n-1$, by Lemma 3.3.17, we have

$$
\begin{aligned}
S_\sigma(G) &= \sum_{i=1}^{\sigma}\mu_i(G) \le \sum_{i=1}^{\sigma}\mu_i(H) + \sum_{i=1}^{\sigma}\mu_i(G\setminus H)\\
&= S_\sigma(KS_{\Delta+1,\omega}) + S_\sigma(G\setminus KS_{\Delta+1,\omega})\\
&\le \Delta+1+(\sigma-1)\omega+2(m(G)-m(KS_{\Delta+1,\omega}))\\
&= (\sigma-1)\omega+2m-(\Delta+1)-\omega^2+3\omega,
\end{aligned}
$$

as $m(KS_{\Delta+1,\omega}) = \frac{\omega^2-3\omega+2(\Delta+1)}{2}$. It is easy to see that equality does not occur in this case.

Now, let $v_1 \notin S$. In this case, suppose that $S \cap N_G(v_1) = \{u_1, u_2, \ldots, u_p\}$. Since ω is the clique number of G, we have $0 \le p \le \omega-1$ (if $p = \omega$, then clique number of G is $\omega+1$, a contradiction). Since $\omega+1 \le \Delta \le n-2$, we have $\Delta-p-1 \ge \Delta-\omega \ge 1$ and G is connected. In this case $H = Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}$ is a subgraph of G. The Laplacian spectrum of $Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}$ is $\{\omega+1, \omega^{[\omega-2]}, \Delta-p+1, 1^{[\Delta-p]}, 0, 0\}$.

Therefore, for $1 \leq \sigma \leq n-1$, by Lemma 3.3.17, we have

$$\begin{aligned}
S_\sigma(G) &= \sum_{i=1}^{\sigma} \mu_i(G) \leq \sum_{i=1}^{\sigma} \mu_i(H) + \sum_{i=1}^{\sigma} \mu_i(G \setminus H) \\
&= S_\sigma(Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}) + S_\sigma(G \setminus Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}) \\
&\leq \omega + 1 + (\sigma-1)\omega + 2(m(G) - m(Ki_{\omega+1,\omega} \cup K_{1,\Delta-p})) \\
&= \omega + 1 + (\sigma-1)\omega + 2m - (\omega^2 - \omega + 2(\Delta + 1 - p) \\
&\leq \Delta + 1 + (\sigma-1)\omega + 2m - (\omega^2 - 3\omega + 2(\Delta+1)) \\
&= (\sigma-1)\omega + 2m - (\Delta+1) - \omega^2 + 3\omega,
\end{aligned}$$

as $2m(Ki_{\omega+1,\omega} \cup K_{1,\Delta-p}) = \omega^2 - \omega + 2(\Delta + 1 - p)$. It is easy to see that equality does not occur in this case as well.

It is clear from the above discussion that the equality holds if $G \cong K_n$ or $G \cong KS_{n,\omega}$.

Conversely, if G is isomorphic to one of the graphs K_n or $KS_{n,\omega}$, then it is easy to see that equality holds in (3.9). $\square$

Remark 3.3.19. We note that the upper bound (3.9) is better than the upper bound (3.8) for $\Delta \geq \omega - 1$.

Now, we obtain a stronger upper bound for $LE(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ and the clique number ω.

Theorem 3.3.20. *Let $G \neq K_n$ be a connected graph of order $n \geq 2$ with m edges, maximum degree Δ and clique number ω. If $\omega \geq \overline{d} = \frac{2m}{n}$, then*

$$LE(G) \leq 2\left(\omega(n-\omega) + 2m - (\Delta+1) - (n-2)\overline{d}\right), \qquad (3.10)$$

with equality if only if $G \cong KS_{n,n-1}$.

Proof. Let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$ be the Laplacian eigenvalues of $G \neq K_n$ and let σ, $(1 \leq \sigma \leq n-2)$ be the number of Laplacian eigenvalues greater than or equal to the average degree $\overline{d} = \frac{2m}{n}$. Since $\omega \geq \overline{d}$, by Theorem 3.3.19, we have

$$\begin{aligned}
LE(G) &= 2\left(S_\sigma(G) - 2\sigma\overline{d}\right)\\
&\leq 2\left(\omega(\sigma-1) + 2m - (\Delta+1) - \omega^2 + 3\omega - 2\sigma\overline{d}\right)\\
&= 2\left(\sigma(\omega-\overline{d}) + 2m - (\Delta+1) - \omega^2 + 2\omega\right)\\
&\leq 2\left((n-2)(\omega-\overline{d}) + 2m - (\Delta+1) - \omega^2 + 2\omega\right), \quad as \;\; \sigma \leq n-2\\
&= 2\left(\omega(n-\omega) + 2m - (\Delta+1) - \overline{d}(n-2)\right).
\end{aligned}$$

Equality occurs in (3.10) if and only if equality occurs in (3.9) and $\sigma = n-2$, that is, if and only if $G \cong KS_{n,n-1}$.

Conversely if $G \cong KS_{n,n-1}$, then it is easy to see that equality occurs in (3.10). □

Remark 3.3.21. For a connected graph $G \neq K_n$ of order $n \geq 2$ having m edges, maximum degree Δ and clique number $\omega \geq \overline{d}$, the upper bound (3.10) is better than the upper bound (3.6) for all $\overline{d}(\omega-3) \geq 2,\ \omega \geq 4$. This can be seen as follows. We have

$$2\left(\omega(n-\omega) + 2m - (\Delta+1) - \overline{d}(n-2)\right) \leq 2\left(2m - \Delta + 1 - \overline{d}\right),$$

that is, $\omega(n-\omega) - 1 \leq (n-3)\overline{d} + 1$, that is, $\overline{d}(n-\omega) - 1 \leq (n-3)\overline{d} + 1$, that is, $\overline{d}(\omega-3) \geq 2$. This shows that the upper bound (3.10) is better than the upper bound (3.5) for $\overline{d}(\omega-3) \geq 2,\ \omega \geq 4$. In fact, it can be seen that, if $\overline{d} = \omega$, then the upper bound (3.10) is better than the upper bound (3.5), for all $\omega \geq 2$.

Remark 3.3.22. If G is a tree with maximum degree $\Delta \geq \frac{n}{2}$ and $n \geq 38$. Then, using $\omega = 2,\ m = n-1, \overline{d} = 2 - \frac{2}{n}$, it is easy to see that the upper bound (3.10) is better than the upper bound (3.2). If G is a unicyclic graph having maximum degree $\Delta \geq \frac{n}{2},\ n \geq 29$ and clique number $\omega = 2$, then the upper bound (3.10) is better than the upper bound (3.2). This can be verified as follows. We have

$$\overline{d} + \sqrt{(n-1)(2m + M_1(G) - 2m\overline{d} - \overline{d}^2)} \geq 2\omega(n-\omega) + 4m - 2(\Delta+1) - 2\overline{d}(n-2)$$

$$2 + \sqrt{(n-1)(M_1(G) - 2n - 4)} \geq 4n - 2\Delta - 2, \ as\ m = n,\ \overline{d} = 2,\ \omega = 2$$

$$(n-1)(M_1(G) - 2n - 4) \geq (4n - 2\Delta - 4)^2$$

$$(n-1)(\frac{n^2}{4} + n + 8) \geq (3n-4)^2, \ as\ M_1(G) \geq \frac{n^2}{4} + n + 8,\ \Delta \geq \frac{n}{2},$$

which is clearly true for $n \geq 29$.

Let $\Gamma_{n,\omega}$ be the family of graphs of order n having clique number ω and $\sigma = \omega - 1$, (where σ is the number of Laplacian eigenvalues greater than or equal to $\overline{d} = \frac{2m}{n}$). The construction of a family of such graphs is given in [140].

The following upper bound can be obtained by proceeding similarly as in Theorem 3.3.20.

Theorem 3.3.23. *Let $G \in \Gamma_{n,\omega}$ be a connected graph of order $n \geq 2$ with m edges and maximum degree Δ. If $\omega \geq \overline{d} = \frac{2m}{n}$, then*

$$LE(G) \leq 2\left(2m + \omega - (\Delta + 1) - (\omega - 1)\overline{d}\right), \tag{3.11}$$

with equality if only if $G \cong KS_{n,\omega}$ or $G \cong K_n$.

Remark 3.3.24. If $G \in \Gamma_{n,\omega}$, it is easy to see that the upper bound (3.11) is better than the upper bound (3.6) for all $\omega \geq 2$. In fact, for $\omega = 2$ (that is, for bipartite graphs) the two bounds are same. Also it is easy to see that the upper bound (3.11) is better than the upper bound (3.10).

By using inequalities $(3.5), (3.6), (3.7)$ and (3.10), we can find the estimates for the Laplacian energy of trees and unicyclic graphs.

Corollary 3.3.25. *If G is a tree on $n \geq 2$ vertices having m edges and maximum degree Δ, then*

$$2\Delta - 2 + \frac{4}{n} \leq LE(G) \leq 4n - 2\Delta - 6 + \frac{4}{n},$$

equality occurs on each side if and only if $G \cong K_{1,n-1}$.

Proof. Since G is tree, we have $m = n - 1$, $\overline{d} = 2 - \frac{2}{n}$, $\omega = 2$. Using inequalities (3.7) and (3.10), the result follows. □

Corollary 3.3.26. *If G is a unicyclic graph on $n \geq 2$ vertices having m edges and maximum degree Δ, then*

$$2\Delta - 2 \leq LE(G) \leq 4n - 2\Delta - 2, \quad if \quad \omega = 2$$
$$2\Delta \leq LE(G) \leq 4n - 2\Delta, \quad if \quad \omega = 3.$$

For $\omega = 3$, equality occurs on the left hand side if and only if $G \cong KS_{n,3}$.

Proof. Since G is unicyclic, we have $m = n$, $\overline{d} = 2$, $\omega = 2$ or 3. Using inequalities (3.6), (3.7) and (3.10), the result follows. $\square$

From this we conclude that, among all the unicyclic connected graphs G with clique number $\omega = 3$, the graph $KS_{n,3}$ is the graph with minimal Laplacian energy.

Let G be a connected graph with $n \geq 2$ vertices and m edges having clique number ω. Let σ be the number of Laplacian eigenvalues greater than or equal to $\overline{d} = \frac{2m}{n}$. It seems that $\sigma \geq \omega - 1$. This is true for $\omega = 2$, follows from the well known fact that $\mu_1 \geq \Delta + 1 \geq \overline{d}$. Also, it is true for $\omega = n$, as in this case $G \cong K_n$ and so $\sigma = \omega - 1$. We note that it is also true for $\omega = n - 1$. If $\omega = n - 1$, then G contains $Ki_{n,n-1}$ as a spanning subgraph. The Laplacian spectrum of $Ki_{n,n-1}$ is $\{n, n-1^{[n-3]}, 1, 0\}$, with average degree $\overline{d}(Ki_{n,n-1}) = n - 3 + \frac{4}{n}$. Now we add edges to $Ki_{n,n-1}$, with out changing the clique number. Let α be the number of edges added, then $0 \leq \alpha \leq n - 3$ and let G^* be the resulting graph. We have $\overline{d}(G^*) = n-3+\frac{2(\alpha+2)}{n}$. Since $n > \overline{d}(G^*)$, therefore for $n-1 > \overline{d}(G^*) = n-3+\frac{2(\alpha+2)}{n}$ implies $\alpha < n-2$, which is true. This shows that the assertion is true in this case. For other values of ω, the problem seems to be difficult. Therefore based on this observation, we leave problem 3.5.1 for the future work.

3.4 Laplacian equienergetic graphs

Two graphs G_1 and G_2 of same order are said to be L-cospectral if they have same L-spectrum and non L-cospectral, otherwise. Just like adjacency matrices, Laplacian matrices of isomorphic graphs are permutation similar and similar matrices have same spectrum. It follows that isomorphic graphs are always L-cospectral. However, there are non isomorphic graphs, which are L-cospectral [28].

Analogous to the definition of equienergetic graphs, two graphs G_1 and G_2 of same order are said to be Laplacian equienergetic (L-equienergetic) if they have the same Laplacian energy. L-cospectral graphs are obviously Laplacian equienergetic, therefore the problem of Laplacian equienergetic graphs is considered only for non L-cospectral graphs. Also, since for regular graphs Laplacian energy is same as energy, therefore for the study of Laplacian equienergetic graphs, we will only consider non regular non L-cospectral graphs.

Let $d_n \leq d_{n-1} \leq \cdots \leq d_1$ be the degree sequence of the graph G and let $d_i^* = |\{i : \mu_i \geq i\}|$. Then the sequence $d_n^* \leq d_{n-1}^* \leq \cdots \leq d_1^*$ is called the conjugate degree sequence of the graph G. It was conjectured by Grone and Merris [62] that

$$\sum_{j=1}^{k} \mu_j \leq \sum_{j=1}^{k} d_j^*,$$

for all $k,\ 1 \leq k \leq n$, with equality for $k = n$. This conjecture was recently proved by Bai [11]. Merris [107] investigated the graphs for which Laplacian spectrum is same as the conjugate degree sequence. It turns out that the class of graphs for which the Laplacian spectrum and the conjugate degree sequence coincide is exactly the class of threshold graphs.

Definition 3.4.1. *Threshold graph.* A graph G which has no induced subgaph isomorphic to P_4 or C_4 or $2K_2$.

Threshold graphs are a simple class of graphs, which due to their wide applicability, keeps reappearing under various names. A good survey on the properties of threshold graphs can be seen in [106]. We may represent a threshold graph on n vertices using a binary sequence $(0 = b_1, b_2 \ldots, b_n)$. Here $b_i,\ 2 \leq i \leq n$, is 0, if vertex v_i was added as an isolated vertex, and b_i is 1, if v_i was added as a dominating vertex. This representation has been called a creation sequence [106]. For convenience, 0 is used as the first character of the string; it represents the first vertex of the graph. This way, the number of characters 1 in the string, called the trace of the graph, indicates the number of dominating vertices in its construction [106]. It is immediate to see from this encoding that two threshold graphs are isomorphic if and only if they have the same binary sequence.

D. Stevanoić [139] was the first who considered Laplacian equienergetic graphs. He [139] showed that for each n, there exists a set of n mutually non L-cospectral connected threshold graphs with equal Laplacian energy and having $O(\sqrt{n})$ vertices. In fact, he proved the following result.

Theorem 3.4.2. *For $k \geq 3$, there exists a set of $k^2 - 4k + 5$ L-equienergetic graphs on $2k$ vertices.*

This large set of graphs with equal Laplacian energy seems to contrast with the case of trees. Stevanović reports that, up to 20 vertices, there exists no pair of non L-cospectral trees with equal Laplacian energy. In fact, to the best of our knowledge, no pair of n vertex non L-cospectral trees with the same Laplacian energy has been identified so far.

Definition 3.4.3. *E-L equienergetic graph.* Two graphs G_1 and G_2 of same order are said to be E-L equienergetic if they are both equienergetic and Laplacian equienergetic. That is, if $E(G_1) = E(G_2)$ and $LE(G_1) = LE(G_2)$.

In 2010, Liu and Liu [101] considered k-iterated double graph of a graph and proved the following result.

Theorem 3.4.4. *There exists a pair of E-L equienergetic graphs of order n, for all $n \equiv 0 \pmod 7$.*

Recently Fritscher et al. [49] introduced a graph operation that affects the Laplacian spectrum of a particular class of graphs in a way that can be controlled. Using this operation, they were able to prove the existence of unicyclic Laplacian equienergetic graphs.

The following result [49] gives the existence of non L-cospectral Laplacian equienergetic unicyclic graphs.

Theorem 3.4.5. *For every $k \geq 2$, there is a family of k non L-cospectral unicyclic graphs with the same Laplacian energy, each with $n = 2k^2 + 2k + 2$ vertices. In particular, for values of n of this type, there is a family of $O(\sqrt{n})$ non L-cospectral unicyclic graphs on n vertices with the same Laplacian energy.*

Let G^{k*}, $k \geq 1$, be the k-th iterated extended double graph of the graph G. It is well known from the definition that G^{k*} is a bipartite graph with $n(G^{k*}) = 2^k n$ vertices. The A-spectrum of G^{k*} was considered in [25]. Here we first study the

L-spectrum of the graph G^{k*}. Let $Q(G) = D(G) + A(G)$ be the signless Laplacian matrix of G and let $\eta(G, x) = |xI_n - Q(G)|$ be the signless Laplacian characteristic polynomial of the graph G. Since the graph G^{k*} is always bipartite for $k \geq 1$, therefore its Laplacian spectrum and signless Laplacian spectrum are same [16, 28].

The following result gives the L-spectrum of the graph G^* in terms of the L-spectrum and Q-spectrum of the graph G.

Lemma 3.4.6. *Let G be an n vertex graph having Laplacian and signless Laplacian spectrum, respectively as $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1$ and $0 \leq q_n \leq q_{n-1} \leq \cdots \leq q_1$. Then the Laplacian spectrum of G^* is $\mu_i, q_i + 2,\ i = 1, 2, \ldots, n$.*

Proof. Let $A(G)$ be the adjacency matrix of the graph G. By a suitable relabelling of vertices it can be seen that the adjacency matrix $A(G^*)$ of the graph G^* is

$$A(G^*) = \begin{pmatrix} 0 & A(G) + I_n \\ A(G) + I_n & 0 \end{pmatrix}.$$

Let $D(G)$ and $D(G^*)$ respectively be the degree matrices of the graphs G and G^*. It is easy to see that

$$D(G^*) = \begin{pmatrix} D(G) + I_n & 0 \\ 0 & D(G) + I_n \end{pmatrix}.$$

Therefore, Laplacian matrix $L(G^*)$ of G^* is

$$L(G^*) = D(G^*) - A(G^*) = \begin{pmatrix} D(G) + I_n & -(A(G) + I_n) \\ -(A(G) + I_n) & D(G) + I_n \end{pmatrix}.$$

So, the Laplacian characteristic polynomial of G^* is

$$\psi(G^*, \lambda) = |\lambda I_{2n} - L(G^*)| = \begin{vmatrix} (\lambda - 1)I_n - D(G) & A(G) + I_n \\ A(G) + I_n & (\lambda - 1)I_n - D(G) \end{vmatrix}$$
$$= |((\lambda - 1)I_n - D(G)) - (A(G) + I_n)|\,|((\lambda - 1)I_n - D(G)) + (A(G) + I_n)|$$
$$= |(\lambda - 2)I_n - (D(G) + A(G))|\,|\lambda I_n - (D(G) - A(G))|$$
$$= \eta(G, \lambda - 2)\psi(G, \lambda).$$

From this the result follows. $\square$

Using Theorem 3.4.6, induction and the fact that $\binom{k}{r}+\binom{k}{r-1}=\binom{k+1}{r}$, for all $0\le r\le k$ and $\binom{s-1}{0}=\binom{s}{0}=\binom{s-1}{s-1}=\binom{s-2}{s-2}=1$, we obtain the L-spectrum of G^{k*} as function of L-spectrum and Q-spectrum of the graph G.

Theorem 3.4.7. *Let G be a graph having L-spectrum μ_i, $1\le i\le n$, and Q-spectrum q_i, $1\le i\le n$. The L-spectrum of the graph G^{k*} is $\mu_i^{[\binom{k}{0}]}$, $\mu_i+2^{[\binom{k-1}{1}]}$, $q_i+2^{[\binom{k-1}{0}]}$, $\mu_i+4^{[\binom{k-1}{2}]}$, $q_i+4^{[\binom{k-1}{1}]},\ldots,\mu_i+2(k-2)^{[\binom{k-1}{k-2}]}$, $q_i+2(k-2)^{[\binom{k-1}{k-3}]}$, $\mu_i+2(k-1)^{[\binom{k-1}{k-1}]}$, $q_i+2(k-1)^{[\binom{k-1}{k-2}]}$, $q_i+2k^{[\binom{k}{k}]}$, where $i=1,2,\ldots,n$.*

For a bipartite graph G, we have the following consequence of Theorem 3.4.7.

