

Variable Sum Exdeg Energy of Graphs



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Dedicated to my Baba and
Mama

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Abstract

In mathematical chemistry, a topological index of a graph is a molecular descriptor which is obtained for a chemical compound from its molecular graph. This graph invariant is a numerical parameter used to characterize the graph topology. The study of energy of a graph was introduced in 1978 by Gutman. Recently, the study on topological indices has gained a lot of significance and is extensively studied concept in spectral graph theory.

Variable Sum exdeg index SEI_ν is the graph property first studied by Vukičević. The author studied the extremal graphs among different classes with respect to SEI_ν , for $\nu > 1$ and the polynomial form of this graph is also introduced. In this thesis the concept of variable sum exdeg energy of graphs is established. The algebraic properties of variable sum exdeg energy of a graph are studied. Some properties related to spectral radius of variable sum exdeg matrix are determined. Nordhaus-Gaddum type results for variable sum exdeg energy and spectral radius are given. Some classes of variable sum exdeg equienergetic graphs are also obtained.

Introduction

Graph Theory is a field of modern mathematics and it has vast range of applications in computer science, genetics, biochemistry, industry, communication science, business, engineering, linguistics, sociology, physics, social sciences and in psychology. It is an advanced field of modern era which is introduced for addressing challenging problems which are very difficult to handle with conventional branches of mathematics such as calculus or algebra. Several other branches of mathematics for example matrix computation, group theory, topology and probability are interconnected with graph theory.

Spectral graph theory is the study of graph properties by means of eigenvalues of a matrix associated to the graph. A matrix associated to a graph can be adjacency matrix, Laplacian matrix, signless Laplacian matrix, incidence matrix and many more. Spectral graph theory was introduced in mid 1900s and has a long history. Till date a lot work has been done on algebraic aspects on spectral graph theory and a lot of literature is available in different papers and books such as , “An Introduction to the Theory of Graph Spectra” (2010), “Algebraic Graph Theory”(1974), “A Textbook of Graph Theory” (2012) etc.

The study of energy of a graph originated from theoretical chemistry in 1978. Ivan Gutman gave the idea of this spectral property of a graph in his paper “The energy of a graph” [19]. It is helpful in determining the total π -electron energy of a molecular compound given by a graph. The roots of this graph invariant go back to the 1940s and a lot of work has been done so far.

The study of topological indices of graphs was established in 1947, when first topological index Wiener index was studied. It is a molecular descriptor which is applied to a molecular structure to convert it into some real number. Topological index is a graph invariant which under graph isomorphism is constant. Many applications of this molecular descriptor are found in theoretical chemistry. This study was extended and related to energy of a graph when Randić energy was defined in 2010.

In 2011 Vukičević defined and introduced Variable sum exdeg index. In this thesis some preliminaries and notations of graph theory are given and some helpful results are included. Some previously done work related to the topic is studied. Some algebraic characteristics of variable sum exdeg index are discussed. The variable sum exdeg energy of some particular graphs is obtained. Moreover, the bounds for variable sum exdeg energy are calculated. Lastly, some results about noncospectral graphs with same variable sum exdeg energy are established.

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Chapter 1

Fundamentals of graph theory

This chapter comprises of basic ideas about graphs and contains some definitions and notations related to graph theory. Various important types of graphs are defined and different basic operations on graphs are discussed.

1.1 Introduction to graphs

Graph is a mathematical diagram that is modeled to depict network of objects and relation or correspondence between them. An ordered triple comprising of finite and disjoint vertex set, edge set and an incidence function, usually represented as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \psi)$ is known as a graph \mathcal{G} . Here in this triple, \mathcal{V} refers to the non-empty, finite set containing vertices (or nodes), \mathcal{E} represents collection of edges (also called links or lines) and ψ is the relation that joins an edge with vertices, that is, it provides with the condition that when two vertices will be adjacent. To make it more convenient it is often rephrased as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. The order (represented by n) of a graph \mathcal{G} is the cardinality of vertex set $\mathcal{V}(\mathcal{G})$, that is, $n = |\mathcal{V}(\mathcal{G})|$, and the number of elements in $\mathcal{E}(\mathcal{G})$ is size (represented by m) of \mathcal{G} , that is, $m = |\mathcal{E}(\mathcal{G})|$.

1.2 Basic definitions and concepts

An edge e linking two vertices, say x and w , of vertex set of a graph \mathcal{G} is an unordered pair written as $e = \{x, w\}$ or simply xw and x and w are called endpoints of the edge xw . If two distinct vertices are endpoints of an edge then they are termed as adjacent vertices; otherwise they are called non-adjacent vertices.

Two edges from $\mathcal{E}(\mathcal{G})$ are said to be adjacent if they are incident on one vertex. Multiple edges are edges which are incident on same end vertices. Loop is an edge which ends at the same vertex from which it begins. A graph free from multiple edges and loops is called simple graph; otherwise it is called multi-graph.

The subset of vertex set $\mathcal{V}(\mathcal{G})$ containing all such vertices that are linked to a vertex $a \in \mathcal{V}(\mathcal{G})$, is termed neighbourhood of a (often written as $N_{\mathcal{G}}(a)$ or simply $N(a)$). The cardinality of neighbourhood of a vertex, say a , is termed as its degree, given by $d_{\mathcal{G}}(a) = |N_{\mathcal{G}}(a)|$, it is often represented by $d(a)$ if there is no ambiguity. A vertex a is a leaf (or pendant vertex) if it is neighbour to only one vertex, that is, $d(a) = 1$ and it is known as an isolated vertex if the number of vertices linked to it is zero, that is, $d(a) = 0$.

A graph is stated as connected if between every two distinct vertices there is a path that connects them. Also, in a connected graph there is no isolated vertex. A graph is called disconnected if it is not connected. A disconnected graph comprises of atleast two or more components.

A graph can be both directed or undirected, in a directed graph (or digraph), all the edges have certain direction from one vertex to another and in an undirected graph edges are directed in both ways. Usually, by a graph in this dissertation we mean a simple, undirected and connected graph, unless mentioned otherwise.

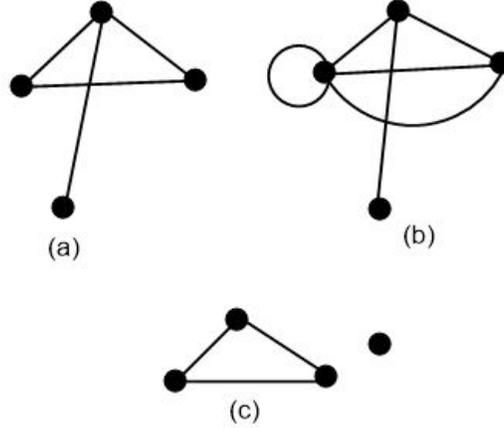


Figure 1.1: Graph $\mathcal{G}(\mathcal{V}(\mathcal{G}), \mathcal{E}(\mathcal{G}))$

Example 1.2.1. *The Figure 1.1(a) demonstrates a graph that is simple, undirected and connected without loops and multiple edges. In (b) the graph is not simple as it contains a loop and multiple edges. In (c) the graph is disconnected with one leaf vertex.*

Definition 1.2.2. *A subset, say $I(\mathcal{G})$, of vertex set $\mathcal{V}(\mathcal{G})$ containing pairwise non-adjacent vertices is called independent set of \mathcal{G} . The cardinality of largest possible independent set is known as independence number of \mathcal{G} .*

Definition 1.2.3. *The maximum degree (represented by $\Delta(\mathcal{G})$) of a graph is maximum value of all the degrees of vertices in \mathcal{G} and mathematically it is defined as*

$$\Delta(\mathcal{G}) = \max\{d_{\mathcal{G}}(v_i) \mid v_i \in \mathcal{V}(\mathcal{G})\}.$$

Definition 1.2.4. *The minimum degree (expressed as $\delta(\mathcal{G})$) of a graph is the smallest value of all the degrees of vertices in \mathcal{G} , mathematically it is defined as*

$$\delta(\mathcal{G}) = \min\{d_{\mathcal{G}}(v_i) \mid v_i \in \mathcal{V}(\mathcal{G})\}.$$

The following is a well-known theorem in graph theory usually called

handshaking lemma which tells us that the sum of degrees of all vertices in a graph equals twice the size of graph.