Corollary 3.4.8. *If G is a bipartite graph having L-spectrum μ_i, $1\le i\le n$, then the L-spectrum of G^{k*} is $\mu_i^{[\binom{k}{0}]}$, $\mu_i+2^{[\binom{k}{1}]},\ldots,\mu_i+2(k-2)^{[\binom{k}{k-2}]}$, $\mu_i+2(k-1)^{[\binom{k}{k-1}]}$, $\mu_i+2k^{[\binom{k}{k}]}$, where $i=1,2,\ldots,n$.*

Proof. Since for a bipartite graph G the Laplacian and the signless Laplacian spectrum are same, we have $\mu_i=q_i$ for all $i=1,2,\ldots,n$. Using this and the fact that $\binom{t}{r}+\binom{t}{r-1}=\binom{t+1}{r}$, $0\le r\le t$ in Theorem 3.4.7, the result follows. $\square$

Since spectrum of a graph G with respect to a given matrix $(L(G),Q(G))$ gives the valuable information about the structural properties of the graph, the importance of considering spectrum with respect to different matrices is that the different matrices give information about different structural properties. It is clear from Lemma 3.4.6, that the structural information one gains from both the L-spectrum and Q-spectrum of the graph G can be obtained from the L-spectrum of the graph G^*. So, instead of considering both the L-spectrum and Q-spectrum of the graph G, one can study the L-spectrum of the graph G^*. Since G^* can be obtained for any graph G, Lemma 3.4.6, gives a connection between the structural properties described by the L-spectrum and Q-spectrum of the graph G and the structural properties described by the L-spectrum of a particular graph, namely G^*.

In [25], three formulae are given for the number of spanning trees of G^* in terms of A-spectrum of the corresponding graph G. We now obtain a formula for the number of spanning trees in terms of the L and Q-spectrum of G^*.

Theorem 3.4.9. *The number of spanning trees $\tau(G^*)$ of the graph G^* is*

$$\tau(G^*) = \frac{1}{2}\tau(G)\prod_{i=1}^{n}(q_i + 2).$$

Proof. Let μ_i and q_i, $(i = 1, 2, \ldots, n)$, be respectively the L-spectrum and the Q-spectrum of the graph G. By Lemma 3.4.6, the L-spectrum of the graph G^* is $\mu_i, q_i + 2$, $(i = 1, 2, \ldots, n)$. By using the fact that the number of spanning trees of a graph of order n is $\frac{1}{n}$ times the product of $(n-1)$ largest Laplacian eigenvalues of the graph, we have

$$\tau(G^*) = \frac{1}{2n}\prod_{i=1}^{n-1}\mu_i\prod_{i=1}^{n}(q_i + 2) = \frac{1}{2}\tau(G)\prod_{i=1}^{n}(q_i + 2) = \frac{1}{2}\tau(G)det(Q(G) + 2I_n).$$

□

In case G is bipartite, $\mu_i = q_i$, so we have

$$\tau(G^*) = \frac{1}{2n}\prod_{i=1}^{n-1}\mu_i\prod_{i=1}^{n}(\mu_i + 2) = \tau(G)\prod_{i=1}^{n-1}(\mu_i + 2).$$

The following observations are the easy consequences of Theorem 3.4.7. The first of these observations gives a method to construct families of non isomorphic L-cospectral graphs from any given pair of non isomorphic L-cospectral graphs and second gives a way to construct families of *Laplacian integral* graphs from any given *Laplacian and signless Laplacian integral* graph.

Corollary 3.4.10. *Two graphs G_1 and G_2 of same order are L-cospectral if and only if the graphs G_1^{k*} and G_2^{k*} are L-cospectral.*

Corollary 3.4.11. *A graph G is Laplacian and signless Laplacian integral if and only if G^{k*} is Laplacian integral graph.*

In [25] it is shown that the graphs G^* and $G \times K_2$ are A-cospectral if and only if $G = K_1$ or G is bipartite. An analogous result holds for the L-spectrum.

Theorem 3.4.12. *The graphs G^* and $G \times K_2$ are L-cospectral if and only if $G = K_1$ or G is bipartite.*

Proof. If $G = K_1$, the graphs G^* and $G \times K_2$ are both isomorphic to K_1, so are L-cospectral. Now if $G \neq K_1$, assume that G is bipartite. Then $\mu_i = q_i$ and so the L-spectrum of G^* is $\mu_i, \mu_i + 2$ for $i = 1, 2, \ldots, n$ which by Lemma 2.4.11, is same as the L-spectrum of $G \times K_2$. Conversely, suppose that the graphs G^* and $G \times K_2$ are L-cospectral. Then $\mu_i = q_i$, which is only possible if and only if G is bipartite. Hence the result. $\square$

Since the extended double cover G^* of the graph G is always bipartite, it follows by Theorem 3.4.12, the graphs G^{**} and $G^* \times K_2$ are non isomorphic L-cospectral and in general the graphs G^{s*} and $G^{(s-1)*} \times K_2$ are non isomorphic L-cospectral. Also, it is easy to see that the graphs $(G \times K_2)^*$ and $G^* \times K_2$ are non isomorphic L-cospectral and in general the graphs $(G \times K_2)^{s*}$ and $G^{s*} \times K_2$ are both non isomorphic L-cospectral as well as Q-cospectral. Moreover, if G is bipartite, then as seen in Theorem 3.4.12, the graphs G^* and $G \times K_2$ are non isomorphic L-cospectral. Using the same argument, it can be seen that the graphs G^{**} and $G \times K_2 \times K_2$ are non isomorphic L-cospectral if and only if G is bipartite. A repeated use of the argument, as used in Theorem 3.4.12, shows the graphs G^{s*} and $(G \times \underbrace{K_2 \times K_2 \times \cdots K_2}_{s}) = (G \times sK_2) = (G \times Q_s)$ are non isomorphic L-cospectral if and only if G is bipartite. From this discussion, it follows that the graphs $G^{s*}, G^{(s-1)*} \times K_2, (G \times K_2)^{(s-1)*}$ and $G \times Q_{s-1}$ are mutually non isomorphic L-cospectral graphs if and only G is bipartite, where Q_n is the hypercube.

Let $D^k[G],\ k \geq 2$, be the k-fold double graph of the graph G. The Laplacian spectrum of $D^k[G]$ was discussed in [103] and is given by the following result.

Lemma 3.4.13. *Let G be a graph with n vertices having vertex degrees $d_i,\ i = 1, 2, \ldots, n$ and Laplacian spectrum $\mu_i, i = 1, 2, \ldots, n$. Then the Laplacian spectrum of $D^k[G]$ is $k\mu_i, kd_i^{[(k-1)]},\ i = 1, 2, \ldots, n$.*

Let $\mu_i,\ i = 1, 2, \ldots, n$, be the L-spectrum of the graph G. Then, by Lemma 3.4.6, the L-spectrum of the extended double cover G^* of the graph G is $\mu_i, q_i +$

$2,\ (1 \leq i \leq n)$. Also the average vertex degree of G^* is $\frac{2m}{n}+1$. Therefore,

$$LE(G^*) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n} - 1| + \sum_{i=1}^{n} |q_i - \frac{2m}{n} + 1|.$$

Using Lemma 3.4.13 and the fact that the average vertex degree of $D^k[G]$ is $k\frac{2m}{n}$, we have

$$\begin{aligned} LE(D^k[G]) &= \sum_{i=1}^{n} |k\mu_i - k\frac{2m}{n}| + (k-1)\sum_{i=1}^{n} |kd_i - k\frac{2m}{n}| \\ &= k\sum_{i=1}^{n} |\mu_i - \frac{2m}{n}| + k(k-1)\sum_{i=1}^{n} |d_i - \frac{2m}{n}| \\ &= kLE(G) + k(k-1)\sum_{i=1}^{n} |d_i - \frac{2m}{n}|. \end{aligned}$$

From this it is clear that $LE(D^k[G]) = kLE(G)$, if G is regular. Also, since the k-fold graph of a regular graph is regular, it follows that, if G_1 and G_2 are r-regular non L-cospectral L-equienergetic graphs then their k-fold graphs $D^k[G_1]$ and $D^k[G_2]$ are always non L-cospectral L-equienergetic.

It can be seen from above that the Laplacian energy of the graph $D[G]$ is twice the Laplacian energy of G, when G is regular. But this need not be true for the graph G^* as is clear from the Laplacian energy of G^* given above. However we have the following observation.

Theorem 3.4.14. *Let G^* be the extended double cover of the bipartite graph G. Then $LE(G^*) = 2LE(G)$ if and only if $|\mu_i - \overline{d}| \geq 1$ for all $1 \leq i \leq n$, where $\overline{d} = \frac{2m}{n}$.*

Proof For the necessary part, using Corollary 3.4.8, for $k = 1$ and the fact

$$|\mu_i - \overline{d} + 1| = \begin{cases} |\mu_i - \overline{d}| + 1, & \text{if } \mu_i \geq \overline{d} \\ |\mu_i - \overline{d}| - 1, & \text{if } \mu_i < \overline{d}, \end{cases}$$

and

$$|\mu_i - \overline{d} - 1| = \begin{cases} |\mu_i - \overline{d}| - 1, & \text{if } \mu_i \geq \overline{d} \\ |\mu_i - \overline{d}| + 1, & \text{if } \mu_i < \overline{d}. \end{cases}$$

The result follows by direct calculation.

For the converse, suppose that $LE(G^*) = 2LE(G)$. We will show that $|\mu_i - \overline{d}| \geq 1$

for all $1 \leq i \leq n$. We prove this by contradiction. Assume that $|\mu_i - \overline{d}| < 1$, for some i. Putting $\beta_i = \mu_i - \overline{d}$, and using the same argument as used in the converse of Theorem 8 in [19] we arrive at a contradiction. $\square$

The *join (complete product)* of graphs G_1 and G_2 is a graph $G = G_1 \vee G_2$ with vertex set $V(G_1) \cup V(G_2)$ and an edge set consisting of all the edges of G_1 and G_2 together with the edges joining each vertex of G_1 with every vertex of G_2. The L-spectrum of the join of graphs is given by the following result [28].

Lemma 3.4.15. *If G_1 and G_2 are two graphs with order $n_i,\ i = 1, 2,$ having L-spectrum respectively as $\mu_1, \mu_2, \ldots, \mu_{n_1-1}, \mu_{n_1} = 0$ and $\sigma_1, \sigma_2, \ldots, \sigma_{n_2-1}, \sigma_{n_2} = 0$, then the L-spectrum of $G = G_1 \vee G_2$ is $n_1+n_2, n_1+\sigma_1, n_1+\sigma_2, \ldots, n_1+\sigma_{n_2-1}, n_2+\mu_1, n_2+\mu_2, \cdots, n_2+\mu_{n_1-1}, 0$.*

Let G^{k*} be the k-th iterated extended double cover of the graph G. The next result gives the Laplacian energy of the graph $G^{k*} \vee \overline{K}_n$.

Theorem 3.4.16. *Let G be a graph of order n with m edges having L and Q-spectrum respectively as μ_i and q_i for $i = 1, 2, \ldots, n$. For $p \geq 2^k n + t$ and $m \leq \frac{(t-k)n}{2} + \frac{t^2}{2^{k+1}},\ t \geq k+2,\ k \geq 1,$ we have $LE(G^{k*} \vee \overline{K_p}) = 2^k n(k+2) + (p - 2^k n)\frac{2m'}{n'} + 2^k(2m)$.*

Proof. Let G^{k*} be the k-th iterated extended double cover of the graph G. By Theorem 3.4.7, the L-spectrum of G^{k*} is $\mu_i^{[\binom{k}{0}]}, \mu_i + 2^{[\binom{k-1}{1}]}, q_i + 2^{[\binom{k-1}{0}]}, \mu_i + 4^{[\binom{k-1}{2}]}, q_i + 4^{[\binom{k-1}{1}]}, \ldots, \mu_i + 2(k-2)^{[\binom{k-1}{k-2}]}, q_i + 2(k-2)^{[\binom{k-1}{k-3}]}, \mu_i + 2(k-1)^{[\binom{k-1}{k-1}]}, q_i + 2(k-1)^{[\binom{k-1}{k-2}]}, q_i + 2k^{[\binom{k}{k}]}$, where $i = 1, 2, \ldots, n$. So, by Lemma 3.4.15, the L-spectrum of $G^{k*} \vee \overline{K_p}$ is $0, p + 2^k n, 2^k n^{[p-1]}, p + \mu_i^{[\binom{k}{0}]}$ $(i = 1, 2, \ldots, n-1), p + \mu_i + 2^{[\binom{k-1}{1}]}, p + q_i + 2^{[\binom{k-1}{0}]}, p + \mu_i + 4^{[\binom{k-1}{2}]}, p + q_i + 4^{[\binom{k-1}{1}]}, \cdots, p + \mu_i + 2(k-2)^{[\binom{k-1}{k-2}]}, p + q_i + 2(k-2)^{[\binom{k-1}{k-3}]}, p + \mu_i + 2(k-1)^{[\binom{k-1}{k-1}]}, p + q_i + 2(k-1)^{[\binom{k-1}{k-2}]}, p + q_i + 2k^{[\binom{k}{k}]},\ i = 1, 2, \ldots, n$, with average vertex degree

$$\overline{d'} = \frac{2m'}{n'} = \frac{2^{k+1}m + 2^k kn + 2^{k+1}pn}{p + 2^k n}.$$

Therefore,

$$LE(G^{k*} \vee \overline{K_p}) = \sum_{i=1}^{n-1} |p + \mu_i - \overline{d'}| + \sum_{r=1}^{k-1} \sum_{i=1}^{n} \binom{k-1}{r} |p + \mu_i + 2r - \overline{d'}|$$
$$+ \sum_{r=1}^{k-1} \sum_{i=1}^{n} \binom{k-1}{r-1} |p + q_i + 2r - \overline{d'}| + \sum_{i=1}^{n} |p + \mu_i + 2k - \overline{d'}|$$
$$+ |p + 2^k n - \overline{d'}| + (p-1)|2^k n - \overline{d'}| + |0 - \overline{d'}|.$$

Now, if $p \geq 2^k n + t$ and $m \leq \frac{(t-k)n}{2} + \frac{t^2}{2^{k+1}}$, $t \geq k+2$, $k \geq 1$, we have for $i = 1, 2, \ldots, n$ and $r = 0, 1, \ldots, t$

$$p + \mu_i + 2r - \overline{d'} = p + \mu_i + 2r - \frac{2^{k+1}m + 2^k kn + 2^{k+1}pn}{p + 2^k n}$$
$$= \frac{p(p - 2^k n) + 2r(p + 2^k n) + (p + 2^k n)\mu_i - 2^{k+1}m - 2^k kn}{p + 2^k n}$$
$$\geq \frac{t(2^k n + t) - t(2^k n + t) + 2^k kn - 2^k kn}{p + 2^k n} = 0.$$

Similarly, it can be seen that $p + q_i + 2r - \overline{d'} \geq 0$. So, we have

$$LE(G^{k*} \vee \overline{K_p})$$
$$= (n-1)(p - \overline{d'}) + \sum_{r=1}^{k-1} \Big(n(p + 2r - \overline{d'}) + 2m\Big) \left[\binom{k-1}{r} + \binom{k-1}{r-1}\right]$$
$$+ (p + 2^k n - \overline{d'}) + (p-1)(\overline{d'} - 2^k n) + \Big(n(p + 2k - \overline{d'}) + 2m\Big) + \overline{d'} + 2m$$
$$= 2^{k+1}n - pn(2^k - 1) + (p-n)\overline{d'} + \sum_{r=1}^{k} \binom{k}{r} \Big(n(p + 2r - \overline{d'}) + 2m\Big) + 2m$$
$$= 2^{k+1}n - pn(2^k - 1) + (p-n)\overline{d'} + n(2^k - 1)(p - \overline{d'}) + (2^k - 1)2m + 2^k kn + 2m$$
$$= 2^k n(k+2) + (p - 2^k n)\frac{2m'}{n'} + 2^k(2m),$$

where we have made use of the fact, $\left[\binom{k-1}{r} + \binom{k-1}{r-1}\right] = \binom{k}{r}$ and $\sum_{r=1}^{k} r\binom{k}{r} = k2^{k-1}$. This proves the result. $\square$

Clearly the Laplacian energy of the graph $G^{k*} \vee \overline{K_p}$ depends only on the parameters p, m, k and n. Therefore all the graphs of the family $\{G_i^{k*} \vee \overline{K_p} : k, i \in \mathbb{N}\}$, with the same parameters p, m, k and n satisfying the conditions in the hypothesis of the Theorem 3.4.16 are mutually non L- cospectral L-equienergetic. Also, since the k-th iterated extended double graph G^{k*} of the graph G is always bipartite Theorem 3.4.16 gives a two way infinite family of L-equienergetic tripartite graphs of independence number p.

Let $D^k[G]$ be the k-fold double graph of the graph G, the next result gives the Laplacian energy of the graph $D^k[G] \vee \overline{K_p}$ and can be proved similar to Theorem 3.4.16.

Theorem 3.4.17. *Let $D^k[G]$ be the k-fold double graph of the graph G. Then for $p \geq kn + t$ and $m \leq \frac{t(kn+t)}{2k^2}$, $t \geq 2k$, $k \geq 2$, we have $LE(D^k[G] \vee \overline{K_p}) = 2kn + (p - nk)\frac{2m'}{n'} + 2mk^2$.*

It is clear from Theorem 3.4.17, that the Laplacian energy of the graph $D^k[G] \vee \overline{K_p}$ depends on the parameters p, k, m and n. Therefore, all the graphs of the family $\{D^k[G_i] \vee \overline{K_p} : i, k \in \mathbb{N}\}$ having the same parameters p, m, k and n, satisfying the conditions of the Theorem 3.4.17, are mutually non L-cospectral L-equienergetic. In fact, Theorem 3.4.17 generates a two way family of L-equienergetic graphs of independence number p.

Both Theorems 3.4.16 and 3.4.17, give a method of constructing families of non L-cospectral L-equienergetic graphs with same number of edges.

Let $SD(G)$ be the strong double graph of the graph G. The next result gives the Laplacian spectrum of the graph $SD(G)$ in terms of the Laplacian spectrum and vertex degrees of the graph G.

Lemma 3.4.18. *If μ_i, d_i, $i = 1, 2, \ldots, n$, are respectively the L-spectrum and vertex degrees of the graph G, then the L-spectrum of the graph $SD(G)$ is $2\mu_i, 2d_i + 2$, $i = 1, 2, \ldots, n$.*

Proof. If d_i is the degree of a vertex v_i in G, then the degree of the corresponding vertex in the graph $SD(G))$ is $2d_i + 1$. Therefore, if D is the degree matrix of the graph G it can be seen by relabelling of vertices (if necessary) that the degree matrix $D(SD(G))$ of the graph $SD(G)$ is

$$D(SD(G)) = \begin{pmatrix} 2D+I_n & 0 \\ 0 & 2D+I_n \end{pmatrix}.$$

Thus Laplacian matrix $L(SD(G))$ of $SD(G)$ is

$$L(SD(G)) = D(SD(G)) - A(SD(G)) = \begin{pmatrix} 2D+I_n-A & -(A+I_n) \\ -(A+I_n) & 2D+I_n-A \end{pmatrix}.$$

So, the Laplacian characteristic polynomial of $SD(G)$ is

$$\begin{aligned}
&\psi(SD(G),x) = |xI_{2n} - L(SD(G))| \\
&= \begin{vmatrix} (x-1)I_n - 2D(G) + A & A+I_n \\ A+I_n & (x-1)I_n - 2D(G) + A \end{vmatrix} \\
&= |((x-1)I_n - 2D + A) - (A+I_n)|\,|((x-1)I_n - 2D + A) + (A+I_n)| \\
&= |(x-2)I_n - 2D|\,|xI_n - 2(D(G) - A(G))| \\
&= \phi\left(D, \frac{x-2}{2}\right)\psi\left(G, \frac{x}{2}\right),
\end{aligned}$$

therefore, the result follows. □

The next result gives the L-spectrum of the graph $SD^k(G)$ and can be proved by using Lemma 3.4.18 and induction principle.

Corollary 3.4.19. *If $\mu_i,\ d_i,\ i = 1, 2, \ldots, n$, are respectively the L-spectrum and vertex degrees of the graph G, then the L-spectrum of the graph $SD^k(G)$ is $2^k\mu_i, 2^k(d_i+1)^{[(2^k-1)]},\ i = 1, 2, \ldots, n$.*

We now obtain the Laplacian energy of the graph $SD(G) \vee \overline{K_p}$.