Theorem 1.2.5 (Vasudev [4]). *For a graph of size m and order n , we have*

$$\sum_{v_i \in V(\mathcal{G})} (d_{\mathcal{G}}(v_i)) = 2m.$$

The above stated result is also referred as **degree-sum formula**.

A vertex is considered to be even (resp., odd) if the number of vertices adjacent to it are even (resp., odd).

The corollary given below is consequence of Theorem 1.2.5.

Corollary 1.2.6 (Vasudev [4]). *In a graph the vertices that are of odd degree are always even in number.*

The next corollaries tells the largest number of edges and largest possible degree of a vertex, respectively, in any simple graph \mathcal{G} .

Corollary 1.2.7 (Vasudev [4]). *The maximum possible number of edges in a simple graph on n vertices is $\frac{n(n-1)}{2}$.*

Corollary 1.2.8 (Vasudev [4]). *The largest possible degree of a vertex in a simple n -vertex graph is $n - 1$.*

The results given below represent the relation of maximum degree of a graph \mathcal{G} with its minimum degree.

Corollary 1.2.9 (Diestel [37]). *If the maximum and minimum degrees of a graph \mathcal{G} of vertex set of size n and edge set of size m are $\Delta(\mathcal{G})$ and $\delta(\mathcal{G})$ respectively, then we have*

$$\delta(\mathcal{G}) \leq \frac{2m}{n} \leq \Delta(\mathcal{G}).$$

Corollary 1.2.10 (Chartrand [14]). *If z is a vertex of a graph \mathcal{G} with vertex set of size n then it is given that,*

$$0 \leq \delta(\mathcal{G}) \leq d_{\mathcal{G}}(z) \leq \Delta(\mathcal{G}) \leq n - 1.$$

1.3 Types of graphs

In this section few basic types of graphs are defined and their notations are mentioned. Some results and remarks about them are also given.

A walk is a simple graph of alternating and finite sequence of vertices and edges, It is written as

$$\mathcal{W} = v_0, e_1, v_1, \dots, e_n, v_n,$$

where $e_k = v_{k-1}v_k$, for $1 \leq k \leq n$. The vertices in a walk need not to be necessarily distinct. The repetition of vertices and edges is allowed in walk. The above mentioned walk is called v_0, v_n -walk. If the edges of a walk do not repeat then it is called v_0, v_n -trail. In a trail, vertices are allowed to repeat. If no vertex is repeating in a trail then it is called a path. The notation used for path of n vertices is \mathcal{P}_n . There are only two pendant vertices in path and all others are of degree two.

A trail $v_0, e_1, v_1, \dots, e_n, v_n$ with $v_0 = v_n$ (same end vertices) is called a closed trail or circuit. A closed circuit with no repetition of vertices except the first and last one is called cycle. The common representation for n -vertex cycle is C_n ($n \geq 3$). For C_n , $d_{C_n}(v_i) = 2$ for all $v_i \in \mathcal{V}(C_n)$. The length of cycle, walk, trail and path is its number of edges. The length of a path \mathcal{P}_n is $n - 1$ and for cycle C_n it is n and $|\mathcal{E}(C_n)| = |\mathcal{V}(C_n)| = n$. A cycle C_n is even or odd when n is even or odd respectively.

A graph that does not contain cycle is an acyclic graph. An acyclic graph (not necessarily connected) is called a forest and an acyclic connected graph is called tree. A tree of order n is expressed as T_n and it comprises of $n - 1$ edges.

If for a simple n -vertex graph \mathcal{G} , each vertex is neighbour of every other vertex in $\mathcal{V}(\mathcal{G})$ then such a graph is termed as a complete graph \mathcal{K}_n .

The corollary stated next tells about the number of edges and degree of vertices in a complete graph.

Remark 1.3.1. In a simple complete graph with vertex set of size n , $d_{\mathcal{K}_n}(v_i) = n - 1$, for all $v_i \in \mathcal{V}(\mathcal{K}_n)$, and the cardinality of $\mathcal{E}(\mathcal{K}_n)$ is $\frac{n(n-1)}{2}$.

If a vertex set of graph \mathcal{G} can be split into two disjoint and independent sets, say \mathcal{X}_1 and \mathcal{X}_2 (called partite sets), so that every edge of graph has one end-vertex in \mathcal{X}_1 and other end-vertex in \mathcal{X}_2 , then such a graph is called bipartite graph.

If in a bipartite graph with partite sets \mathcal{X}_1 and \mathcal{X}_2 , every vertex of \mathcal{X}_1 is linked to each vertex of \mathcal{X}_2 , then such a graph is termed as complete bipartite graph. If $|\mathcal{V}(\mathcal{X}_1)| = \mathcal{s}$ and $|\mathcal{V}(\mathcal{X}_2)| = \mathcal{z}$, then complete bipartite graph is given by $\mathcal{K}_{\mathcal{s},\mathcal{z}}$.

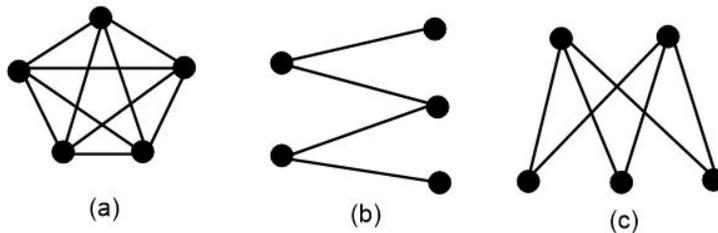


Figure 1.2: (a) Complete graph (\mathcal{K}_5) (b) Bipartite graph (c) Complete Bipartite Graph ($\mathcal{K}_{2,3}$).

Theorem 1.3.1 (Vasudev [4]). In a bipartite graph all the cycles are of even length.

Also, if it is possible for a graph to split its vertex set into \mathcal{s} partite sets, then such a graph is termed as \mathcal{s} -partite graph.

A star of order n , denoted by \mathcal{S}_n , is a graph with one central vertex adjacent to $n - 1$ pendant vertices. A star with vertex set of size n is a complete bipartite graph and hence it may be expressed as $\mathcal{K}_{n-1,1}$.

If in a graph \mathcal{G} the number of vertices connected to every vertex is \mathcal{s} , that

is, $d_{\mathcal{G}}(a) = s$ for every $a \in \mathcal{V}(\mathcal{G})$, then \mathcal{G} is known as s -regular graph. Note that, $\Delta(\mathcal{G}) = \delta(\mathcal{G}) = s$ for a s -regular graph \mathcal{G} .

Remark 1.3.2. (1). An s -regular graph with vertex set of size n has $\frac{1}{2}(ns)$ edges.

(2). Every cycle C_n is 2-regular.

(3). A complete graph \mathcal{K}_n is $(n - 1)$ -regular.

A line graph, represented by $\mathcal{L}_{\mathcal{G}}$, of a \mathcal{G} is another graph comprising of set of vertices $\mathcal{V}(\mathcal{L}_{\mathcal{G}}) = \mathcal{E}(\mathcal{G})$ and its edges are defined as: for every pair of edges in \mathcal{G} having a common vertex there is an edge in $\mathcal{L}_{\mathcal{G}}$ between their corresponding vertices. Note that a line graph of \mathcal{G} is a simple graph in any case.

Remark 1.3.3. (1). Line graph of a star of order n is a complete graph with vertex set of size $n - 1$, that is, $\mathcal{L}_{\mathcal{K}_{1,n-1}} = \mathcal{K}_{n-1}$.

(2). If \mathcal{G} is a path \mathcal{P}_n , then $\mathcal{L}_{\mathcal{P}_n}$ is the path \mathcal{P}_{n-1} .

(3). For a cycle C_n , the line graph is again a cycle C_n .

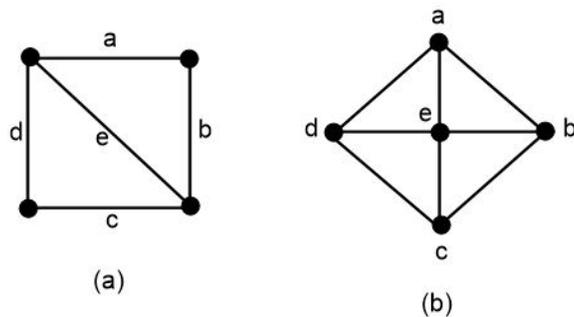


Figure 1.3: The graph in (b) is Line graph $\mathcal{L}_{\mathcal{G}}$ of graph \mathcal{G} in (a)

1.4 Operations on graphs

Graph operations create a new graph from the existing one by defining some basic or advanced changes in the graph. In this section few graph operations are discussed and elaborated with examples.