Theorem 3.4.20. *If G is a graph of order n having m edges, then for $p \geq 2n+k$ and $m \leq \frac{n(k-1)}{4} + \frac{k^2}{8},\ k \geq 5$ we have $LE(SD(G) \vee \overline{K_p}) = 6n + (p-2n)\frac{2m'}{n'} + 8m$.*

Proof. For $i = 1, 2, \ldots, n$ let μ_i and d_i be respectively the L-spectrum and vertex degrees of the graph G. By Lemmas 3.4.15 and 3.4.19, the L-spectrum of the graph $SD(G) \vee \overline{K_p}$ is $p+2n, p+2\mu_i\ (1 \leq i \leq n-1), p+2d_i+2,\ (1 \leq i \leq$

$n), 2n^{[(p-1)]}, 0$, with average degree $\frac{2m'}{n'} = \frac{8m+2n+4pn}{p+2n}$. Therefore, if $p \geq 2n + k$ and $m \leq \frac{(k-1)n}{4} + \frac{k^2}{8}$, $k \geq 5$, we have for $i = 1, 2, \ldots, n$,

$$\begin{aligned} p + 2\mu_i - \frac{2m'}{n'} &= p + 2\mu_i - \frac{8m + 4pn + 2n}{p + 2n} \\ &= \frac{p(p - 2n) + 2(2n + p)\mu_i - 8m - 2n}{p + 2n} \\ &\geq \frac{k(2n + k) - 2(k - 1)n - k^2 - 2n}{p + 2n} = 0. \end{aligned}$$

Similarly, we have $p + 2d_i + 2 - \frac{2m'}{n'} \geq 0$. So using these observations, we obtain by direct calculation, $LE(SD(G) \vee \overline{K_p}) = 6n + (p - 2n)\frac{2m'}{n'} + 8m$. $\square$

From Theorem 3.4.19, it is clear that the Laplacian energy of the graph $SD(G) \vee \overline{K_p}$ is a function of the parameters n, m and p. Therefore, it follows that all the graphs of the family $\{SD(G_i) \vee \overline{K_p} : i,\ p \in \mathbb{N}\}$ with the parameters n, m and p satisfying the conditions of the Theorem 3.4.20 are non L-cospectral L-equienergetic.

3.5 Conclusion

We conclude this chapter with the following problems which will be of interest in future.

Problem 3.5.1. *Let G be a connected graph with $n \geq 2$ vertices and m edges having clique number ω. If σ is the number of Laplacian eigenvalues greater than or equal to $\overline{d} = \frac{2m}{n}$, then $\sigma \geq \omega - 1$.*

Problem 3.5.2. *Characterize the graphs for which $\sigma = \omega - 1$.*

Problem 3.5.3. *Prove or disprove that there exists a pair of non L-cospectral L-equienergeric trees. If such a pair exists, give the construction of a family of such trees.*

CHAPTER 4

Relation between energy and Laplacian energy of graphs

In this chapter, we discuss the relation between energy and Laplacian energy of a graph G. We present some well known results on the relation between energy and Laplacian energy of graphs. We give various constructions of the families of graphs G for which energy is greater than the corresponding Laplacian energy. We also give a construction of non bipartite graphs for which energy is less than the corresponding Laplacian energy.

4.1 Introduction

Let $E(G)$ be the energy and $L(G)$ be the Laplacian energy of the graph G. Gutman et al. [75] computed the energy and Laplacian energy of various known families of graphs like *complete bipartite graph* $K_{a,b}$, union of two complete graphs $K_a \cup K_b$, *coalescence* of complete graphs $K_n * K_n$, $Kb_n(k)$ the graph obtained from K_n by deleting k independent edges, $Kc_n(k)$ the graph obtained from K_n by deleting edges of the clique K_k etc and found that energy is always less than or equal to the Laplacian energy for these families of graphs. This observation made Gutman et al. to believe that energy of a graph G is always less than or equal to the corresponding Laplacian energy and so, they made the following conjecture.

Conjecture 4.1.1. *For any graph G,*

$$E(G) \leq LE(G). \tag{4.1}$$

Proving the inequality (4.1) (in case it happens to be correct) may be a much more difficult task than disproving it, a single counterexample would suffice.

It was Stevanović et al. [135] who disproved the conjecture by furnishing an infinite family of graphs G, namely $G = KK_n^2$, for which the reverse inequality holds for all $n \geq 8$. By direct calculation, it can be seen that the inequality (4.1) is true for all graphs of order $n \leq 6$. For $n = 7$, there is only one graph (see graph H in Figure 1) for which the reverse inequality holds. Using this graph, Liu and Liu [102] constructed an infinite family of disconnected graphs for which the reverse inequality holds. Although from [135, 102], it was clear that conjecture is not true in general, it is of interest to characterize the graphs for which the conjecture holds. Clearly characterizing all the graphs for which (4.1) holds or does not hold is not an easy task and is still an open problem. However some families of graphs have been characterized for which (4.1) holds and some families have been characterized for which (4.1) does not hold.

4.2 Inequality (4.1) is true for bipartite graphs

In this section, we will show the inequality (4.1) is true for bipartite graphs. Nikiforov [110] recognized that the energy of the graph G is equal to the sum of the singular values (Recall that the singular values of a real matrix M are equal to the positive square roots of the eigenvalues of MM^t) of its adjacency matrix $A(G)$. This observation seems to be of great importance for the theory of graph energy, because of the following Theorem, first proven by Fan [43].

Theorem 4.2.1. *Let A and B be two square matrices of order n, such that $A + B = C$. Then*

$$\sum_{i=1}^{n} s_i(C) \leq \sum_{i=1}^{n} s_i(A) + \sum_{i=1}^{n} s_i(B),$$

where $s_i(X)$ is the i^{th} singular value of X. Equality holds if and only if there exists an orthogonal matrix P, such that PA and PB are both positive semi-definite.

Using Theorem 4.2.1, various lower and upper bounds have been obtained for both energy and Laplacian energy see [128].

We now show that the inequality (4.1) is true for bipartite graphs.

Theorem 4.2.2. *For a bipartite graph G the inequality* (4.1) *holds.*

Proof. Let $L(G)$ be the Laplacian matrix and $Q(G)$ be the signless Laplacian matrix of the graph G. We have

$$L(G) = D(G) - A(G) \tag{4.2}$$

and

$$Q(G) = D(G) + A(G). \tag{4.3}$$

Subtracting equation (4.2) from equation (4.3), we get

$$Q(G) - L(G) = 2A(G)$$

or

$$\left(Q(G) - \frac{2m}{n}I_n\right) - \left(L(G) - \frac{2m}{n}I_n\right) = 2A(G).$$

Now using Theorem 4.1.1 and the fact that $s_i(X) = s_i(-X)$, it follows that

$$QE(G) + LE(G) \geq 2E(G).$$

Since for a bipartite graph Laplacian and signless Laplacian spectrum are same, therefore, for a bipartite graph G, we have $QE(G) = LE(G)$. This proves the result. □

It is clear from the proof of the Theorem 4.2.2, that the inequality (4.1) also holds for the graphs G, for which $QE(G) < LE(G)$. For instance, consider the graph G_1 as shown in Figure 1. By direct calculation, it can be seen that $QE(G_1) = 5.1233 < 6 = LE(G_1)$. We now show how an infinite family of non bipartite graphs can be constructed for which inequality (4.1) holds from any given non bipartite graph G satisfying $QE(G) < LE(G)$.

Let $D^k[G],\ k \geq 2$, be the k-fold double graph of the graph G having vertex degrees d_i and Q-spectrum $q_i,\ i = 1, 2, \ldots, n$. Proceeding similarly as in [103], it can be seen that Q-spectrum of the graph $D^k[G]$ is $kq_i, kd_i^{[(k-1)]}$, d_i, for $i = 1, 2, \ldots, n$. Also the average vertex degree of $D^k[G]$ is $k\frac{2m}{n}$, so we have

$$\begin{aligned} QE(D^k[G]) &= \sum_{i=1}^{n} |kq_i - k\frac{2m}{n}| + (k-1)\sum_{i=1}^{n} |kd_i - k\frac{2m}{n}| \\ &= k\sum_{i=1}^{n} |q_i - \frac{2m}{n}| + k(k-1)\sum_{i=1}^{n} |d_i - \frac{2m}{n}| \qquad (4.4) \\ &= kQE(G) + k(k-1)\sum_{i=1}^{n} |d_i - \frac{2m}{n}|. \end{aligned}$$

Similarly,

$$LE(D^k[G]) = kQE(G) + k(k-1)\sum_{i=1}^{n}|d_i - \frac{2m}{n}|. \tag{4.5}$$

It is clear from equations (4.4) and (4.5) that $LE(D^k[G]) \geq QE(D^k[G])$ if and only if $LE(G) \geq QE(G)$. Since, the k-fold graph of a non bipartite graph G is non bipartite, it follows that if G is a non bipartite graph with $LE(G) > QE(G)$, then $LE(D^k[G]) > QE(D^k[G])$, for all $k \geq 2$. Thereby, constructing an infinite family of such graphs.

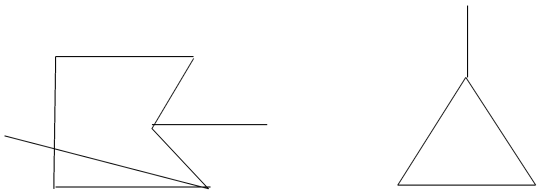


Figure 1: The graph H, for which energy is greater than Laplacian energy and the graph G_1 for which Laplacian energy is greater than signless Laplacian energy

4.3 Graphs for which inequality (4.1) does not hold

In this section, we obtain various families of graphs for which the inequality (4.1) does not hold.

Let KK_n^j, $1 \leq j \leq n$, be the graph defined in section 2.3. The L-spectrum of the graph KK_n^j, $1 \leq j \leq n$, was considered in [46] and is given by the following result.

Lemma 4.3.1. *If $1 \leq j \leq n$,$n \geq 3$, the L-characteristic polynomial of KK_n^j is $x(x-n)^{2n-j-2}(x-n-1)^{j-1}g(x)$, where $g(x) = x^2 - (n+1+j)x + 2j$.*

Stevanović et al. [135] considered the graph KK_n^2 and proved the following result.

Theorem 4.3.2. *If $G = KK_n^2$, then*

$$E(KK_n^2) > LE(KK_n^2),$$

for all $n \geq 9$.

By Lemma 4.3.1, the L-spectrum of the graph KK_n^j is $\{n^{[2n-j-2]}, n+1^{[j-1]}, \frac{(n+j+1)+\sqrt{(n+j+1)^2-8j}}{2}, \frac{(n+j+1)-\sqrt{(n+j+1)^2-8j}}{2}, 0\}$, with average vertex degree $n-1+\frac{j}{n}$. Therefore for any $j,\ 1 \leq j \leq n$, the Laplacian energy of the graph KK_n^j is

$$LE(KK_n^j) = 3n - j + \frac{4j}{n} - 5 + \sqrt{(n+j+1)^2 - 8j}. \tag{4.6}$$

It is easy to see that $LE(KK_n^j)$ is an increasing function of $j,\ 1 \leq j \leq n$. Therefore, it follows that $\{KK_n^j,\ \ 1 \leq j \leq n\}$ gives a family of graphs where adding an edge one by one, increases the Laplacian energy monotonically. So we have the following observation.

Theorem 4.3.3. *Among the family $\{KK_n^j : n \in \mathbb{N},\ 1 \leq j \leq n\}$, the graph KK_n^1 has the minimal Laplacian energy and the graph KK_n^n has the maximal Laplacian energy.*

For $j = n$, we have $LE(KK_n^n) = 3n - n + \frac{4n}{n} - 5 + \sqrt{(n+n+1)^2 - 8n} = 4n - 2 = LE(K_{2n})$. Since the L-spectrum of the graph K_{2n} is $\{2n^{[2n-1]}, 0\}$, it follows by Lemma 4.3.2, these graphs are non L-cospectral. Therefore we have the following observation.

Theorem 4.3.4. *For $j \in \mathbb{N},\ 1 \leq j \leq n$, the graphs KK_n^n and K_{2n} are non L-cospectral, L-equienergetic graphs.*

Theorem 4.3.2 shows that inequality (4.1) does not hold for the graph KK_n^2. Here we first show that this inequality does not hold for the graphs KK_n^3 and KK_n^4 also. Using this we prove a general result in Theorem 4.3.6, which generalizes Proposition 1 (of [135]) and Theorem 4.3.5.

Theorem 4.3.5. *For any graph $G = KK_n^j$ of order $2n$ and $j = 3, 4$, we have*

$$E(KK_n^j) > LE(KK_n^j),$$

for all $n \geq 8$.

Proof. For $j = 3$, it follows from Lemma 2.3.7, that the A-characteristic polynomial $P(KK_n^3, x)$ of the graph KK_n^3 is $P(KK_n^3, x) = (x+1)^{2n-4}h(x)$, where $h(x) = x^4 - 2(n-2)x^3 + (n^2 - 6n + 3)x^2 + (2n^2 - 14)x + (16n - 23 - 2n^2)$.

For $n \geq 8$, we have $h(n) = n^2 + 2n - 23 > 0$, $h(n-1) = -9 < 0$, $h(n-2) = (n-1)^2 > 0$, $h(1) = n^2 + 8n - 29 > 0$, $h(0) = -2n^2 + 16n - 23 < 0$, $h(-2.3) = -1.31n^2 + 8.594n + 4.3861 < 0$, $h(-3) = n^2 + 16n + 19 > 0$.

Therefore, $h(x)$ has three positive roots, one in each of the intervals $(0, 1)$, $(n-2, n-1)$ and $(n-1, n)$, and a single negative root in the interval $(-3, -2.3)$. Assume that x_1, x_2, x_3, x_4 are the roots of $h(x)$ with $x_1, x_2, x_3 > 0$ and $x_4 < 0$. Therefore the A-spectrum of the graph KK_n^3 is $\{-1^{[2n-4]}, x_1, x_2, x_3, x_4\}$, with $x_1 + x_2 + x_3 + x_4 = 2(n-2)$. We have

$$\begin{aligned} E(KK_n^3) &= (2n-4)|-1| + |x_1| + |x_2| + |x_3| + |x_4| \\ &= 2n - 4 + x_1 + x_2 + x_3 - x_4 \\ &= 2n - 4 + 2n - 4 - 2x_4 \\ &> 4n - 3.4. \end{aligned}$$

By equation (4.6), the Laplacian energy of KK_n^3 is

$$LE(KK_n^3) = 3n - 8 + \frac{12}{n} + \sqrt{n^2 + 8n - 8}.$$

So $E(KK_n^3) - LE(KK_n^3) = n + 4.6 - \frac{12}{n} - \sqrt{n^2 + 8n - 8} = g(n)$. It is easy to see that $g(n) > 0$, for all $n \geq 8$. That is, $E(KK_n^3) > LE(KK_n^3)$, for all $n \geq 8$.

Using the same argument as above, it can be seen, for $j = 4$, that the polynomial $h(x)$ has three positive roots, one in each of the intervals $(0, 1)$, $(n-2, n-1)$ and $(n-1, n)$, and a single negative root in the interval $(-3, -2.4)$. So proceeding similarly the result follows. $\square$

In general, the following result gives a sufficient condition for energy of the graph KK_n^j to be greater than the corresponding Laplacian energy.

Theorem 4.3.6. *For $k \in \mathbb{N} - \{1\}$ and $(k-1)^2 < j \leq k^2$, we have*

$$E(KK_n^j) \; > \; LE(KK_n^j),$$

for all $n \geq ((k-1)^2+2)^2 - (k-1)^2$.

Proof. For $k = 2$, we have $j = 2, 3, 4$ and $n \geq 8$, the result follows by Proposition 1 (of [135]) and Theorem 4.3.5. So assume that $k \geq 3$. By equation (4.6) and Corollary 2.3.9, we have

$$\begin{aligned} E(KK_n^j) - LE(KK_n^j) &= 4n - 8 + 2\sqrt{j} - 3n + j - \frac{4j}{n} + 5 - \sqrt{(n+j+1)^2 - 8j} \\ &= n + 2\sqrt{j} + j - 3 - \frac{4j}{n} - \sqrt{(n+j+1)^2 - 8j} = g(n). \end{aligned}$$

It is easy to see that $g(n) > 0$, for $n \geq ((k-1)^2+2)^2 - (k-1)^2, \; k \geq 3$. Therefore, the result follows. $\square$

By a suitable labelling of vertices, the adjacency matrix $A = A(KK_n^j)$ of the graph $KK_n^j, \; 1 \leq j \leq n$, can be put in the form

$$A = \begin{pmatrix} 0 & x_{2n-1} \\ x_{2n-1}^t & B \end{pmatrix},$$

where x_{2n-1} is a $(2n-1)$-vector having first $(n-1+j)$-entries equal to 1 and rest 0 and B is the adjacency matrix of the graph $K_{n-1} \cup K_n$.

Suppose that the eigenvalues of A are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2n-1} \geq \lambda_{2n}$. Since the spectrum of B is $\{n-1, n-2, -1^{[2n-3]}\}$, by interlacing inequalities for principal submatrix, we have

$$\lambda_1 \geq n-1 \geq \lambda_2 \geq n-2 \geq \lambda_3 \geq -1 \geq \lambda_4 \geq -1 \geq \cdots \geq -1 \geq \lambda_{2n-1} \geq -1 \geq \lambda_{2n}.$$

From this it follows that $\lambda_1 \in (n-1, 2n-1), \lambda_2 \in (n-2, n-1), \lambda_3 \in (-1, n-2), \lambda_{2n} \in (-1, -2n+1)$ and $\lambda_4 = \lambda_5 = \cdots = \lambda_{2n-1} = -1$. This shows that the eigenvalue $\lambda_1, \; \lambda_2$ are always positive and λ_{2n} always negative. While as λ_3 may be positive or negative. Also it is clear from this and Lemma 2.3.7, that $\lambda_1, \lambda_2, \lambda_3, \lambda_{2n}$ are the zeros of the polynomial $h(x) = x^4 + (4-2n)x^3 + (n^2-6n+6-j)x^2 + (2n^2-6n+2nj-j^2-3j+4)x + (1+nj^2-2j^2+n^2-2n-2j+3jn-jn^2)$. So $\lambda_1+\lambda_2+\lambda_3+\lambda_{2n} = 2n-4$ and $\lambda_1\lambda_2\lambda_3\lambda_{2n} = 1+nj^2-2j^2+n^2-2n-2j+3jn-jn^2$.

Since $\lambda_1, \lambda_2 > 0$ and $\lambda_{2n} < 0$, it follows that $\lambda_3 > 0$ if and only if $1 + nj^2 - 2j^2 + n^2 - 2n - 2j + 3jn - jn^2 < 0$, which is so if and only if $2 \leq j \leq n-3$. Therefore, we have the following result.

Theorem 4.3.7. *For $5 \leq j \leq n-3,\ n \geq 9$, we have $E(KK_n^j) > LE(KK_n^j)$, if and only if $n > \frac{j^2-3j+16+\sqrt{(j^2-3j+16)^2+4(j-4)(j^2-2j+16)}}{2(j-4)}$.*

Proof. Since, for $5 \leq j \leq n-3$, the eigenvalue $\lambda_3 > 0$, therefore we have

$$\begin{aligned} E(KK_n^j) &= (2n-4)|-1| + |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_{2n}| \\ &= 2n - 4 + \lambda_1 + \lambda_2 + \lambda_3 - \lambda_{2n} \\ &= 2n - 4 + 2n - 4 - 2\lambda_{2n} \\ &= 4n - 8 - 2\lambda_{2n}. \end{aligned}$$

Also, by Theorem 4.3.3, we have $4n - 4 = LE(KK_n^0) < LE(KK_n^1) < LE(KK_n^j) < LE(KK_n^n) = 4n - 2$, for all $5 \leq j \leq n-3$. So instead of showing $E(KK_n^j) > LE(KK_n^j)$, we will show $E(KK_n^j) > LE(KK_n^n)$. We have,

$$\begin{aligned} E(KK_n^j) - LE(KK_n^n) &= 4n - 8 - 2\lambda_{2n} - 4n + 2 \\ &= -6 - 2\lambda_{2n} > 0 \end{aligned}$$

if and only if $\lambda_{2n} < -3$ which, by the Intermediate Value Theorem, is equivalent to $h(-3) < 0$, that is $(j-4)n^2 - (j^2 - 3j + 16)n - (j^2 - 2j + 16) > 0$, that is, $n > \frac{j^2-3j+16+\sqrt{(j^2-3j+16)^2+4(j-4)(j^2-2j+16)}}{2(j-4)}$. □

Theorem 4.3.7 gives another sufficient condition for the energy of the graph KK_n^j to be greater than the corresponding Laplacian energy.