Definition 1.4.1. *The complement of a simple graph \mathcal{G} , given by $\overline{\mathcal{G}}$, is the graph having the same vertex set as \mathcal{G} , that is, $\mathcal{V}(\overline{\mathcal{G}}) = \mathcal{V}(\mathcal{G})$, and two vertices are connected by an edge in $\overline{\mathcal{G}}$ if and only if they are not connected in \mathcal{G} .*

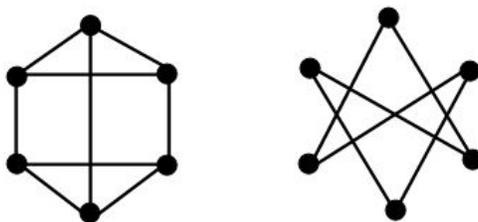


Figure 1.4: A graph \mathcal{G} and its complement $\overline{\mathcal{G}}$.

Remark 1.4.2. (1) *The complement of \mathcal{K}_n is a graph comprising of n isolated vertices.*

(2) $\overline{\overline{\mathcal{G}}} = \mathcal{G}$.

(3) *If complement of a graph is isomorphic to itself then such a graph is called self-complementary.*

Definition 1.4.3. *Let us consider graphs \mathcal{D}_1 and \mathcal{D}_2 with disjoint vertex sets $\mathcal{V}(\mathcal{D}_1)$ and $\mathcal{V}(\mathcal{D}_2)$. Then the **union** of graphs $\mathcal{D}_1 \cup \mathcal{D}_2$ is a graph with vertex set $\mathcal{V}(\mathcal{D}_1) \cup \mathcal{V}(\mathcal{D}_2)$ and edge set $\mathcal{E}(\mathcal{D}_1) \cup \mathcal{E}(\mathcal{D}_2)$. And, also $d_{\mathcal{D}_1 \cup \mathcal{D}_2}(a) = d_{\mathcal{D}_1}(a)$ if $a \in \mathcal{V}(\mathcal{D}_1)$ and $d_{\mathcal{D}_1 \cup \mathcal{D}_2}(a) = d_{\mathcal{D}_2}(a)$ if $a \in \mathcal{V}(\mathcal{D}_2)$.*

Definition 1.4.4. *Let $\mathcal{V}(\mathcal{G})$ be the set containing vertices of a graph \mathcal{G} and consider a set \mathcal{W} for which $\mathcal{V}(\mathcal{G}) \cap \mathcal{W} = \phi$ and $|\mathcal{V}(\mathcal{G})| = |\mathcal{W}|$. Suppose $t : \mathcal{V}(\mathcal{G}) \rightarrow \mathcal{W}$ be a bijection, that is, for $a \in \mathcal{V}(\mathcal{G})$, $t(a) = \acute{a}$. The **duplication***

of \mathcal{G} , represented by \mathcal{G}^* , is the graph with $\mathcal{V}(\mathcal{G}^*) = \mathcal{V}(\mathcal{G}) \cup \mathcal{W}$ and $e_1e_2 \in \mathcal{E}(\mathcal{G})$ if and only if $e_1e_2 \in \mathcal{E}(\mathcal{G})^*$ and $e_1e_2 \in \mathcal{E}(\mathcal{G}^*)$, where $e_1, e_2 \in \mathcal{V}(\mathcal{G})$ and $e_1, e_2 \in \mathcal{V}(\mathcal{G}^*)$.