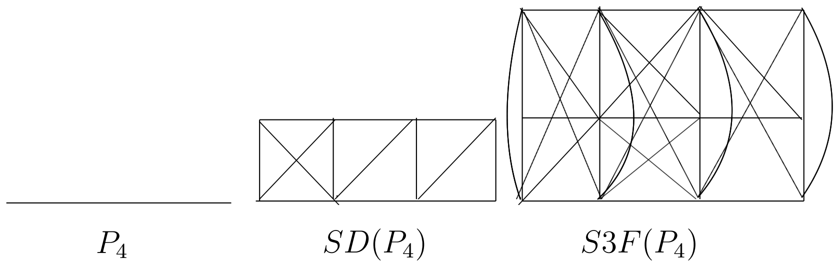


Figure 2: The graph P_4 its strong double graph $SD(P_4)$ and 3-fold graph $S3F(P_4)$.

Let $SD(G)$ be the strong double graph of the graph G. We have the following observation.

Theorem 3.4.8. *If $SD(KK_n^2)$ is the strong double graph of the graph KK_n^2, then we have $LE(SD(KK_n^2)) < E(SD(KK_n^2))$, for all $n \geq 9$.*

Proof. The adjacency spectrum of the graph KK_n^2 is $\{-1^{[2n-4]}, \lambda_1, \lambda_2, \lambda_3, \lambda_4\}$, where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the zeros of the polynomial $P(x) = x^4 - 2(n-2)x^3 + (n^2 - 6n + 4)x^2 + 2(n^2 - n - 3)x - (n^2 - 8n + 11)$. We have $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 2(n-2)$, being the sum of zeros of the polynomial $P(x)$. As shown in [135] one among the four zeros of the polynomial $P(x)$, say λ_4, lies in the interval $(-3, -2.2)$ and so is negative and the rest $\lambda_1, \lambda_2, \lambda_3$ are positive, for all $n \geq 9$. Therefore, it follows by Theorem 2.4.15, that the A-spectrum of the graph $SD(KK_n^2)$ is $2\lambda_1 + 1, 2\lambda_2 + 1, 2\lambda_3 + 1, 2\lambda_4 + 1, -1^{[4n-4]}$, where $2\lambda_4 + 1 \in (-5, -3.2)$ and therefore is negative. So the energy of the graph $SD(KK_n^2)$ is

$$\begin{aligned}
E(SD(KK_n^2)) &= (4n-4)|-1| + |2\lambda_1 + 1| + |2\lambda_2 + 1| + |2\lambda_3 + 1| + |2\lambda_4 + 1| \\
&= 4n - 4 + 2\lambda_1 + 1 + 2\lambda_2 + 1 + 2\lambda_3 + 1 - 2\lambda_4 - 1 \\
&= 8n - 10 - 4\lambda_4 \\
&> 8n - 1.2.
\end{aligned}$$

Also, the L-spectrum of the graph KK_n^2 is $n^{[2n-4]}, n+1, \frac{n+3\pm\sqrt{n^2+6n-7}}{2}, 0$, with average vertex degree $\frac{2m_1}{n_1} = n - 1 + \frac{2}{n}$, where $m_1 = n(n-1) + 2$ and $n_1 = 2n$ are respectively the number of edges and vertices in the graph KK_n^2. Also the degree sequence of the graph KK_n^2 is $[d_i]$, $i = 1, 2, \ldots, 2n$, where

$$d_i = \begin{cases} n+1, & \text{if } i = 1 \\ n, & \text{if } i = 2, 3 \\ n-1 & \text{if } 4 \leq i \leq 2n. \end{cases}$$

Therefore, by Lemma 3.4.19, the L-spectrum of the graph $SD(KK_n^2)$ is $2n^{[4n-7]}, 2n + 2^{[3]}, 2n + 4, (n+3) \pm \sqrt{n^2 + 6n - 7}, 0$, with average vertex degree $\frac{2m_2}{n_2} = 2(\frac{2m_1}{n_1}) + 1 = 2n - 1 + \frac{4}{n}$. So, by direct calculation, it can be seen that the Laplacian energy of the graph $SD(KK_n^2)$ is

$$LE(SD(KK_n^2)) = 6n - 10 + \frac{16}{n} + 2\sqrt{n^2 + 6n - 7}.$$

Therefore,

$$E(SD(KK_n^2) - LE(SD(KK_n^2)) = 2n + 8.8 - \frac{16}{n} - 2\sqrt{n^2+6n-7} = g(n).$$

It is easy to see that the derivative of the function $g(n)$ is positive for $n > 1$. Therefore, it follows that the function $g(n)$ is increasing in the interval $(1, \infty)$, moreover $g(3) = 0.5227281 > 0$ implies that $g(n) > 0$ for all $n \geq 3$. Thus we conclude that $E(SD(KK_n^2)) > LE(SD(KK_n^2))$, for all $n \geq 9$. $\square$

We observe that the strong double graph $SD(KK_n^2)$ of the graph KK_n^2 does not belong to the family of graphs $\{KK_n^2 : n \in \mathbb{N}\}$, for any n.

For a graph G with vertex set $\{v_1, v_2, \ldots, v_n\}$, let $SPF(G)$ be the graph obtained by taking p-copies of the graph G and joining each vertex v_i in one copy with the closed neighbourhood $N[v_i] = N(v_i) \cup \{v_i\}$ of the corresponding vertex in every other copy (see Figure 2). By a suitable labelling of vertices, it can be seen that the adjacency matrix $\widehat{A}$ of the graph $SPF(G)$ is

$$\widehat{A} = \begin{pmatrix} A & A+I & \cdots & A+I \\ A+I & A & \cdots & A+I \\ \vdots & \vdots & \cdots & \vdots \\ A+I & A+I & \cdots & A \end{pmatrix},$$

where A is the adjacency matrix of G and I is the identity matrix of order equal to the order of A.

Therefore the characteristic polynomial of $SPF(G)$ is

$$|\lambda I_{pn} - \widehat{A}| = \begin{vmatrix} \lambda I_n - A & -(A+I) & \cdots & -(A+I) \\ -(A+I) & \lambda I_n - A & \cdots & -(A+I) \\ \vdots & \vdots & \cdots & \vdots \\ -(A+I) & -(A+I) & \cdots & \lambda I_n - A \end{vmatrix}.$$

Using elementary transformations $C_1 \to C_1 + C_2 + \cdots + C_p$ and then $R_i \to R_i - R_1$, for $i = 2, 3, \ldots, p$, it can be seen that the spectrum of the matrix $\widehat{A}$ and so the A-spectrum of the graph $SPF(G)$ is

$$\{-1^{[n(p-1)]}, px_1 + p - 1, px_2 + p - 1, \ldots, px_n + p - 1\}, \tag{4.7}$$

where $x_1, x_2, \ldots, x_n$ are the adjacency eigenvalues of the graph G.

Also, the degree matrix $\widehat{D}$ of the graph $SPF(G)$ is

$$\widehat{D} = \begin{pmatrix} pD+(p-1)I & 0 & \cdots & 0 \\ 0 & pD+(p-1)I & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & pD+(p-1)I \end{pmatrix}.$$

So, the Laplacian matrix $\widehat{L}$ of the graph $SPF(G)$ is

$$\widehat{L} = \begin{pmatrix} pD+(p-1)I-A & -(A+I) & \cdots & -(A+I) \\ -(A+I) & pD+(p-1)I-A & \cdots & -(A+I) \\ \vdots & \vdots & \cdots & \vdots \\ -(A+I) & -(A+I) & \cdots & pD+(p-1)I-A \end{pmatrix}.$$

Proceeding similarly as above, it can be seen that the L-spectrum of the graph $SPF(G)$ is

$$\{p\mu_1, p\mu_2, \ldots, p\mu_n, pd_1 + p^{[p-1]}, pd_2 + p^{[p-1]}, \ldots, pd_n + p^{[p-1]}\}, \tag{4.8}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of G and $d_1, d_2, \ldots, d_n$ are the degrees of the vertices in G.

The next result gives a two way infinite families of graphs G for which the inequality (4.1) does not hold.

Theorem 4.3.9. *For $j = 2, 3, 4,\ p = 2, 3$ and $n \geq 9$ and for $j = 2, 3, 4,\ p \geq 4$ and $n > pj$, we have*

$$E(SPF(KK_n^j)) \quad > \quad LE(SPF(KK_n^j)),$$

where $SPF(G)$ is the p-fold graph of the graph G.

Proof. For $p = 2$ and $j = 2, 3, 4$, it is clear from the definition of strong p-fold graph that $SPF(KK_n^j) \cong SD(KK_n^2),\ SD(KK_n^3),\ SD(KK_n^4)$. If $SPF(KK_n^j) \cong SD(KK_n^2)$, then the result follows by Theorem 4.3.8. If $SPF(KK_n^j) \cong SD(KK_n^3)$ or $SD(KK_n^4)$, then proceeding similarly as in Theorem 4.3.8, it can be seen that the result is true in this case as well. Also for $p = 3$ and $j = 2, 3, 4$, we have

$SPF(KK_n^j) \cong KK_n^2 \circ K_3,\ KK_n^3 \circ K_3,\ KK_n^4 \circ K_3$, where $\circ$ denotes the composition of graphs. We will show that the result holds if $SPF(KK_n^j) \cong KK_n^2 \circ K_3$, and then proceed similarly for the other two cases.

The A-spectrum of the graph $KK_n^2 \circ K_3$ is $\{-1^{[6n-4]}, 3x_1+2, 3x_2+2, 3x_3+2, 3x_4+2\}$, where x_1, x_2, x_2, x_4 are the zeros of $h(x) = x^4 - 2(n-2)x^3 + (n^2-6n+4)x^2 + 2(n^2-n-3)x - (n^2-8n+11)$. Proceeding similarly as in Theorem 4.3.5, it can be seen that $x_1, x_2, x_3 > 0$ and $x_4 \in (-3, -2.2)$ for all $n \geq 9$. So, we have

$$E(KK_n^2 \circ K_3) = 12n - 6x_4 - 12 > 12n + 1.2.$$

Also, the L-spectrum of the graph $KK_n^2 \circ K_3$ is $\{3n^{[6n-10]}, 3n+3^{[5]}, 3n+6^{[2]}, \frac{3(n+3)\pm\sqrt{n^2+6n-7}}{2}, 0\}$, with average vertex degree $3n-1+\frac{6}{n}$. We have

$$LE(KK_n^2 \circ K_3) = 9n - 13 + \frac{24}{n} + 3\sqrt{n^2+6n-7}.$$

Therefore, $E(KK_n^2 \circ K_3) - LE(KK_n^2 \circ K_3) = 3n + 14.2 - \frac{24}{n} - 3\sqrt{n^2+6n-7} = g(n)$. It is easy to see that $g(n) > 0$, for all $n \geq 9$.

So, assume that $p \geq 4$ and $j = 2, 3, 4$. Using equation (4.7) and Lemma 2.3.7, it follows that the A-spectrum of the graph $SPF(KK_n^j)$ is

$$\{-1^{[2pn-4]}, px_1 + (p-1), px_2 + (p-1), px_3 + (p-1), px_4 + (p-1)\},$$

where x_1, x_2, x_3, x_4 are the zeros of the polynomial $h(x) = x^4 - 2(n-2)x^3 + (n^2 - 6n+6-j)x^2 + (2n^2-6n+2nj-j^2-3j+4)x + (1+nj^2-2j^2+n^2-2n-2j+3nj-jn^2)$.

For $n > pj,\ p \geq 4$ and $j = 2, 3, 4$, we have $h(n) = n^2 + 2n - 2j^2 - 2j + 1 > 0$, $h(n-1) = -j^2 < 0$, $\quad h(n-2) = (n-1)^2 > 0$, $\quad h(1) = 16 - 6j - 3j^2 - 16n + 5jn + nj^2 + 4n^2 - jn^2 > 0$, $\quad h(0) = 1 + nj^2 - 2j^2 + n^2 - 2n - 2j + 3nj - jn^2 < 0$, $h(-3) = 16 - 2j + j^2 + 16n - 3jn + nj^2 + 4n^2 - jn^2 > 0$,

$$h(-2.j) = h(-(2+0.j)) = \begin{cases} -0.56n^2 + 4.656n + 2.3936 < 0, & \text{if } j = 2 \\ -1.31n^2 + 8.594n + 4.3861 < 0, & \text{if } j = 3 \\ -2.04n^2 + 14.288n + 8.0016 < 0 & \text{if } j = 4. \end{cases}$$

Therefore, $h(x)$ has three positive roots, one in each of the intervals $(0,1)$, $(n-2, n-1)$ and $(n-1, n)$, and a single negative root in the interval $(-3, -2.j)$. Assume that $x_1, x_2, x_3 > 0$ and $x_4 < 0$. We have

$$\begin{aligned} E(SPF(KK_n^j)) &= (2pn-4)|-1| + |px_1+p-1| + |px_2+p-1| \\ &\quad + |px_3+p-1| + |px_4+p-1| \\ &= 2pn-4+p(x_1+x_2+x_3)-px_4+2p-2 \\ &= 4pn-2p-2px_4-6 \\ &> 4pn+2p(1.j)-6. \end{aligned}$$

Also, by Lemma 4.3.1, equation (4.8) and the fact that the degree sequence of the graph KK_n^j is $[n+j-1, n^{[j]}, (n-1)^{[2n-j-1]}]$, it follows that the L-spectrum of the graph $SPF(KK_n^j)$ is
$\{pn^{[2pn-p(j+1)-1]}, p(n+1)^{[pj-1]}, p(n+j)^{[p-1]}, \frac{p((n+j+1)\pm\sqrt{(n+j+1)^2-8j)}}{2}, 0\}$
with average vertex degree $pn-1+\frac{pj}{n}$. Therefore, by direct calculation, we have

$$LE(SPF(KK_n^j) == 3pn - p(j+1) - 4 + \frac{4pj}{n} + p\sqrt{(n+j+1)^2-8j}.$$

For $n > pj, \quad p \geq 4$ and $j = 2, 3, 4$, it is easy to see that $E(SPF(KK_n^j)) - LE(SPF(KK_n^j)) = pn+p(2(1.j)+j+1)-2-\frac{4pj}{n}-p\sqrt{(n+j+1)^2-8j} > 0$. That is, $E(SPF(KK_n^j)) > LE(SPF(KK_n^j))$, for all $n > pj, \quad p \geq 4$ and $j = 2, 3, 4$. □

Although all graphs for which the inequality (4.1) does not hold are not so common, Theorem 4.3.9 shows the existence of families of such graphs.

4.4 Conclusion

Although the conjecture that "the inequality $LE(G) \geq E(G)$ holds for all G" has been disproved. This inequality holds for most of the graphs as shown in [75] and [135]. Therefore the following problem will be of great interest.

Problem 4.4.1. *Characterize all non-bipartite graphs G for which the inequality $LE(G) \geq E(G)$ holds.*

CHAPTER 5

Laplacian-energy-like invariant and Kirchhoff index

In this chapter, we consider *Laplacian-energy-like invariant* $LEL(G)$ and *Krichhoff index* $Kf(G)$ of a graph G. We mention some well known results on these Laplacian spectrum based graph invariants. We obtain a lower bound for $LEL(G)$ and an upper bound for $Kf(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ and a positive real number k. We consider the relation between $LEL(G)$ and $Kf(G)$ and obtain some sufficient conditions for a graph G or its complement $\overline{G}$ to satisfy the inequality $LEL(G) > Kf(G)$. As a consequence, we arrive at a complete comparison of $LEL(G)$ and $Kf(G)$ for the complement of a tree, unicyclic graphs, bicyclic graphs, tricyclic graphs and tetracyclic graphs.

5.1 Introduction

Let $L(G)$ be the Laplacian matrix of the graph G and let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$ be the Laplacin spectrum of G. As discussed in Chapter 3, the idea of Gutman and Zhou [65] was to conceive a graph energy like quantity that instead of adjacency eigenvalues is defined in terms of Laplacian eigenvalues and that hopefully would preserve the main features of the original graph energy. The definition of Laplacian energy $LE(G)$ was therefore so chosen that all the properties possessed by graph energy $E(G)$ should be preserved. In fact, they were successful, as most of the properties possessed by $E(G)$ are also possessed by $LE(G)$, but there are some dissimilarities also. Liu and Liu [98] put forward a new Laplacian spectrum based graph invariant, which they called *Laplacian-energy-like invariant* $LEL(G)$ of a graph. It was shown in [70, 98] that this graph invariant possesses all the properties of graph energy. Gutman et al. [70] pointed out that $LEL(G)$ is more similar to $E(G)$ than to $LE(G)$. In fact, Stevanoić et al. [134] showed that $LEL(G)$ of a graph describes well the properties which are accounted by the majority of molecular descriptors: motor octane number, entropy, molar volume, molar refraction, particularly the acentric factor AF parameter, but also more difficult properties like boiling point, melting point and partition coefficient *Log P*. In a set of polycyclic aromatic hydrocarbons, $LEL(G)$ of a graph was proved [134] to be as good as the Randić index (a connectivity index) and better than the Wiener index (a distance based index). Moreover, it is well defined mathematically and shows interesting relations in particular classes of graphs, these recommending $LEL(G)$ of a graph as a new and powerful topological index (Numbers reflecting certain structural features of a molecule that are derived from its molecular graph are known as topological indices, these are used in theoretical chemistry for design of chemical compounds with given physicochemical properties or given pharmacological and biological activities).

For a connected graph G with vertex set $V(G) = \{v_1, v_2 \ldots, v_n\}$, the (ordinary) distance between vertices v_i and v_j, denoted by d_{ij}, is the length of a shortest path connecting them. The original index based on distance in a graph G is the Wiener index $W(G)$ [143], which counts the sum of distances between the pairs of vertices in G, that is,

$$W(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_{ij}.$$

In 1993, Klein and Randić [91] defined a new distance function named resistance distance, framed in terms of electrical network theory. However, this concept has been discussed much earlier (1949) for another purpose by Foster [45] as recently pointed out by Palacios [113]. The resistance distance between vertices v_i and v_j of G, denoted by r_{ij}, is defined to be the effective resistance between the nodes v_i and v_j as computed with Ohm's and Kirchhoff's laws when all the edges of G are considered to be unit resistors. As an analogue to the Wiener index, the sum

$$Kf(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} r_{ij}$$

was proposed in [91], later was called the Kirchhoff index of G in [18]. Klein and Randić [91] proved that $r_{ij} \leq d_{ij}$ with equality if and only if there is exactly one path between v_i and v_j, and so $Kf(G) \leq W(G)$ with equality if and only if G is a tree. As the Wiener index $W(G)$ of a tree has been extensively studied [37], therefore the Krichhoff index is primarily of interest in the case of of cycle-containing graphs. This index is also named as total effective resistance [90] or the effective graph resistance [40], and like the Wiener index have found applications in chemistry, electrical network, Markov chains, averaging networks, experiment design, and Euclidean distance embeddings, see [18, 90, 91]. It is well known that the resistance distance between two arbitrary vertices in an electrical network can be obtained in terms of the eigenvalues and eigenvectors of the combinatorial Laplacian matrix $L(G)$ and normalized Laplacian matrix associated with the network (when considered as a graph). By studying Laplacian matrix, researchers have obtained many properties of resistance distances [144, 145]. At almost exactly the same time, Gutman and Mohar [64] and Zhu et al. [161] showed that, for a connected graph G the *Krichhoff index* $Kf(G)$ can be expressed as function of Laplacian eigenvalues of G.

5.2 Laplacian-energy-like invariant of a graph

Definition 5.2.1. *Laplacian-energy-like invariant of a graph.* Let G be a graph of order n with m edges having Laplacian eigenvalues $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$. The Laplacian-energy-like invariant of G is denoted by $LEL(G)$ and is defined as

$$LEL(G) = \sum_{j=1}^{n} \sqrt{\mu_j} = \sum_{j=1}^{n-1} \sqrt{\mu_j}. \tag{5.1}$$

The concept of *Laplacian-energy-like invariant* $LEL(G)$ was first introduced in 2008 by Liu and Liu [98], where it is shown that it has similar features as earlier studied graph energy.

Let $C = C(G)$ be the oriented vertex-edge incidence matrix of the graph G, defined in Section 3.1, then as seen in [28], we have $C(G)C(G)^t = D(G) - A(G) = L(G)$. As the singular values of the matrix X are the positive square roots of the eigenvalues of the matrix XX^t, it follows that the singular values of the matrix $C(G)$ are the positive square roots of the eigenvalues of the matrix $L(G)$. That is, the singular values of the matrix $C(G)$ are $0 = \sqrt{\mu_n} \leq \sqrt{\mu_{n-1}} \leq \cdots \leq \sqrt{\mu_2} \leq \sqrt{\mu_1}$. So, following the definition of matrix energy by Nikifrov [110], the energy of the matrix $C(G)$ is given by

$$E(C(G)) = \sum_{j=1}^{n} s_i(C(G)) = \sum_{j=1}^{n} \sqrt{\mu_j} = LEL(G).$$

Using this coincidence, Stevanoić et al. [138] called *Laplacian-energy-like invariant* $LEL(G)$, the oriented incidence energy of the graph G. This provides a new interpretation of $LEL(G)$ and therefore, offers a new insight into its possible physical or chemical meaning.

Let $B = B(G)$ be the matrix obtained from the matrix $C(G)$ by replacing each -1 by $+1$ and leaving the rest of entries unchanged. This matrix $B(G)$ is called vertex-edge incidence matrix of the graph G. It is well known [28] that $B(G)B(G)^t = D(G) + A(G) = Q(G)$. So, following the definition of matrix energy by Nikifrov [110], the energy of the matrix $B(G)$ was called *incidence energy* $IE(G)$ [88] of the graph G and is given by

$$E(B(G)) = \sum_{j=1}^{n} s_i(B(G)) = \sum_{j=1}^{n} \sqrt{\mu_j} = IE(G),$$

where $0 \leq q_n \leq q_{n-1} \leq \cdots \leq q_2 \leq q_1$ are the eigenvalues of $Q(G)$. Using a well known fact, that the Laplacian and the signless Laplacian spectrum of a graph are same for a bipartite graph, we have the following observation.

Theorem 5.2.1 *For a bipartite graph G, the incidence and oriented incidence energy are same, that is,*

$$LEL(G) = IE(G).$$

In general, the following relation exists between the *Laplacian-energy-like invariant* $LEL(G)$ and the *Incidence energy* $IE(G)$ of a graph G [5].

Theorem 5.2.2 *For a graph G, we have*

$$LEL(G) \leq IE(G),$$

with equality if and only if G is bipartite.

From this it follows that any lower bound to $LEL(G)$ is a lower bound for $IE(G)$.

5.3 Bounds for Laplacian-energy-like invariant

Various lower and upper bounds for the Laplacian-energy-like invariant $LEL(G)$ are known, which give its connection with the different parameters of a graph. Here, we list some of the well known bounds.

The following [98] is an upper bound for *Laplacian-energy-like invariant* $LEL(G)$ as a function of the number of vertices n and the number of edges m.

Theorem 5.3.1. *Let G be a graph with n vertices and m edges. Then*

$$LEL(G) \leq \sqrt{2m(n-1)},$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

Since, for a graph G we always have $m \leq \frac{n(n-1)}{2}$. Therefore, we have the following consequence of Theorem 5.3.1.

Corollary 5.3.2. *Let G be a graph with n vertices. Then*

$$LEL(G) \leq (n-1)\sqrt{n},$$

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

Let $G - e$ be the graph obtained from the graph G by deleting the edge e of G. Since, the Laplacian eigenvalues of G and $G-e$ satisfying Interlacing property, we have by Lemma 3.3.11,

$$\sum_{j=1}^{n} \mu_j(G) - \sum_{j=1}^{n} \mu_j(G-e) = 2.$$

As an immediate consequence to this, we have the following observation [159].

Theorem 5.3.3. *Let G be a graph and e be any edge in G. Then*

$$LEL(G-e) < LEL(G).$$

A repeated application of Theorem 5.3.3, shows that the empty graph $\overline{K_n}$ has the minimal and the complete graph K_n has the maximal Laplacian-energy-like invariant over all the graphs G of order n, that is,

$$LEL(\overline{K_n}) \leq LEL(G) \leq LEL(K_n).$$

If G is a bipartite graph having cardinalities of partite sets equal to r and s, then G is a spanning subgraph of the complete bipartite graph $K_{r,s}$ and so by Theorem 5.3.3, we have the following observation.

Corollary 5.3.4. *Let G be a bipartite graph having cardinalities of partite sets equal to r and s. Then*

$$LEL(G) \leq \sqrt{r+s} + (r-1)\sqrt{s} + (s-1)\sqrt{r},$$

with equality if and only if $G \cong K_{r,s}$.

From this, it follows that among bipartite graphs G having cardinalities of partite sets equal to r and s, complete bipartite graph $K_{r,s}$ has the maximal Laplacian-energy-like invariant.

The following is an upper bound [98] for the *Laplacian-energy-like invariant* $LEL(G)$ in terms of the number of vertices n, the number of edges m and maximum vertex degree Δ.

Theorem 5.3.5. *Let G be a graph with n vertices and $m \geq 1$ edges having 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 $G \cong K_{1,n-1}$.

The *Laplacian-energy-like invariant* $LEL(G)$ as a function of the number of edges satisfies the following inequalities [98].

Theorem 5.3.6. *If G is a graph with n vertices and m edges, then*

$$\sqrt{2m} \leq LEL(G) \leq \sqrt{2}m,$$

with equality on the left if and only if $G \cong \overline{K_n}$ *or* $K_2 \cup (n-2)K_1$*, and equality on the right if and only if* $G \cong rK_2 \cup (n-2r)K_1$*, where* $r = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$.

The following is a lower bound for *Laplacian-energy-like invariant* $LEL(G)$ [78] as a function of number of vertices n.

Theorem 5.3.7. *If* G *is a graph with* n *vertices, then*

$$LEL(G) \geq \sqrt{n-1} + n - 2,$$

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

From Theorems 5.3.3 and 5.3.7, it is clear that among connected graphs on n vertices, the complete graph K_n is the graph with maximal $LEL(G)$ and the star graph $K_{1,n-1}$ is the graph with minimal $LEL(G)$.

The following is the lower bound [78] for $LEL(G)$, in terms of the number of vertices n and the number of edges m.

Theorem 5.3.8. *If* G *is a graph with* n *vertices and* m *edges, then*

$$LEL(G) \geq \frac{2m}{\sqrt{n}}, \tag{5.2}$$

with equality if and only if $G \cong K_n$ *or* $\overline{K_n}$.

The next result gives the lower bound [78, 141] for $LEL(G)$, in terms of the number of vertices n and the number of edges m and first *Zagreb index* $M_1(G)$.

Theorem 5.3.9. *If* G *is a graph with* n *vertices and* m *edges, then*

$$LEL(G) \geq \sqrt{\frac{(2m)^3}{M_1(G) + 2m}}, \tag{5.3}$$

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

It is shown in [141] that the lower bounds (5.2) and (5.3) are incomparable.

If G is a graph free from K_{r+1}, $2 \leq r \leq n$ (that is, G has no subgraph isomorphic to K_{r+1}), then it is well known that [153]

$$M_1(G) \leq \frac{2r-2}{r} mn.$$

Using this we have the following consequence of Theorem 5.3.9.

Corollary 5.3.10. *If G is a K_{r+1}-free graph $(2 \leq r \leq n)$ with n vertices and m edges, then*

$$LEL(G) \geq \frac{2m}{\sqrt{\frac{n(r-1)}{r}+1}},$$

with equality if and only if $G \cong \overline{K_n}$ or $r = n$ and $G \cong K_n$.

The next result is a Cauchy-Bunyakovsky-Schwarz type discrete inequality and can be found in [38].

Lemma 5.3.11.*(Pólya-Szegö inequality) Let $(a_1, a_2, \ldots, a_n)$ and $(b_1, b_2, \ldots, b_n)$ be two sequences of positive real numbers such that there exist positive numbers A, a, B, b satisfying*

$$0 < a \leq a_i \leq A < \infty, \quad 0 < b \leq b_i \leq B < \infty,$$

for all $i = 1, 2, \ldots, n$. Then

$$\frac{\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2}{(\sum_{i=1}^{n} a_i b_i)^2} \leq \frac{(ab+AB)^2}{4abAB}. \tag{5.4}$$

The equality holds in (5.4) if and only if $p = \frac{n.\frac{A}{a}}{(\frac{A}{a}+\frac{B}{b})}, q = \frac{n.\frac{B}{b}}{(\frac{A}{a}+\frac{B}{b})}$ are integers and if p of the numbers $a_1, a_2, \ldots a_n$ are equal to a, and q of these numbers are equal to A, and if the corresponding numbers b_i are equal to b and B, respectively.

We now obtain a lower bound for $LEL(G)$ in terms of the number of vertices n, the number of edges m and a positive real number k.

Theorem 5.3.12. *Let G be a connected graph with n vertices and m edges having algebraic connectivity $\mu_{n-1} \geq k$. Then,*

$$LEL(G) \geq \sqrt{\frac{8m(n-1)\sqrt{kn}}{(\sqrt{n}+\sqrt{k})^2}}, \tag{5.5}$$

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

Proof. Setting in (5.4) $n = n-1$, $a_i = \sqrt{\mu_i}, b_i = 1$, for $i = 1, 2, \ldots, n-1$ and $a = \sqrt{\mu_{n-1}}, A = \sqrt{\mu_1}, b = 1, B = 1$, we get

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

This gives,

$$LEL(G) \geq \sqrt{\frac{8m(n-1)\sqrt{\mu_1 \mu_{n-1}}}{(\sqrt{\mu_1} + \sqrt{\mu_{n-1}})^2}}.$$

Since,

$$\sqrt{\frac{8m(n-1)\sqrt{\mu_1 \mu_{n-1}}}{(\sqrt{\mu_1} + \sqrt{\mu_{n-1}})^2}} \geq \sqrt{\frac{8m(n-1)\sqrt{k\mu_1}}{(\sqrt{\mu_1} + \sqrt{k})^2}},$$

it follows that,

$$LEL(G) \geq \sqrt{\frac{8m(n-1)\sqrt{k\mu_1}}{(\sqrt{\mu_1} + \sqrt{k})^2}}.$$

For $x \leq n$, consider the function $f(x) = \dfrac{8m(n-1)\sqrt{kx}}{(\sqrt{x} + \sqrt{k})^2}$. For this function, we have $f'(x) = \dfrac{4m(n-1)\sqrt{k}(\sqrt{k} - \sqrt{x})}{\sqrt{x}(\sqrt{x} + \sqrt{k})^3} \leq 0$. That is, $f(x)$ is a decreasing function for $x \leq n$. So $f(x) \geq f(n) = \dfrac{8m(n-1)\sqrt{kn}}{(\sqrt{n} + \sqrt{k})^2}$. This gives,

$$LEL(G) \geq \sqrt{\frac{8m(n-1)\sqrt{kn}}{(\sqrt{n} + \sqrt{k})^2}}.$$

Equality occurs in (5.5) if and only if equality occurs in (5.4) and $\mu_1 = n$. That is, by Lemma 3.3.10 and Lemma 5.3.11, if and only if G is a join of two graphs and p, q are integers, where $p + q = n - 1$ with p of the numbers in $\mu_1, \mu_2, \ldots, \mu_{n-1}$ equal to μ_1 and q of them equal to μ_{n-1}. For p, q integers there are $n-1$ solutions of the equation $p + q = n - 1$ and for any of these integral solutions it follows, from Lemma 5.3.11, that equality occurs if and only if G has two distinct Laplacian eigenvalues. That is, if and only if $G \cong K_n$ [28].

Conversely, if $G \cong K_n$, then it is easy to see that equality holds in (5.5). $\square$

Remark 5.3.13.

(i). Let T be a tree of order n, $n \geq 6$ with algebraic connectivity $\mu_{n-1} \geq 0.07$. We will show that the lower bound (5.5) is better than the lower bound in (5.2) for a tree T. We have, $\frac{8m(n-1)\sqrt{(0.07)n}}{(\sqrt{n}+\sqrt{0.07})^2} \geq (\frac{2m}{\sqrt{n}})^2$, that is, $\frac{80(n-1)^2\sqrt{7n}}{(10\sqrt{n}+\sqrt{7})^2} \geq \frac{4(n-1)^2}{n}$, as $m = n-1$, that is, $20n\sqrt{7n} \geq (10\sqrt{n}+\sqrt{7})^2$, which is true for $n \geq 6$. Since, for almost all trees, algebraic connectivity $\mu_{n-1} \geq 0.07$, it follows that lower bound (5.5) is better than bound (5.2) for almost all trees.

(ii). Let G be graph of order n having $m \leq \frac{2n(n-1)\sqrt{n}}{(\sqrt{n}+1)^2}$ edges and algebraic connectivity $\mu_{n-1} \geq 1$, then the lower bound (5.5) is better than the lower bound (5.2) for G, we have $\sqrt{\frac{8m(n-1)\sqrt{kn}}{(\sqrt{n}+\sqrt{k})^2}} \geq \frac{2m}{\sqrt{n}}$, that is, $\frac{8m(n-1)\sqrt{n}}{(\sqrt{n}+1)^2} \geq \frac{4m^2}{n}$, that is,

$$2n(n-1)\sqrt{n} \geq m(\sqrt{n}+1)^2, \tag{5.6}$$

which is true. In particular if G is a unicyclic, a bicyclic, a tricyclic, a tetracyclic graph, then $m = n, n+1, n+2, n+3$ (respectively). It is easy to see that (5.6) holds for $n \geq 5$.

Remark 5.3.14.

(i). Let T be a tree of order n, $n \geq 3$ with maximum degree $\Delta \geq \frac{n}{2}$ and algebraic connectivity $\mu_{n-1} \geq 0.07$, then the lower bound (5.5) is better than the lower bound (5.3) for T. We have, $\sqrt{\frac{8m(n-1)\sqrt{kn}}{(\sqrt{n}+\sqrt{k})^2}} \geq \sqrt{\frac{(2m)^3}{2m+n\Delta^2}}$, that is, $\frac{80(n-1)^2\sqrt{7n}}{(10\sqrt{n}+\sqrt{7})^2} \geq \dfrac{8(n-1)^3}{2(n-1)+n\Delta^2}$, as $m = n-1$, that is, $n\Delta^2 \geq \dfrac{(n-1)(10\sqrt{n}+\sqrt{7})^2}{10\sqrt{7n}} - 2(n-1)$, which is true for $\Delta \geq \frac{n}{2}$, $n \geq 3$.

(ii). Let G be graph of order n with maximum degree $\Delta \geq \sqrt{\frac{m^2(\sqrt{n}+1)^2}{n(n-1)\sqrt{n}} - \frac{2m}{n}}$ and algebraic connectivity $\mu_{n-1} \geq 1$. It can be seen by proceeding similarly as in part (i) that the lower bound (5.5) is better than the bound (5.3) for G. In particular, if G is a unicyclic, a bicyclic, a tricyclic graph, then $m = n, n+1, n+2$. It can be seen by direct calculation, that (5.5) is better than (5.3) for $\Delta \geq \frac{n}{2}$, $n \geq 6$.

The following result characterizes the graphs with three distinct Laplacian eigenvalues and is due to Das [31].

Lemma 5.3.15. *Let G be a graph on $n > 3$ vertices whose distinct Laplacian eigenvalues are $0 < \alpha < \beta$. Then the following hold.*
(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 $K_n - e$.

We now obtain another lower bound for $LEL(G)$ in terms of the number of vertices n, the number of edges m and a positive real number k, which improves the lower bound (5.5).

Theorem 5.3.16. *Let G be a connected graph of order n having m edges with maximum degree Δ and algebraic connectivity $\mu_{n-1} \geq k$. Then*

$$LEL(G) \geq \frac{(n-1)\sqrt{kn} + 2m}{\sqrt{n} + \sqrt{k}}, \tag{5.7}$$

with equality if and only if $k = n$ and $G \cong K_n$ or $k = n-2$ and $G \cong K_n - e$.
Proof. Let $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_2 \leq \mu_1$ be the Laplacian spectrum of G with algebraic connectivity $\mu_{n-1} \geq k$.

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

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

Consider the function

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

for which

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

As $2m = \sum_{i=1}^{n} \mu_i = \mu_1 + \mu_2 + \cdots + \mu_{n-1} > (n-1)\mu_{n-1} \geq (n-1)k$, we have $f'(x) < 0$. This shows that the function $f(x)$ is decreasing for $\Delta + 1 \leq x \leq n$. Therefore,

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

implying

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

Equality in (5.7) 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 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 5.3.15, we have $G \cong K_n - e$.

Conversely, if G is isomorphic to K_n or $K_n - e$, then it is easy to see that equality holds in (5.7). $\square$

Remark 5.3.17. Using the fact that the arithmetic mean is greater than or equal to the geometric mean, it follows that

$$\frac{(n-1)\sqrt{nk} + 2m}{\sqrt{n} + \sqrt{k}} \geq \sqrt{\frac{8m(n-1)\sqrt{kn}}{(\sqrt{n} + \sqrt{k})^2}}.$$

This shows that the lower bound (5.7) always improves the lower bound (5.5).

From the definition, one can immediately get the *Laplacian-energy-like-invariant* $LEL(G)$ of a graph by computing the Laplacian eigenvalues of the graph. However, it is rather hard to deal directly with Laplacian matrix $L(G)$ even for special graphs. So, researchers established several lower and upper bounds to estimate this invariant for some classes of graphs. Wang et al. [141] obtained the bounds for line graph, subdivision graph and total graph of a graph. Stevanović [136] obtained the upper and lower bounds for $LEL(G)$ of trees. Similarly, Stevanović and Ilić [137] gave the upper and lower bounds for $LEL(G)$ of unicyclic graphs. He and Shan [81] presented the lower bound for $LEL(G)$ of bicyclic graphs. For further details, see the comprehensive survey [100].

We now obtain lower and upper bounds for *Laplacian-energy-like-invariant* of some graphs derived from regular graphs.

A bipartite graph G with a bipartition $V(G) = U \cup W$ is called an (r,s)-semiregular graph if all vertices in U have degree r and all vertices in W have degree s. The following result gives the relationship between Laplacian characteristic polynomial $\psi(\mathscr{L}(G),x)$ of the line graph of G and the Laplacian characteristic polynomial $\psi(G,x)$ of G.

Lemma 5.3.18. *If G is an (r,s)-semiregular graph with n vertices and $m = \frac{nrs}{r+s}$ edges, then*

$$\psi(\mathscr{L}(G),x) = (x-(r+s))^{m-n}\psi(G,r+s-x),$$

where $\mathscr{L}(G)$ is the line graph of G.

Proof. Let $B(G)$ be the vertex-edge incidence matrix of the graph G. Then [28]

$$B(G)B(G)^t = Q(G) \quad \text{and} \quad B(G)^tB(G) = 2I_m + A(\mathscr{L}(G)), \tag{5.8}$$

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

It is well known that the line graph $\mathscr{L}(G)$ of an (r,s)-semiregular graph G is $(r+s-2)$-regular. Therefore, we have

$$L(\mathscr{L}(G)) = (r+s-2)I_m - A(\mathscr{L}(G)).$$

Using (5.8), we have

$$(r+s)I_m - L(\mathscr{L}(G)) = B(G)^tB(G). \tag{5.9}$$

Using the fact that the matrices XX^t and X^tX have the same non-zero eigenvalues, it follows from (5.8) and (5.9) that $Q(G)$ and $(r+s)I_m - L(\mathscr{L}(G))$ have the same non-zero eigenvalues. Note that the difference between the dimension of $L(\mathscr{L}(G))$ and $Q(G)$ is $m-n$. The proof now follows by using the fact that the leading coefficient of the characteristic polynomial is equal to one and Laplacian and signless Laplacian spectrum coincides if and only if G is bipartite. $\square$

By Lemma 5.3.18, the Laplacian spectrum of line graph $\mathscr{L}(G)$ of an (r,s)-semiregular graph G is $\{(r+s)^{m-n}, r+s-\mu_1, r+s-\mu_2, \ldots, r+s-\mu_n\}$, where

$\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of the graph G.

Now we obtain an upper bound for $LEL(\mathscr{L}(G))$ of an (r,s)-semiregular graph G.

Theorem 5.3.19. *Let G be an (r,s)-semiregular graph with n vertices. Then*

$$LEL(\mathscr{L}(G)) \leq (\frac{nrs}{r+s} - n + 1)\sqrt{r+s} + \sqrt{(n-2)((n-1)(r+s) - \frac{2nrs}{r+s})},$$

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

Proof. Let m be the number of edges in G, then $m = \frac{nrs}{r+s}$ and $\sum_{i=1}^{n-1} \mu_i = 2m$. Also $\mu_1(G) = r+s$ and $\mu_n(G) = 0$. Using Cauchy-Schwarz inequality, we have

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

Equality occurs if and only if $r+s = \mu_1, \mu_2 = \mu_3 = \cdots = \mu_{n-1}$. Since G is (r,s)-semiregular, it follows by Lemma 5.3.15, G is either $K_{1,n-1}$ or $K_{\frac{n}{2},\frac{n}{2}}$.