Definition 1.4.5. Consider a graph \mathcal{G} and let $\mathcal{V}(\mathcal{G})$ be its vertex set. Let $\mathcal{G}_1, \mathcal{G}_2, \dots, \mathcal{G}_q$ be q copies of \mathcal{G} with vertex sets $\mathcal{V}^1(\mathcal{G}_1), \mathcal{V}^2(\mathcal{G}_2), \dots, \mathcal{V}^q(\mathcal{G}_q)$. Let $\mathcal{V}^l(\mathcal{G}_l) = \{v_{1l}, v_{2l}, \dots, v_{ml}\}$, $l = 1, \dots, q$ and v_{il} represents the vertex on i th position in l th copy of graph \mathcal{G} and $i = 1, \dots, m$. The q -double graph \mathcal{G}^q of \mathcal{G} is the graph with the vertex set $\mathcal{V}(\mathcal{G}^q) = \mathcal{V}^1(\mathcal{G}_1) \cup \dots \cup \mathcal{V}^q(\mathcal{G}_q)$ and its edges includes initial edges of \mathcal{G} and remaining edges are defined as $x_1x_2 \in \mathcal{E}(\mathcal{G})$ (where $x_1, x_2 \in \mathcal{V}(\mathcal{G})$) if and only if $v_{1l}v_{2k} \in \mathcal{E}(\mathcal{G}^q)$ with $l \neq k$, and $k = 1, \dots, q$.

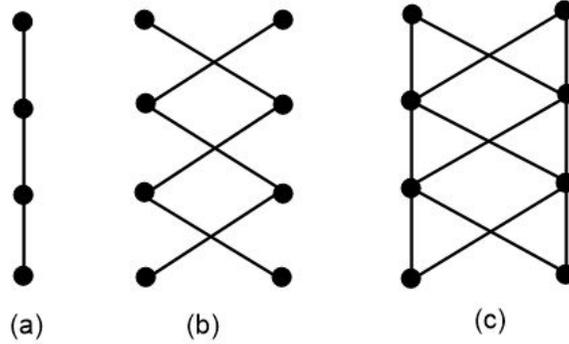


Figure 1.5: (a) \mathcal{P}_4 (b) \mathcal{P}_4^* (Duplication of \mathcal{P}_4) (c) \mathcal{P}_4^2 (2-double graph of \mathcal{P}_4)

Chapter 2

Spectral graph theory and topological indices

In this chapter, spectral graph theory is briefly discussed and some helpful results related to the topic are mentioned. The concept of graph energy and its bounds for simple graphs are included. This chapter also includes introduction of topological indices and definitions of some extensively used indices. Lastly, it is briefed that how a topological index matrix is associated to a graph to calculate its energy.

2.1 Spectral graph theory

In the current section the concept of spectral graph theory is illustrated. Some results showing the properties of eigenvalues of a graph are mentioned. Spectral graph theory is a branch in mathematics in which the relation of a graph with the matrix associated to it is studied and also its relationship with its characteristic polynomial, eigenvalues and eigenvectors is studied. The most commonly studied matrix in spectral graph theory is adjacency matrix. The adjacency matrix associated to an n -vertex graph \mathcal{G} , represented

by $\mathcal{A}(\mathcal{G}) = [b_{ij}]_{n \times n}$, is obtained as:

$$b_{ij} = \begin{cases} 1 & \text{if } u_i u_j \in \mathcal{E}(\mathcal{G}), \\ 0 & \text{otherwise.} \end{cases}$$

The adjacency characteristic polynomial, denoted by $\psi(\mathcal{G}, \sigma)$, is of the form:

$$\psi(\mathcal{G}, \sigma) = \det(\mathcal{A}(\mathcal{G}) - \sigma \mathcal{I}_n), \quad (2.1)$$

where \mathcal{I}_n represents the $n \times n$ identity matrix. The zeros of the equation (2.1) are called eigenvalues of $\mathcal{A}(\mathcal{G})$ or adjacency eigenvalues. The set of eigenvalues of adjacency matrix along with its algebraic multiplicity is adjacency spectrum of \mathcal{G} , denoted by $\text{spec}_{\mathcal{A}}(\mathcal{G})$. Suppose $\sigma_1, \sigma_2, \dots, \sigma_l$ are the distinct eigenvalues of $\mathcal{A}(\mathcal{G})$ and m_1, m_2, \dots, m_l be their respective multiplicities, then the adjacency spectrum is given as: $\text{spec}_{\mathcal{A}}(\mathcal{G}) = \{\sigma_1^{(m_1)}, \sigma_2^{(m_2)}, \dots, \sigma_l^{(m_l)}\}$.