Conversely, it is easy to see that if G is one of the graphs $K_{1,n-1}$ or $K_{\frac{n}{2},\frac{n}{2}}$, then equality holds. $\square$

For a graph G, the paraline graph, denoted by $\mathscr{C}(G)$, is defined as a line graph of the subdivision graph $S(G)$ (the subdivision graph $S(G)$ of a graph G is the graph obtained from G by inserting a vertex to every edge of G) of G. The concept of the paraline graph (or clique-inserted graph [151]) of a graph was first introduced by Shirai [131], who obtained the spectrum of the paraline 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 paraline graph of an r-regular graph is the line graph of an $(r, 2)$-semiregular graph. It is clear that paraline graph of a regular r-graph is an r-regular graph.

The following result gives the L-spectrum of the graph $\mathscr{C}(G)$ in terms of the L-spectrum of the graph G.

Lemma 5.3.20. *If G is an r-regular graph with n vertices, then*

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

If $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of G, then from Lemma 5.3.20, it follows that the Laplacian spectrum of $\mathscr{C}(G)$ is $\{(r+2)^{m-n}, r^{m-n}, \frac{(r+2)\pm\sqrt{(r+2)^2-4\mu_i}}{2}\}$, where $i = 1, 2, \ldots, n$.

Now, we obtain the bounds for $LEL(\mathscr{C}(G))$ in terms of the number of vertices n, the number of edges m and the degree of regularity r of G.

Theorem 5.3.21. *Let G be a connected r-regular graph with n vertices. Then*

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

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

Proof. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the Laplacian eigenvalues of the graph G. Using the fact $\mu_i = r - \lambda_{n+i-1},\ i = 1, 2, \ldots, n$ and $\lambda_1 = r$, where λ_i are the adjacency eigenvalues of G, we have

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

By Perron-Frobenius Theorem [21], $-r \leq x < r$, for $i = 2, 3, \ldots, n$. For $-r \leq x < r$, consider the function

$$f(x) = \sqrt{\frac{(r + 2) + \sqrt{r^2 + 4x + 4}}{2}} + \sqrt{\frac{(r + 2) - \sqrt{r^2 + 4x + 4}}{2}}.$$

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

$$\begin{aligned} LEL(\mathscr{C}(G)) &> (m-n)\sqrt{r} + (m-n+1)\sqrt{r+2} + \sum_{i=2}^{n} \sqrt{r+2} \\ &= (m-n)\sqrt{r} + m\sqrt{r+2}, \end{aligned}$$

and

$$\begin{aligned} LEL(\mathscr{C}(G)) &\leq (m-n)\sqrt{r} + (m-n+1)\sqrt{r+2} + \sum_{i=2}^{n} (\sqrt{r} + \sqrt{2}) \\ &= (m-1)\sqrt{r} + (m-n+1)\sqrt{r+2} + (n-1)\sqrt{2}. \end{aligned}$$

Equality occurs 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. So G must be a complete graph. Note that the sum of the adjacency eigenvalues of G is equal to zero; that is, $r + (n-1)(-r) = 0$. It follows that G is a complete graph with two vertices; that is, $G \cong K_2$. $\square$

5.4 Kirchhoff index of a graph

As already pointed out, the Laplacian matrix $L(G)$ is singular and therefore has no inverse. In case of the singular matrices, instead of inverses (which do not exist) one can sometimes use the so-called generalized inverses. Several types of generalized inverses are known in the mathematical literature [13]. In the theory of electrical networks, the Moore-Penrose generalized inverse is encountered [13]. We outline it in some detail.

Let X be a real, symmetric square matrix of order n. Then the eigenvalues of X are real numbers. Let S_0 be the vector space, spanned by those eigenvectors of X whose eigenvalues are equal to zero. Let S_+ be the vector space, spanned by the eigenvectors of X whose eigenvalues are non zero. The Moore-Penrose generalized inverse of a matrix X is denoted by X^+. In case of the symmetric square matrices, X^+ is defined [13] so that $XX^+ = X^+X$ is an orthogonal projector on the vector space S_+. That is,

$$(XX^+)u = (X^+X)u = 0, \quad for\ all\ vectors\ u \in S_0,\ and$$
$$(XX^+)v = (X^+X)v = v, \quad for\ all\ vectors\ v \in S_+.$$

These two conditions uniquely determine Moore-Penrose generalized inverse X^+ of the matrix X. Using the theory of electric networks, Klein and Randić [91] showed that $Kf(G) = ntr(L^+)$, where $tr(L^+)$, denotes the trace of Moore-Penrose generalized inverse L^+ of the matrix $L(G)$. Using this, Gutman and Mohar [64] and Zhu et al. [161] in 1996 put forward the following definition.

Definition 5.3.1. *Kirchhoff index of a graph.* Let G be a connected graph of order n with m edges having Laplacian eigenvalues $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_2 \leq \mu_1$. The Kirchhoff index of G is denoted by $Kf(G)$ and is defined as

$$Kf(G) = n\sum_{j=1}^{n-1}\frac{1}{\mu_j}. \tag{5.10}$$

Various variations of *Kirchhoff index* $Kf(G)$ have been put forward of which the additive and multiplicative *Kirchhoff index* [26] have been mostly studied [66].

5.5 Bounds for Kirchhoff index

Various bounds for the *Kirchhoff index* $Kf(G)$ are known, which give its connection with the different parameters of a graph. Here, we list some of the well known bounds.

The following is a lower bound [158] for *Kirchhoff index* $Kf(G)$ as a function of the number of vertices n and vertex degrees d_i $i = 1, 2 \ldots, n$.

Theorem 5.5.1. *Let G be a graph with n vertices having vertex degrees d_i, $i = 1, 2, \ldots, n$. Then*

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

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

As for r-regular graph G, we have $d_i = r$ for all $i,\ i = 1, 2, \ldots, n$. Therefore, we have the following consequence of Theorem 5.5.1.

Corollary 5.5.2. *Let G be an r-regular graph with n vertices. Then*

$$Kf(G) \geq -1 + \frac{n(n-1)}{r},$$

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

The following is a lower bound [158] for *Kirchhoff index* $Kf(G)$ in terms of the number of vertices n, the number of edges m and maximum vertex degree Δ.

Theorem 5.5.3. *Let G be a connected graph with $n \geq 3$ vertices, m edges and maximum vertex degree Δ. Then*

$$Kf(G) \geq \frac{n}{\Delta + 1} + \frac{n(n-2)^2}{2m - \Delta - 1}, \tag{5.11}$$

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

Das et al. [33] obtained the following lower bound for *Kirchhoff index* $Kf(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ, second maximum degree Δ_2 and minimum degree δ, which is better than the lower bound (5.11).

Theorem 5.5.4. *Let G be a connected graph with $n \geq 3$ vertices, m edges, maximum degree Δ, second maximum degree Δ_2 and minimum degree δ. Then*

$$Kf(G) \geq \frac{n}{\Delta + 1} + \frac{n}{2m - \Delta - 1}\left((n-2)^2 + \frac{(\Delta_2 - \delta)^2}{\Delta_2 \delta}\right),$$

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

Indeed, the two bounds are same for regular graphs.

Let $G - e$ be the graph obtained from the graph G by deleting the edge e of G. Since the Laplacian eigenvalues of G and $G - e$ satisfy Interlacing property, so using Lemma 3.3.11, we have the following observation.

Theorem 5.5.5. *Let G be a connected graph and e be any edge in G. Then*

$$Kf(G-e) > Kf(G).$$

A repeated application of Theorem 5.5.5, shows that the path P_n has the maximal and complete graph K_n has the minimal Kirchhoff index over all the connected graphs G of order n, that is,

$$Kf(K_n) \leq Kf(G) \leq Kf(P_n).$$

As an application of Theorem 5.5.5, to bipartite graphs G [147, 148], we have the following observation.

Corollary 5.5.6. *Let G be a connected bipartite graph on n vertices having partite sets of cardinalities r and s with $r+s=n$. Then*

$$\frac{(r+s-1)(r^2+s^2)-rs}{rs} \leq Kf(G) \leq \frac{n(n^2-1)}{6},$$

with equality on the left if and only if $G \cong K_{r,s}$ and on the right if and only if $G \cong P_n$.

From this, it follows that, among connected bipartite graphs of order n, complete bipartite graph $K_{r,s}$ $r+s=n$ has the minimal and path P_n has the maximal *Kirchhoff index.*

We now obtain an upper bound for *Kirchhoff index* $Kf(G)$ in terms of the number of vertices n, the number of edges m, maximum degree Δ and a positive real number k.

Theorem 5.5.7. *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*

$$Kf(G) \leq \frac{n(\Delta+1)+nk(n-1)+n^2(n-2)-2mn}{k(\Delta+1)}, \tag{5.12}$$

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

Proof. Let $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_2 \leq \mu_1$ be the Laplacian spectrum of G with $\mu_{n-1} \geq k$.

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

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

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

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

that is, the function $f(x)$ is decreasing for $k \leq x$. Therefore,

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

implying

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

Equality occurs in (5.12) if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-2}$, $n = \mu_1 = \Delta + 1$ and $\mu_{n-1} = k$. That is, if G is the 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 the join of two graphs having three distinct Laplacian eigenvalues with $\mu_1 = \Delta + 1$, then by Lemma 5.3.15, $G \cong K_{1,n-1}$.

Conversely, if G is one of the graphs $K_{1,n-1}$ or K_n, then it is easy to see that equality occurs in (5.12). $\square$

The exact formulae for Kirchhoff index of various families of graphs (like cycles, complete graphs, geodetic graphs, distance transitive graphs etc) are known. The Kirchhoff index of certain composite operations between two graphs was studied, such as product, lexicographic product [146] and join, corona, cluster [150]. Kirchhoff index of graphs derived from a single graph, such as the line graph, the subdivision graph, the total graph were considered in [53].

We now obtain bounds for *Kirchhoff index* of some graphs derived from regular graphs.

Let $\mathscr{L}(G)$ be the line graph of the (r,s)-semiregular graph defined in Section 5.3. The following is the lower bound for $Kf(\mathscr{L}(G))$ in terms of the number of vertices n, the number of edges m and degrees of regularities r, s of the graph G.

Theorem 5.5.8. *Let G be an (r,s)-semiregular graph with n vertices. Then*

$$Kf(\mathscr{L}(G)) \geq \frac{m(m+n-1)}{r+s} + \frac{m(n-2)^2}{(n-1)(r+s)-2m},$$

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

Proof. Let $m = \frac{nrs}{r+s}$ be the number of edges in G. Since $\mu_1(G) = r+s$ and $\mu_n(G) = 0$, it follows by equation (5.10) and A.M-H.M inequality that

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

Equality occurs if and only if $r+s = \mu_1, \mu_2 = \mu_3 = \cdots = \mu_{n-1}$. Since G is (r,s)-semiregular graph, it follows by Lemma 5.3.17, G is either $K_{1,n-1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Conversely, if G is one of the graphs $K_{1,n-1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, then it is easy to see that equality occurs. $\square$

Since $\mu_{n-1}(\mathscr{L}(G)) > 1$, we have the following observation, which follows from Theorem 5.5.7.

Corollary 5.5.9. *Let G be an (r,s)-semiregular graph with n vertices. Then*

$$Kf(\mathscr{L}(G)) \leq n + \frac{n^3 - n^2 - n - 2mn}{r+1},$$

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

Let $\mathscr{C}(G)$ be the paraline graph of the graph G defined in Section 5.3. The following result gives the *Kirchhoff index* $Kf(\mathscr{C}(G))$ of the graph $\mathscr{C}(G)$ in terms of the *Kirchhoff index* $Kf(G)$ of the graph G.

Theorem 5.5.10. *If G is a connected r-regular graph with n vertices, then*

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

Proof. Let $\mathscr{C}(G)$ be the paraline graph of the r-regular graph G having n vertices and $m = \frac{nr}{2}$ edges. Then the number of vertices in $\mathscr{C}(G)$ is nr. Therefore, by (5.10), we have

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

$\square$

The following is an immediate consequence of Theorems 5.5.1 and 5.5.10.

Corollary 5.5.11. *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 $G \cong K_{\frac{n}{2},\frac{n}{2}}$, $\quad n$ even.

5.6 Relation between Laplacian-energy-like invariant and Kirchhoff index

In this Section, we consider the relation between two Laplacian spectrum based graph invariants, namely the *Laplacian-energy-like invariant $LEL(G)$* and *Kirchhoff index $Kf(G)$* of a graph G. As both these graph invariants are based on Laplacian spectrum, it is of interest to establish a relation between them. This problem was first considered by Das et al. [36]. Since for the complete graph K_n, the Laplacian spectrum is $\{n^{[n-1]}, 0\}$, we have

$$LEL(K_n) = (n-1)\sqrt{n} > n-1 = n\frac{(n-1)}{n} = Kf(K_n).$$

It is natural to raise the question, "*characterize the graphs G for which the relation $LEL(G) < Kf(G)$ or $LEL(G) > Kf(G)$ holds*". Das et al. [36] considered this question and established some sufficient condition for the relation $LEL(G) < Kf(G)$, to hold for a graph G. As a consequence to these sufficient conditions, the relations between $Kf(G)$ and $LEL(G)$ was completely solved for trees, unicyclic graphs, bicyclic graphs, tricyclic graphs, and tetracyclic graphs.

The following [36] is a sufficient condition for the inequality $LEL(G) < KF(G)$, in terms of number of vertices n, number of edges m and minimum degree δ of G.

Theorem 5.6.1. *Let G be a connected graph of order n with m edges and minimum degree δ. If $2m \leq (n-2)n^{\frac{2}{3}} + \delta$, then*

$$LEL(G) < Kf(G). \tag{5.13}$$

As, for a tree T, $m = n-1$, $\delta = 1$ and $2(n-1) \leq (n-2)n^{\frac{2}{3}} + 1$, for all $n \geq 4$, see [36], we have the following consequence of Theorem 5.6.1.

Corollary 5.6.2. *Let T be a tree of order n. Then $LEL(T) > Kf(T)$, for $n = 2$ and $LEL(T) < Kf(T)$, for all $n \geq 3$.*

As, for a unicyclic graph U, $m = n$, $\delta = 1$ *or* 2 and $2n \leq (n-2)n^{\frac{2}{3}} + 1$, for all $n \geq 6$, see [36], we have the following consequence of Theorem 5.6.1.

Corollary 5.6.3. *Let U be a unicyclic graph of order n. Then $LEL(U) > Kf(U)$, for $n = 3$ and $LEL(U) < Kf(U)$, for all $n \geq 4$.*

Similarly, using the facts, for a bicyclic graph B, $m = n+1$, $\delta \geq 1$ and $2(n+1) \leq (n-2)n^{\frac{2}{3}} + 1$, for $n \geq 6$, see [36]. For a tricyclic graph TC, $m = n+2$, $\delta \geq 1$ and $2(n+2) \leq (n-2)n^{\frac{2}{3}} + 1$, for $n \geq 7$, see [9], and for a tetracyclic graph QC, $m = n+3, \delta \geq 1$ and $2(n+3) \leq (n-2)n^{\frac{2}{3}} + 1$, for $n \geq 7$, see [9]. We have the following observations, which follow from Theorem 5.6.1.

Corollary 5.6.4. *Let B be a bicyclic graph of order n. Then $LEL(B) < Kf(B)$, except for $B \cong K_4 - e$.*

Corollary 5.6.5. *Let TC be a tricyclic graph of order n. Then $LEL(TC) < Kf(TC)$, except for $TC \cong H_{14},\ H_{16},\ H_{17},\ H_{18}$.*

Corollary 5.6.6. *Let QC be a tetracyclic graph of order n. Then $LEL(QC) < Kf(QC)$, except for $QC \cong H_{41},\ H_{42},\ H_{43},\ H_{44}$.*

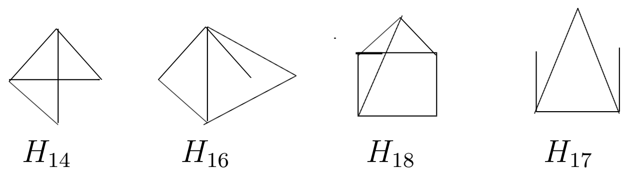
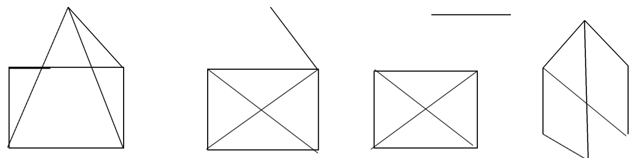


Figure 3: The tricyclic graphs of Corollary 5.6.5.



H_{41} H_{42} H_{43} H_{44}

Figure 4: The tetracyclic graphs of Corollary 5.6.6.

The following [36] is a sufficient condition for the inequality $LEL(G) < KF(G)$, in terms of the number of vertices n and the number of edges m of G.

Theorem 5.6.7. *Let G be a connected graph of order n with m edges. If $2m \leq (n-1)n^{\frac{2}{3}}$, then*

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

Let $Ki_{n,\omega}$ be the graph obtained by attaching a pendent path on $n-\omega$ vertices to a vertex of the complete graph on ω vertices and let $\Gamma_{n,k}$ be the class of graphs of order n obtained by attaching a pendent path on $n-k$ vertices to a vertex of a connected graph of order k. In particular, $Ki_{n,k} \in \Gamma_{n,k}$.

The following is a sufficient condition [36] for the inequality $LEL(G) < KF(G)$ in the class of graphs $\Gamma_{n,k}$.

Theorem 5.6.8. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq 1$. If $k^3 < (\frac{3n}{8}-2)^2(n-k)^2$, then*

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

Since, for $n \geq 12$, $(\frac{3n}{8}-2)^2 > \frac{n}{2}$, gives $(\frac{3n}{8}-2)^2(n-k)^2 > k^3$, if $k < \frac{n}{2}$, we have the following observation [36], which is immediate from Theorem 5.6.8.

Corollary 5.6.9. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq 2$. If $k < \frac{n}{2}$, $n \geq 12$, then*

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

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

Liu et al. [99] determined the nine graphs with the largest *Laplacian-energy-like invariant* among all connected graphs. In fact, they proved the following.

Theorem 5.6.10. *Let G be a connected graph of order $n \geq 6$ different from $K_n, G_1(n), G_2(n), G_3(n), G_4(n), G_5(n), G_6(n), G_7(n), G_8(n)$, then*

$$LEL(K_n) > LEL(G_1(n)) > LEL(G_2(n)) > LEL(G_3(n)) > LEL(G_4(n)) > \\ LEL(G_5(n)) > LEL(G_6(n)) > LEL(G_7(n)) > LEL(G_8(n)) > LEL(G).$$

Using a similar procedure, Das et al. [36] determined the nine graphs with smallest *Kirchhoff index* among all the connected graphs. In fact, they proved the following result.

Theorem 5.6.11. *Let G be a connected graph of order $n \geq 11$ different from $K_n, G_1(n), G_2(n), G_3(n), G_4(n), G_5(n), G_6(n), G_7(n), G_8(n)$, then*

$$Kf(K_n) < Kf(G_1(n)) < Kf(G_2(n)) < Kf(G_3(n)) < Kf(G_4(n)) < \\ Kf(G_5(n)) < Kf(G_6(n)) < Kf(G_7(n)) < Kf(G_8(n)) < Kf(G).$$

The following observation is immediate from Theorem 5.6.11 and Theorem 5.6.12 [9].

Corollary 5.6.12. *For any graph $G \in \{K_n, G_1(n), G_2(n), G_3(n), G_4(n), G_5(n), G_6(n), G_7(n), G_8(n)\}$, we have*

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

Let $G-e$ be the graph obtained by deleting the edge e of the graph G. If $G-e$ is connected, the next observation [9], follows from Theorem 5.3.3 and Theorem

5.5.5.

Theorem 5.6.13. *Let G be a connected graph and e be an edge in G, such that $G - e$ is connected. If $Kf(G) > LEL(G)$, then $Kf(G-e) > LEL(G-e)$.*

Let $G+e$ be the graph obtained from G by adding an edge e. Using the fact, Laplacian eigenvalues of $G+e$ and G interlace, we have the following observation [9].

Theorem 5.6.14. *Let G be a connected graph and e be an edge in G. If $Kf(G) < LEL(G)$, then $Kf(G+e) < LEL(G+e)$.*

The following is a lower bound for *algebraic connectivity* μ_{n-1} of G in terms of minimum degree δ [64].

Lemma 5.6.15. *Let $G \ncong K_n$ be a connected graph of order n and let δ be its smallest vertex degree. Then $\mu_{n-1} \leq \delta$.*

Let $\overline{G}$ be the complement of the graph G. The following result gives the relation between the Laplacian spectrum of $\overline{G}$ and the Laplacian spectrum of G [44].

Lemma 5.6.16. *If $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_1$, are the Laplacian eigenvalues of the graph G, then the Laplacian eigenvalues of its complement $\overline{G}$ are $0 = \mu_n < n - \mu_1 \leq n - \mu_2 \leq \cdots \leq n - \mu_{n-1}$.*

Das et al. [36] raised the reverse question, whether it is "possible to find a constant c (which may depend on the number of vertices n and maximum vertex degree Δ), such that for any connected graph G with $m \geq c$ edges, $LEL(G) > Kf(G)$ holds". We studied this problem and obtained various sufficient conditions for the relation $LEL(G) > Kf(G)$, to hold. As a consequence, to these sufficient conditions, the relations between $Kf(G)$ and $LEL(G)$ is completely solved for complements of trees, unicyclic graphs, bicyclic graphs, tricyclic graphs, and tetracyclic graphs.

The following is a sufficient condition for the inequality $LEL(G) > Kf(G)$, in terms of the number of vertices n, the number of edges m, maximum degree Δ of a graph G and a positive real number k.

Theorem 5.6.17. *Let G be a connected graph with algebraic connectivity $\mu_{n-1} \geq k$. Let m be the number of edges and Δ the maximum degree of G. If*

$$2m > \frac{k(\sqrt{n}+\sqrt{k})}{k+\sqrt{n}+\sqrt{k}} \left(\frac{(n+k)(n-1)}{k} - \frac{(n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}} \right) \tag{5.14}$$

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

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

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

Recall Lemma 5.6.15, for $k \leq x \leq \delta$, consider the function

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

for which

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

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

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

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

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

that is,

$$LEL(G) \geq \frac{2m + (n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}} \ . \tag{5.15}$$

We also have

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

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

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

resulting in

$$Kf(G) \leq \frac{(n+k)(n-1) - 2m}{k} \ . \tag{5.16}$$

Suppose that inequality (5.14) holds. By direct calculation, it can be transformed into

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

Bearing in mind the inequalities (5.15) and (5.16), it follows that $LEL(G) > Kf(G)$. □

In particular, if $\mu_{n-1} \geq 1$, then we have the following consequence of Theorem 5.6.17.

Corollary 5.6.18. *Let G be a connected graph G with algebraic connectivity $\mu_{n-1} \geq 1$. Let m be the number of edges and Δ the maximum degree of G. If*

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

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

Corollary 5.6.18 provides a partial answer to the question whether it is "possible to find a constant c (which may depend on the number of vertices n and maximum vertex degree Δ), such that for any connected graph G with $m \geq c$ edges, $LEL(G) > Kf(G)$ holds", raised by Das et al. in [36] .

Since a tree T of order n has minimum degree $\delta = 1$ and $m = n-1$ edges, we have the following observation.

Corollary 5.6.19. *Let T be a tree and $\overline{T}$ be its complement. If the order of T is $n \geq 12$ and $\Delta(T) \leq n-2$, then $LEL(\overline{T}) > Kf(\overline{T})$.*

Proof. Since any tree T of order n has minimum degree one and $n-1$ edges, it follows that $\Delta(\overline{T}) = n-2$ and $2m(\overline{T}) = (n-1)(n-2)$. Because of $\mu_1(T) \leq n-1$, by Lemma 5.6.16, $\mu_{n-1}(\overline{T}) = n - \mu_1(T) \geq 1$. Therefore,

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

if
$$n-2 > \left(\frac{(n+1)(\sqrt{n}+1)-\sqrt{n-1}}{\sqrt{n}+2}\right),$$
that is, $n+\sqrt{n-1} > 3\sqrt{n}+5$, which is true for $n \geq 13$.

Therefore, by Corollary 5.6.18, $LEL(\overline{T}) > Kf(\overline{T})$, for $n \geq 13$. Also for $n = 12$, it can be checked directly that $LEL(\overline{T}) > Kf(\overline{T})$. $\square$

As a unicyclic graph U of order n has minimum degree $\delta = 1$ or 2 and $m = n$ edges, we have the following observation.

Corollary 5.6.20. *Let U be a unicyclic graph and $\overline{U}$ its complement. If the order of U is $n \geq 14$ and $\Delta(U) \leq n-2$, then $LEL(\overline{U}) > Kf(\overline{U})$.*

As a bicyclic graph B of order n has minimum degree $\delta = 1$ *or* 2 and $m = n+1$ edges, we have the following observation.

Corollary 5.6.21. *Let B be a bicyclic graph and $\overline{B}$ its complement. If the order of B is $n \geq 15$ and $\Delta(B) \leq n-2$, then $LEL(\overline{B}) > Kf(\overline{B})$.*

Since a tricyclic graph of order n has minimum degree $\delta = 1$ *or* 2 *or* 3 and $m = n+2$ edges, we have the following observation.

Corollary 5.6.22. *Let TC be a tricyclic graph and $\overline{TC}$ its complement. If the order of TC is $n \geq 16$ and $\Delta(TC) \leq n-2$, then $LEL(\overline{TC}) > Kf(\overline{TC})$.*

Since a tetracyclic graph QC of order n has minimum degree $\delta \geq 1$ and $m = n+2$ edges, we have following observation.

Corollary 5.6.23. *Let QC be a tetracyclic graph and $\overline{QC}$ its complement. If the order of QC is $n \geq 17$ and $\Delta(QC) \leq n-2$, then $LEL(\overline{QC}) > Kf(\overline{QC})$.*

Let $\mathscr{L}(G)$ be the line graph of the graph G. The following is the lower bound [7] for largest Laplacian eigenvalue μ_1 of a graph G in terms of the largest vertex degree of its line graph $\mathscr{L}(G)$.

Lemma 5.6.24. *Let $0 = \mu_n < \mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_1$ be the Laplacian eigenvalues of the graph G and let $t_1 \geq t_2 \geq \cdots \geq t_n$ be the degree sequence of its line graph $\mathscr{L}(G)$. Then $\mu_1 \leq t_1 + 2$, with equality if and only if G is regular or semiregular bipartite.*

The next result gives a sufficient condition for the complement of a graph to satisfy the inequality $LEL(G) > Kf(G)$.

Theorem 5.6.25. *If G is a graph for which $\mu_1 < n - n^{2/3}$, then $LEL(\overline{G}) > Kf(\overline{G})$.*

Proof. Apply Lemma 5.6.16, we have

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

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

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

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

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

that is,

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

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

Remark 5.6.26. By Lemma 5.6.24, $\mu_1 \leq t_1 + 2$, where t_1 is the maximum vertex degree of the line graph $\mathscr{L}(G)$ of G. Then from Theorem 5.6.25, it follows $f(x) \geq f(t_1+2) = \frac{(n-t_1-2)^{3/2}-n}{n-t_1-2}$, which gives $LEL(\overline{G}) > Kf(\overline{G})$, if $t_1 < n - n^{2/3} - 2$.

Let $\Gamma_{n,k}$ be the family of graphs obtained by attaching a path on $n-k$ vertices to a graph of order k, we have the following consequence of Theorem 5.6.25.

Corollary 5.6.27. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq n^{2/3}+2$. Then $LEL(\overline{G}) > Kf(\overline{G})$.*

The complement $\overline{G}$ and line graph $\mathscr{L}(G)$ of an r-regular graph G are respectively, $(n-1-r)$-regular and $(2r-2)$-regular. The following result gives a sufficient condition for a regular graph and its complement to satisfy the inequality $LEL(G) > Kf(G)$.

Corollary 5.6.28. *Let $G \ncong K_n$ be an r-regular graph with n vertices. If $r < (n-n^{2/3})/2$, then $LEL(\overline{G}) > Kf(\overline{G})$. If $r > (n+n^{2/3}-2)/2$, then $LEL(G) > Kf(G)$.*

The following is another sufficient condition for a graph G to satisfy the inequality $LEL(G) > Kf(G)$.

Theorem 5.6.29. *For $p \geq 4$ and $1 \leq r \leq p$, let $K_p \vee \overline{K_r}$ be a spanning subgraph of a graph G of order $n = p+r$. Then $LEL(G) > Kf(G)$.*

Proof. The Laplacian spectrum of K_p and $\overline{K_r}$ are $\{p^{p-1}, 0\}$ and $\{0^r\}$, respectively. Therefore, by Lemma 3.4.15, the Laplacian spectrum of $K_p \vee \overline{K_r}$ is $\{(p+r)^p, p^{r-1}, 0\}$. This implies

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

and

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

resulting in $LEL(K_p \vee \overline{K_r}) \geq Kf(K_p \vee \overline{K_r})$. The result follows now from Theorem 5.6.14. $\square$

The Laplacian spectrum of the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ is $\left\{n, (\frac{n}{2})^{n-2}, 0\right\}$. For $n \geq 5$, this yields

$$Kf(K_{\frac{n}{2},\frac{n}{2}}) = 2n - 3 < \sqrt{n} + (n-2)\sqrt{\frac{n}{2}} = LEL(K_{\frac{n}{2},\frac{n}{2}}).$$

Using Theorem 5.6.14, we have the following observation.

Theorem 5.6.30. *If $K_{\frac{n}{2},\frac{n}{2}}$ is a spanning subgraph of a graph G of order n, then $Kf(G) < LEL(G)$, for all $n \geq 5$.*

5.7 Conclusion

Although we have solved the problem "is it possible to find a constant c (which may depend on the number of vertices n and maximum vertex degree Δ), such that for any connected graph G with $m \geq c$ edges, $LEL(G) > Kf(G)$" asked in [36] partially. It will be of interest in future to find more sufficient conditions for the inequality $LEL(G) > Kf(G)$.

CHAPTER 6

On the Laplacian energy of digraphs

In this chapter, we consider the Laplacian energy of digraphs. We mention different approaches of Laplacian energy of a digraph, put forward by different researchers. We will consider the skew Laplacian energy of a digraph as given in [22] and we obtain some bounds in this regard.

6.1 Introduction

Let $\mathscr{D}$ be a digraph with n vertices $v_1, v_2, \ldots, v_n$ and m arcs. Let $d_i^+ = d^+(v_i)$, $d_i^- = d^-(v_i)$ and $d_i = d_i^+ + d_i^-$, $i = 1, 2, \ldots, n$ be the outdegree, indegree and degree of the vertices of $\mathscr{D}$, respectively. The out-adjacency matrix $A^+(\mathscr{D}) = (a_{ij})$ of a digraph $\mathscr{D}$ is the $n \times n$ matrix, where $a_{ij} = 1$, if (v_i, v_j) is an arc and $a_{ij} = 0$, otherwise. The in-adjacency matrix $A^-(\mathscr{D}) = (a_{ij})$ of a digraph $\mathscr{D}$ is the $n \times n$ matrix, where $a_{ij} = 1$, if (v_j, v_i) is an arc and $a_{ij} = 0$, otherwise. It is clear that $A^-(\mathscr{D}) = (A^+(\mathscr{D}))^t$.

The skew adjacency matrix $S(\mathscr{D}) = (s_{ij})$ of a digraph $\mathscr{D}$ is the $n \times n$ matrix, where

$$s_{ij} = \begin{cases} 1, & \text{if there is an arc from } v_i \text{ to } v_j, \\ -1, & \text{if there is an arc from } v_j \text{ to } v_i, \\ 0, & \text{otherwise.} \end{cases}$$

It is clear that $S(\mathscr{D})$ is a skew symmetric matrix, so all its eigenvalues are zero or purely imaginary. The energy of the matrix $S(\mathscr{D})$ was considered in [2], and is defined as

$$E_s(\mathscr{D}) = \sum_{i=1}^{n} |\xi|,$$

where $\xi_1, \xi_2, \ldots, \xi_n$ are the eigenvalues of $S(\mathscr{D})$. This energy of a digraph $\mathscr{D}$ is called the skew energy by Adiga et al. [2]. For recent developments in the theory of skew energy, see the survey [97].

Let $D^+(G) = diag(d_1^+, d_2^+, \ldots, d_n^+)$, $D^-(G) = diag(d_1^-, d_2^-, \ldots, d_n^-)$ and $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex outdegrees, vertex indegrees and vertex degrees of $\mathscr{D}$, respectively.

In an effort to extend the concept of Laplacian energy to digraphs, Adiga and Smitha [4] in 2009, while following the definition of Laplacian energy by Lazic [95] put forward the skew Laplacian energy of a simple digraph $\mathscr{D}$, which is defined as

$$SLE_l(\mathscr{D}) = \sum_{i=1}^{n} \nu_i^2, \tag{6.1}$$

where $\nu_1, \nu_2, \ldots, \nu_n$ are the eigenvalues of the skew Laplacian matrix $SL(\mathscr{D}) = D(\mathscr{D}) - S(\mathscr{D})$ of $\mathscr{D}$. In analogy to Theorem 2 and 4 in [95], they obtained the following result.

Theorem 6.1.1.

(i) For any simple digraph $\mathscr{D}$ on n vertices whose vertex degrees are $d_1, d_2 \ldots, d_n$, $SLE_l(\mathscr{D}) = \sum\limits_{i=1}^{n} d_i(d_i + 1)$.

(ii) For any connected simple digraph $\mathscr{D}$ on $n \geq 2$ vertices, $2n-4 \leq SLE_l(\mathscr{D}) \leq n(n-1)(n-2)$, where the left equality holds if and only if $\mathscr{D}$ is the directed path on n vertices and the right equality holds if and only if $\mathscr{D}$ is the complete digraph on n vertices.

Theorem 6.1.1 shows that the skew Laplacian energy of a simple digraph defined in this way is independent of its orientation, which does not reflect the adjacency of the digraph. Being aware of this and the definition of Laplacian energy of a graph as put forward by Gutman and Zhou [65], Adiga and Khoshbakht [3] gave another definition of the skew Laplacian energy of a digraph as

$$SLE_g(\mathscr{D}) = \sum_{i=1}^{n} |\nu_i - \frac{2m}{n}|, \tag{6.2}$$

where $\nu_1, \nu_2, \ldots, \nu_n$ are the eigenvalues of the skew Laplacian matrix $SL(\mathscr{D}) = D(\mathscr{D}) - S(\mathscr{D})$ of $\mathscr{D}$. In analogy to the bounds for Laplacian energy of a graph established by Gutman et al. [65], they obtained the following result.

Theorem 6.1.2. *Let $\mathscr{D}$ be simple digraph with n vertices and m arcs. Assume that $d_1, d_2, \ldots, d_n$ are the vertex degrees and $\nu_1, \nu_2, \ldots, \nu_n$ are the eigenvalues of the skew Laplacian matrix $SL(\mathscr{D}) = D(\mathscr{D}) - S(\mathscr{D})$. Let $\gamma_i = \nu_i - \frac{2m}{n}$ and $|\gamma_1| \leq |\gamma_2| \leq \cdots \leq |\gamma_n| = k$. Then* *(i)* $2\sqrt{M} \leq SLE_g(\mathscr{D}) \leq \sqrt{2M_1 n}$.

(ii) $SLE_g(\mathscr{D}) \leq k + \sqrt{(n-1)(2M_1 - k^2)}$.

(iii) If $\mathscr{D}$ *has no isolated vertices, then* $SLE_g(\mathscr{D}) \leq 2M_1$, *where* $M = -m + \frac{1}{2}\sum_{i=1}^{n}(d_i - \frac{2m}{n})^2$ *and* $M_1 = M + 2m = m + \frac{1}{2}\sum_{i=1}^{n}(d_i - \frac{2m}{n})^2$.

In 2010, Kissani and Mizoguchi [89] introduced a different approach for the Laplacian energy for digraphs, in which only the outdegrees of the vertices are considered rather than both the outdegrees and indegrees. Let $\mathscr{D}$ be a digraph on n vertices and let $\nu_1, \nu_2, \ldots, \nu_n$ be the eigenvalues of the matrix $L^+(\mathscr{D}) = D^+(\mathscr{D}) - A^+(\mathscr{D})$. They [89] defined the Laplacian energy of a digraph $\mathscr{D}$ as

$$LE_k(\mathscr{D}) = \sum_{i=1}^{n} \nu_i^2, \tag{6.3}$$

and obtained the following result.

Theorem 6.1.3. *Let* $\mathscr{D}$ *be a digraph with* n *vertices and vertex out degrees* $d_1^+, d_2^+, \ldots, d_n^+$. *Then*

(i) If $\mathscr{D}$ *is a simple digraph, then* $LE_k(\mathscr{D}) = \sum_{i=1}^{n}(d_i^+)^2$.

(ii) If $\mathscr{D}$ *is a symmetric digraph,. then* $LE_k(\mathscr{D}) = \sum_{i=1}^{n} d_i^+(d_i^+ + 1)$.

Moreover, Kissani and Mizoguchi [89] established some relation between the Laplacian energy of a graph (as put forward by Lazic [95]) and the Laplacian energy $LE_k(\mathscr{D})$ of the corresponding digraph $\mathscr{D}$ and used the so-called minimization maximum out-degree (MMO) algorithm [10] to determine the digraphs with minimum Laplacian energy. The shortage of this definition is that it does not make use of the in-adjacency information of a digraph.

Recently (in 2013) Cai et al. [22] defined a new type of skew Laplacian matrix $\widetilde{SL}(\mathscr{D})$ of a digraph $\mathscr{D}$ as follows.

Let $D^+(\mathscr{D})$ and $D^-(\mathscr{D})$ respectively be the diagonal matrices of vertex outdegree and vertex indegree and let $A^+(\mathscr{D})$ and $A^-(\mathscr{D})$ respectively be the outadjacency and in-adjacency matrix of a digraph $\mathscr{D}$. If $A(G)$ is the adjacency matrix of the underlying graph G of the digraph $\mathscr{D}$, then it is clear that $A(G) =$

$A^+(\mathscr{D})+A^-(\mathscr{D})$ and $S(\mathscr{D}) = A^+(\mathscr{D}) - A^-(\mathscr{D})$, where $S(\mathscr{D})$ is the skew adjacency matrix of $\mathscr{D}$. Therefore, following the definition of Laplacian matrix of a graph, Cai et al. called the matrix

$$\begin{aligned}\widetilde{SL}(\mathscr{D}) &= (D^+(\mathscr{D}) - D^-(\mathscr{D})) - (A^+(\mathscr{D}) - A^-(\mathscr{D}))\\ &= \widetilde{D}(\mathscr{D}) - S(\mathscr{D}),\end{aligned}$$

where $\widetilde{D}(\mathscr{D}) = D^+(\mathscr{D}) - D^-(\mathscr{D})$, as the skew Laplacian matrix of the digraph $\mathscr{D}$. It is clear that the matrix $\widetilde{SL}(\mathscr{D})$ is not symmetric, so its eigenvalues need not be real. However, we have the following observation.

Theorem 6.1.4.

(i) $\nu_1, \nu_2, \ldots, \nu_n$ *are the eigenvalues of* $\widetilde{SL}(\mathscr{D})$*, then* $\sum\limits_{i=1}^{n} \nu_i = 0$.

(ii) 0 *is an eigenvalue of* $\widetilde{SL}(\mathscr{D})$ *with multiplicity* p*, where* p *is the number of components of* $\mathscr{D}$ *with all ones vector* $(1, 1, \ldots, 1)$ *as the corresponding eigenvector.*

Following the definition of matrix energy given by Nikifrov [110], Cai et al. [22] defined the skew Laplacian energy of a digraph $\mathscr{D}$, as the sum of the absolute values of the eigenvalues of the matrix $\widetilde{SL}(\mathscr{D})$ and obtained various bounds.

In this chapter, we will confine ourselves to the definition of Laplacian energy of a digraph given by Cai et al. [22].

6.2 Laplacian energy of digraphs

Definition 6.2.1. *Skew Laplacian energy of a digraph.* Let $\mathscr{D}$ be a digraph of order n with m arcs and having skew Laplacian eigenvalues $\nu_1, \nu_2, \ldots, \nu_n$. The skew Laplacian energy of $\mathscr{D}$ is denoted by $SLE(\mathscr{D})$ and is defined as

$$SLE(\mathscr{D}) = \sum_{j=1}^{n} |\nu_j|. \tag{6.4}$$

This concept was introduced in 2013 by Cai et al. [22]. The idea of Cai et al. was to conceive a graph energy like quantity for a digraph, that instead of skew adjacency eigenvalues is defined in terms of skew Laplacian eigenvalues and that hopefully would preserve the main features of the original graph energy. The definition of $SLE(\mathscr{D})$ was therefore so chosen that all the properties possessed by graph energy should be preserved.