The spectrum of adjacency matrix of a complete graph and complete bipartite graph is given as:

$$\begin{aligned} \text{spec}_{\mathcal{A}}(\mathcal{K}_n) &= \{(-1)^{n-1}, (n-1)\}, \\ \text{spec}_{\mathcal{A}}(\mathcal{K}_{\iota, \delta}) &= \{(0)^{\iota+\delta-2}, \pm\sqrt{\iota\delta}\}. \end{aligned} \quad (2.2)$$

According to the definition of an adjacency matrix it is clear that $a_{kk} = 0$, for $k = 1, 2, \dots, n$. As $\text{tr}(\mathcal{A}(\mathcal{G})) = \sum_{k=1}^n \sigma_k$, then for the eigenvalues of adjacency matrix we get,

$$\text{tr}(\mathcal{A}(\mathcal{G})) = \sum_{k=1}^n \sigma_k = 0.$$

The trace of the square of adjacency matrix is given as:

$$\text{tr}(\mathcal{A}^2(\mathcal{G})) = \sum_{k=1}^n \sigma_k^2 = 2m.$$

The result stated next establishes the connection between a symmetric matrix and its eigenvalue.

Lemma 2.1.1 (Zhang [12]). *Suppose that \mathcal{K} be a symmetric and n -square matrix and its eigenvalues be $\mu_1 \geq \dots \geq \mu_n$, then for any $x \in \mathbb{R}^n$ with $x \neq 0$.*

$$x^T \mathcal{K} x \leq \mu_1 x^T x,$$

where x^T is the transpose of x . The above equality is obtained when x is an eigenvector corresponding to the eigenvalue μ_1 of \mathcal{K} .

The following lemma establishes the relation between largest eigenvalues of two matrices.

Lemma 2.1.2 (Horn and Johnson[36]). *Let $\mathcal{S} = [s_{ij}]_{n \times n}$ and $\mathcal{T} = [t_{ij}]_{n \times n}$ be $n \times n$ symmetric and non-negative matrices, respectively. If $\mathcal{S} \geq \mathcal{T}$, that is, $s_{ij} \geq t_{ij}$ for all $i, j = 1, \dots, n$, then $\mu_1(\mathcal{S}) \geq \sigma_1(\mathcal{T})$, where μ_1 and σ_1 is the largest eigenvalue of the \mathcal{S} and \mathcal{T} respectively.*

The bounds on largest eigenvalue of an adjacency matrix associated to a graph \mathcal{G} is obtained in next two theorems.

Theorem 2.1.1 (Hong [45]). *Consider a graph \mathcal{G} with edge set of size m and vertex set of size n and let $\sigma_1 \geq \dots \geq \sigma_n$ be its adjacency eigenvalues. Then*

$$\sigma_1 \leq \sqrt{2m - n + 1},$$

and the equality holds when \mathcal{G} is star \mathcal{S}_n . It also holds for a complete graph \mathcal{K}_n .

Theorem 2.1.2 (Cao [6]). *Let \mathcal{G} be a graph with vertex set of size n and its minimum and maximum degree be $\delta(\mathcal{G})$ and $\Delta(\mathcal{G})$ respectively. Let eigenvalues of an adjacency matrix of \mathcal{G} be $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n$ and $\delta(\mathcal{G}) \geq 1$. Then*

$$\sigma_1 \leq \sqrt{2m - \delta(n - 1) + (\delta - 1)\Delta} .$$

2.2 Energy of graphs

One of the most significant concepts in the spectral graph theory is energy of graphs. This concept was established by Ivan Gutman in 1978 [19]. This invariant of graph is determined from its eigenvalues. Let the matrix associated to \mathcal{G} be adjacency matrix and its eigenvalues be $\sigma_1, \sigma_2, \dots, \sigma_n$. The energy of a graph \mathcal{G} is represented by $\xi(\mathcal{G})$ and is obtained as:

$$\xi(\mathcal{G}) = \sum_{k=1}^n |\sigma_k|.$$

This spectral graph quantity is widely used in chemistry as it is helpful in approximating the total π energy of electrons of a molecule which is represented by a graph [11]. In the last decade research in this field of graph theory is extended significantly and several different kinds of energy of graph are introduced. Gutman and Zhou [23] gave Laplacian energy of a graph as sum of eigenvalues of Laplacian matrix. It was also defined for other variants like signless Laplacian matrix [35], general matrix that is not associated to any graph [43] and also for incidence matrix [34]. Many bounds on energy of a graph are proved. Next theorem gives bounds for energy of a graph of size m .