A digraph $\mathscr{D}$ is said to be Eulerian if $d_i^+ = d_i^-$, for all $i = 1, 2, \ldots, n$. Therefore, for an Eulerian digraph $\mathscr{D}$, we always have $\widetilde{D}(\mathscr{D}) = 0$, which gives $\widetilde{SL}(\mathscr{D}) = -S(\mathscr{D})$. Using this, we have the following observation.

Theorem 6.2.1. *For an Eulerian digraph $\mathscr{D}$, $SLE(\mathscr{D}) = E_s(\mathscr{D})$, where $E_s(\mathscr{D})$ is the skew energy of $\mathscr{D}$.*

As an immediate consequence to Theorem 6.2.1, we have the following result.

Corollary 6.2.2. *For a directed cycle C_n, $SLE(C_n) = E_s(C_n)$, where $E_s(\mathscr{D})$ is the skew energy of $\mathscr{D}$.*

We show that every even positive integer is indeed the skew Laplacian energy of some digraph.

Theorem 6.2.3. *Every even positive integer $2(n-1)$ is the skew Laplacian energy of a directed star.*

Proof. Let $V(K_{1,n}) = \{v_1, v_2, \ldots, v_{n+1}\}$ be the vertex set of $K_{1,n}$. If v_{n+1} is the center of $K_{1,n}$, orient all the edges toward v_{n+1}. Then

$$S(K_{1,n}) = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ -1 & -1 & \cdots & -1 & 0 \end{pmatrix} \text{ and } \widetilde{D}(K_{1,n}) = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & -n \end{pmatrix}.$$

Therefore,

$$\widetilde{SL}(K_{1,n}) = \begin{pmatrix} 1 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & -1 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -1 \\ 1 & 1 & \cdots & 1 & -n \end{pmatrix}.$$

It is easy to see that the eigenvalues of this matrix are $\{-(n-1), 0, 1^{[n-1]}\}$, and so $SLE(K_{1,n}) = 2(n-1)$. On the other hand, if we orient the edges away from v_{n+1}, then it can be seen that $\widetilde{SL}(K_{1,n}) = \begin{pmatrix} -1 & 0 & \cdots & 0 & 1 \\ 0 & -1 & \cdots & 0 & 1 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 1 \\ -1 & -1 & \cdots & -1 & n \end{pmatrix}$, having eigenvalues $\{(n-1), 0, -1^{[n-1]}\}$, so $SLE(K_{1,n}) = 2(n-1)$. Thus, for a directed star $K_{1,n}$, we have $SLE(K_{1,n}) = 2(n-1)$. □

If all the edges of the star $K_{1,n}$ are oriented away from the center v_{n+1} except $k,\ 1 \leq k \leq n-1$, edges which are oriented towards the center v_{n+1}, then it can be seen that the skew Laplacian matrix of $K_{1,n}$ is

$$\widetilde{SL}(K_{1,n}) = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & 0 & \cdots & 0 & -1 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & \cdots & 0 & -1 \\ 0 & 0 & \cdots & 0 & -1 & \cdots & 0 & 1 \\ \vdots & \vdots & \cdots & 0 & 0 & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & -1 & 1 \\ 1 & 1 & \cdots & 1 & -1 & \cdots & -1 & n-2k \end{pmatrix}.$$

By direct calculation, it can be seen that the skew Laplacian characteristic polynomial of this matrix is $x(x-1)^{k-1}(x+1)^{n-k-1}\,(x^2-(n-2k)x+n-1)$ and so its eigenvalues are $\{0, 1^{[k-1]}, -1^{[n-k-1]}, \frac{n-2k+\sqrt{(n-2k)^2-4(n-1)}}{2}, \frac{n-2k-\sqrt{(n-2k)^2-4(n-1)}}{2}\}$. Therefore, $SLE(K_{1,n}) = n-2+\sqrt{(n-2k)^2-4(n-1)}$. Thus, using Theorem 6.2.3, we have
$SLE(K_{1,n}) = 2(n-1)$, if all the edges are oriented towards or away from the center, and $SLE(K_{1,n}) = n-2+\sqrt{(n-2k)^2-4(n-1)}$, otherwise, where $k,\ 1 \leq k \leq n-1$ is the number of edges oriented towards the center,
giving the complete description of the skew Laplacian energy of orientations of $K_{1,n}$. It is clear that unlike the skew energy of any orientation of $K_{1,n}$, which is same as the corresponding energy, the skew Laplacian energy of orientations of $K_{1,n}$ is not same as the corresponding Laplacian energy.

Moreover, it is also clear that any two orientations which contain edges directed from and directed to, the center of $K_{1,n}$ are mutually non cospectral digraphs.

6.3 Bounds for skew Laplacian energy

In this section, we mention some well known bounds for skew Laplacian energy $SLE(\mathscr{D})$, which gives its connection to various graph parameters.

For a digraph with n vertices, m arcs having vertex outdegrees d_i^+ and vertex indegrees d_i^-, $i = 1, 2, \ldots, n$, let $M = -m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^+ - d_i^-\right)^2$ and $M_1 = M + 2m = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^+ - d_i^-\right)^2$. Clearly, $M_1 \geq m$, with equality if and only if $\mathscr{D}$ is Eulerian.

The following bounds are obtained in the basic paper [22] for skew Laplacian energy $SLE(\mathscr{D})$ of a digraph $\mathscr{D}$, which are analogues to the corresponding bounds on Laplacian energy $LE(G)$.

Theorem 6.3.1. *Let $\mathscr{D}$ be a simple digraph possessing n vertices, m arcs and p components. Assume that d_i^+ and d_i^- respectively are the outdegree and indegree of the vertex v_i, $i = 1, 2, \ldots, n$ and $\nu_1, \nu_2, \ldots, \nu_n$ are the skew Laplacian eigenvalues of $\mathscr{D}$. Then*

$$2\sqrt{|M|} \leq SLE(\mathscr{D}) \leq \sqrt{2M_1(n-p)}. \tag{6.5}$$

Equality occurs on the left if and only if for each pair of $\nu_{i_1}\nu_{j_1}$ and $\nu_{i_2}\nu_{j_2}$ $(i_1 \neq j_1, i_2 \neq j_2)$, there exists a non-negative real number k such that $\nu_{i_1}\nu_{j_1} = k\nu_{i_2}\nu_{j_2}$; and for each pair of $\nu_{i_1}^2$ and $\nu_{i_2}^2$, there exists a non-negative real number l such that $\nu_{i_1}^2 = l\nu_{i_2}^2$. Equality occurs on the right if and only if $\mathscr{D}$ is 0-regular or for each $v_i \in V(\mathscr{D}), d_i^+ = d_i^-$, and the eigenvalues of $\widetilde{SL}(\mathscr{D})$ are $0^{[p]}, ai^{[\frac{n-p}{2}]}, -ai^{[\frac{n-p}{2}]} (a > 0)$.

As an immediate consequence to Theorem 6.3.1, we have the following result.

Corollary 6.3.2. *Let $\mathscr{D}$ be a simple digraph possessing p components $C_1, C_2, \ldots, C_p$. If $SLE(\mathscr{D}) = \sqrt{2M_1(n-p)}$, then each component C_i is Eulerian with odd number of vertices.*

Since $n-p \leq n$, we have the following consequence of Theorem 6.3.1.

Corollary 6.3.3. *For any simple digraph $\mathscr{D}$, $SLE(\mathscr{D}) \leq \sqrt{2M_1 n}$.*

If $\mathscr{D}$ has no isolated vertices, then $n \leq 2m$, and so $\sqrt{2M_1 n} \leq 2\sqrt{M_1 m} \leq 2M_1$. Thus we have the following observation.

Corollary 6.3.4. *For any simple digraph $\mathscr{D}$, $SLE(\mathscr{D}) \leq 2M_1$.*

We now obtain a Koolen type upper bound (see Theorem 2.3.6) for $SLE(\mathscr{D})$.

Theorem 6.3.5. *Let $\mathscr{D}$ be a simple connected digraph with n vertices, m arcs and p components. Assume that $t = |\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_{n-p}| \geq 0$, where $\nu_1, \nu_2, \ldots, \nu_{n-p}, 0^{[p]}$ are the eigenvalues of $\widetilde{SL}(\mathscr{D})$. Then*

$$SLE(\mathscr{D}) \leq t + \sqrt{(n-p-1)(2M_1 - t^2)}.$$

Equality occurs if and only if $\mathscr{D}$ is 0-regular or for each $v_i \in V(\mathscr{D}), d_i^+ = d_i^-$, and the eigenvalues of $\widetilde{SL}(\mathscr{D})$ are $0^{[p]}, ai^{[\frac{n-p}{2}]}, -ai^{[\frac{n-p}{2}]} (a > 0)$.

Proof. Let $\widetilde{SL}(\mathscr{D}) = (l_{ij})$. By Schur's triangularization theorem [82], there exists a unitary matrix U such that $U^*\widetilde{SL}(\mathscr{D})U = T$, where $T = (t_{ij})$ is an upper triangular matrix with diagonal entries $t_{ii} = \nu_i,\ i = 1, 2, \ldots, n$. Therefore,

$$\sum_{i,j=1}^{n} |l_{ij}|^2 = \sum_{i,j=1}^{n} |t_{ij}|^2 \geq \sum_{i=1}^{n} |t_{ii}|^2 = \sum_{i=1}^{n} |\nu_i|^2,$$

that is,

$$\sum_{i=1}^{n} |\nu_i|^2 \leq \sum_{i,j=1}^{n} |l_{ij}|^2 = \sum_{i,j=1}^{n} (d_i^+ - d_i^-)^2 + 2m = 2M_1. \tag{6.6}$$

Now, applying Cauchy-Schwarz's inequality to vectors $(|\nu_2|, |\nu_3|, \ldots, |\nu_{n-p}|)$

and $(1, 1, \ldots, 1)$ and using (6.6), we have

$$SLE(\mathscr{D}) - |\nu_1| = \sum_{i=2}^{n} |\nu_i| = \sum_{i=2}^{n-p} |\nu_i| \leq \sqrt{(n-p-1)\sum_{i=2}^{n-p} |\nu_i|^2}$$
$$= \sqrt{(n-p-1)\sum_{i=2}^{n} |\nu_i|^2} \leq \sqrt{(n-p-1)(2M_1 - |\nu_1|^2)}.$$

This gives,

$$SLE(\mathscr{D}) \leq t + \sqrt{(n-p-1)(2M_1 - t^2)}.$$

Equality case can be discussed similarly as in Theorem 6.3.1. □

The following arithmetic-geometric mean inequality can be found in [92].

Lemma 6.3.6. *If $a_1, a_2, \ldots, a_n$ are non-negative numbers, then*

$$n\left[\frac{1}{n}\sum_{j=1}^{n} a_j - \left(\prod_{j=1}^{n} a_j\right)^{\frac{1}{n}}\right] \leq n\sum_{j=1}^{n} a_j - \left(\sum_{j=1}^{n} \sqrt{a_j}\right)^2$$
$$\leq n(n-1)\left[\frac{1}{n}\sum_{j=1}^{n} a_j - \left(\prod_{j=1}^{n} a_j\right)^{\frac{1}{n}}\right].$$

Moreover equality occurs if and only if $a_1 = a_2 = \cdots = a_n$.

The following inequality was obtained by Furuichi [51].

Lemma 6.3.7. *For $a_1, a_2, \ldots, a_n \geq 0$ and $p_1, p_2, \ldots, p_n \geq 0$ such that $\sum\limits_{j=1}^{n} p_i = 1$,*

$$\sum_{j=1}^{n} a_j p_j - \prod_{j=1}^{n} a_j^{p_j} \geq n\lambda\left(\frac{1}{n}\sum_{j=1}^{n} a_j - \prod_{j=1}^{n} a_j^{\frac{1}{n}}\right),$$

where $\lambda = \min\{p_1, p_2, \ldots, p_n\}$. Moreover equality occurs if and only if $a_1 = a_2 = \cdots = a_n$.

For a connected digraph $\mathscr{D}$, let $K = \prod_{j=1}^{n-1} |\nu_j|$, where $|\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_{n-1}| \geq 0$ are the absolute values of the eigenvalues of $\widetilde{SL}(\mathscr{D})$.

We first obtain a lower bound for $SLE(\mathscr{D})$ in terms of the number of vertices n and the number K.

Theorem 6.3.8. *Let $\mathscr{D}$ be a simple connected digraph with n vertices and m arcs having skew Laplacian eigenvalues $\nu_1, \nu_2, \ldots, \nu_{n-1}, 0$ with $t = |\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_{n-1}| \geq 0.$. Then*

$$SLE(\mathscr{D}) \geq t + (n-2)K^{\frac{1}{n-1}} \left(\frac{K^{\frac{1}{2(n-1)(n-2)}}}{t^{\frac{1}{2n-4}}} - 1 \right), \tag{6.7}$$

with equality if and only if $t = |\nu_1| = |\nu_2| = \cdots = |\nu_{n-1}|$.

Proof. Setting $n = n-1$, $a_j = |\nu_j|$, for $j = 1, 2, \ldots, n-1$, $p_1 = \frac{1}{2(n-1)}, p_j = \frac{2n-3}{2(n-1)(n-2)}$, for $j = 2, 3, \ldots, n-1$ in Lemma 6.3.7, we have

$$\begin{aligned} &\frac{|\nu_1|}{2(n-1)} + \frac{2n-3}{2(n-1)(n-2)} \sum_{j=2}^{n-1} |\nu_j| - |\nu_1|^{\frac{1}{2(n-1)}} \prod_{j=2}^{n-1} |\nu_j|^{\frac{2n-3}{2(n-1)(n-2)}} \\ &\geq \frac{1}{2(n-1)} \sum_{j=1}^{n-1} |\nu_j| - \frac{1}{2} \prod_{j=1}^{n-1} |\nu_j|^{\frac{1}{n-1}}, \end{aligned}$$

that is,

$$\begin{aligned} &\frac{|\nu_1|}{2(n-1)} + \frac{2n-3}{2(n-1)(n-2)} \left(SLE(\mathscr{D}) - |\nu_1|\right) - |\nu_1|^{\frac{-1}{2(n-2)}} K^{\frac{2n-3}{2(n-1)(n-2)}} \\ &\geq \frac{1}{2(n-1)} SLE(\mathscr{D}) - \frac{1}{2} K^{\frac{1}{n-1}}, \end{aligned}$$

this gives,

$$SLE(\mathscr{D}) \geq 2(n-2) \left(\frac{|\nu_1|}{2(n-1)} + \frac{K^{\frac{2n-3}{2(n-1)(n-2)}}}{|\nu_1|^{\frac{1}{2(n-2)}}} - \frac{1}{2} K^{\frac{1}{n-1}} \right),$$

from this the result follows.

Equality occurs in (6.7) if and only if equality occurs in Lemma 6.3.7, that is if and only if $t = |\nu_1| = |\nu_2| = \cdots = |\nu_{n-1}|$. $\square$

We now obtain the bounds for $SLE(\mathscr{D})$ in terms of the number of vertices n, the numbers $K,\ M$ and M_1.

Theorem 6.3.9. *Let $\mathscr{D}$ be a simple connected digraph with n vertices and m arcs having skew Laplacian eigenvalues $\nu_1, \nu_2, \ldots, \nu_{n-1}, 0$ with $|\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_{n-1}| \geq 0$. Then*

$$\sqrt{2|M| + (n-1)(n-2)K^{\frac{2}{n-1}}} \leq SLE(\mathscr{D}) \leq \sqrt{2M_1(n-2) + (n-1)K^{\frac{2}{n-1}}}, \tag{6.8}$$

with equality on the left if and only if for each pair $\nu_{i_1}^2$ and $\nu_{i_2}^2$, there exists a non-negative real number l such that $\nu_{i_1}^2 = l\nu_{i_2}^2$ and the equality on right occurs if and only if $\mathscr{D}$ is 0-regular or for each $v_i \in V(\mathscr{D}), d_i^+ = d_i^-$, and the eigenvalues of $\widetilde{SL}(\mathscr{D})$ are $0^{[p]}, ai^{[\frac{n-p}{2}]}, -ai^{[\frac{n-p}{2}]} (a > 0)$.

Proof. Setting $n = n-1$ and $a_j = |\nu_j|^2$, for $j = 1, 2, \ldots, n-1$ in Lemma 6.3.6, we have

$$\alpha \leq (n-1)\sum_{j=1}^{n-1}|\nu_j|^2 - \left(\sum_{j=1}^{n-1}|\nu_j|\right)^2 \leq (n-2)\alpha,$$

that is,

$$\alpha \leq (n-1)\sum_{j=1}^{n-1}|\nu_j|^2 - (SLE(\mathscr{D}))^2 \leq (n-2)\alpha, \tag{6.9}$$

where

$$\begin{aligned}\alpha &= (n-1)\left[\frac{1}{n-1}\sum_{j=1}^{n-1}|\nu_j|^2 - \left(\prod_{j=1}^{n-1}|\nu_j|^2\right)^{\frac{1}{n-1}}\right]\\ &= \sum_{j=1}^{n-1}|\nu_j|^2 - (n-1)\left(\prod_{j=1}^{n-1}|\nu_j|\right)^{\frac{2}{n-1}}\\ &= \sum_{j=1}^{n-1}|\nu_j|^2 - (n-1)K^{\frac{2}{n-1}}.\end{aligned}$$

Using (6.6) and the value of α, we have from the left inequality of (6.9)

$$(SLE(\mathscr{D}))^2 \leq (n-2)\sum_{j=1}^{n-1} |\nu_j|^2 + (n-1)K^{\frac{2}{n-1}},$$

that is,

$$SLE(\mathscr{D}) \leq \sqrt{2M_1(n-2) + (n-1)K^{\frac{2}{n-1}}},$$

this proves the right inequality.

Now, using (7) from [22] (Theorem 3.1) and the value of α, we have from the right inequality of (6.9)

$$(SLE(\mathscr{D}))^2 \geq \sum_{j=1}^{n-1} |\nu_j|^2 + (n-1)(n-2)K^{\frac{2}{n-1}},$$

that is,

$$SLE(\mathscr{D}) \geq \sqrt{2|M| + (n-1)(n-2)K^{\frac{2}{n-1}}},$$

this proves the left inequality.

Equality case can be discussed similarly as in Theorem 6.3.1. □

Remark 6.3.10. The upper bound given by Theorem 6.3.9, is better than the upper bound given by Theorem 6.3.1 for all connected digraphs $\mathscr{D}$. As by arithmetic-geometric mean inequality, we have

$$2M_1 \geq \sum_{j=1}^{n-1} |\nu_j|^2 \geq (n-1)\left(\prod_{j=1}^{n-1} |\nu_j|\right)^{\frac{2}{n-1}} = (n-1)K^{\frac{2}{n-1}},$$

adding $2M_1(n-2)$ on both sides, we obtain

$$2M_1(n-1) \geq 2M_1(n-2) + (n-1)K^{\frac{2}{n-1}},$$

from which the result follows.

Remark 6.3.11. The lower bound given by Theorem 6.3.9, is better than the lower bound given by Theorem 6.3.1 for all connected digraphs $\mathscr{D}$, with $2|M| \leq (n-1)(n-2)K^{\frac{2}{n-1}}$.

6.4 Conclusion

We conclude this chapter with the following problems, which will of interest for the future research.

Problem 6.4.1. *Interpret all the coefficients of the characteristic polynomial of* $\widetilde{SL}(\mathscr{D})$ *in terms of* $\mathscr{D}$.

Problem 6.4.2. *Establish the possible relations between the largest and smallest skew Laplacian eigenvalue of a digraph* $\mathscr{D}$ *with the parameters associated with the digraph.*

Problem 6.4.3. *Establish the possible relations between the skew Laplacian spectrum of a digraph* $\mathscr{D}$ *and the Laplacian spectrum of the corresponding underlying graph* $G_{\mathscr{D}}$.

Problem 6.4.4. *For any orientation, give the complete description for the skew Laplacian energy of the cycle* C_n.

Problem 6.4.45. *Characterise all the non-Eulerian digraphs* $\mathscr{D}$ *for which* $SLE(\mathscr{D}) = E_s(\mathscr{D})$.

Problem 6.4.6. *If possible, interpret skew Laplacian energy in chemistry and other disciplines.*

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