Theorem 2.2.1 (Caporossi et al. [13]). *Let \mathcal{G} be a graph with edge set of size m . The bound is calculated as:*

$$2\sqrt{m} \leq \xi(\mathcal{G}) \leq 2m.$$

The lower bound for $\xi(\mathcal{G})$ is given in next theorem.

Theorem 2.2.2 (Gutman [20]). *Consider a graph \mathcal{G} with vertex set of size n . The lower bound for $\xi(\mathcal{G})$ is given as:*

$$\xi(\mathcal{G}) \geq 2\sqrt{n-1}.$$

The equality holds only in the case $\mathcal{G} \cong \mathcal{K}_{n-1,1}$.

The idea of energy of digraphs was established in 2008 by Peña and Rada [25] and the energy of a sigraph was given by Germina et al. [28]. In 2014, Bhat and Pirzada [42] proposed the generalization of the energy of a digraph to the sidigraphs.

Let \mathcal{D}_n be an n -vertex digraph. The adjacency matrix associated to \mathcal{D}_n is not always symmetric and hence the eigenvalues of a digraph can also be complex numbers. Let τ_i , for $i = 1, \dots, n$, be the eigenvalues of matrix $\mathcal{A}(\mathcal{D}_n)$. For a digraph \mathcal{D}_n , its energy is defined as:

$$\xi(\mathcal{D}_n) = \sum_{i=1}^n |Re(\tau_i)|,$$

here $|Re(\tau_i)|$ represents the absolute value of real part of τ_i .

In next theorem a well known result for maximal and minimal energy among unicyclic digraphs is given.

Theorem 2.2.3 (Peña and Rada [25]). *The minimal energy among all unicyclic digraphs with vertex set of size n , is of a digraph that contains a directed cycle $\mathcal{C}_2, \mathcal{C}_3$ or \mathcal{C}_4 . The maximal energy among all unicyclic digraphs on n vertices is attained for directed cycle \mathcal{C}_n .*

If between every two vertices of the digraph \mathcal{D}_n there is a directed path, then such a digraph is termed as a strongly connected . The maximal strong connected subdigraphs of a digraph are called its strong components.

The following theorem gives the result about strong components of a digraph.

Theorem 2.2.4. *Let $\mathcal{K}_1, \mathcal{K}_2, \dots, \mathcal{K}_\ell$ be the strong components of a digraph. Then energy of a digraph \mathcal{D}_n is given as:*

$$\xi(\mathcal{D}_n) = \sum_{i=1}^{\ell} \xi(\mathcal{K}_i).$$

2.3 Topological indices

Topological index [15] is a mathematical formula that is applied to graphs for conversion of a molecular structure into a real number. Topological index is also called molecular descriptor or connectivity index. It is constant under graph isomorphism. Topological indices have applications in molecular topology, mathematical chemistry and chemical graph theory [2].

The study of topological indices started in 1947 and now at present there are more than 120 topological indices [5]. The relation between chemical characteristics of a molecular compound and their structures is shown in various studies. Topological indices are either defined on the basis of connectivity or topological distances in the graph. For the further study reader may refer to [7]. Early topological indices were based on distances.

Wiener index

Wiener index, represented by $\mathcal{W}(\mathcal{G})$, was introduced by Harold Wiener in 1947 [16]. At first it was named path invariant but then in 1971 this notion was defined by Hosoya [15]. Wiener index is based on distance and it is calculated for a graph \mathcal{G} by taking summation of distance between all the vertices of \mathcal{G}

$$\mathcal{W}(\mathcal{G}) = \sum_{\{x, \xi\} \in \mathcal{V}(\mathcal{G})} d_{\mathcal{G}}(x, \xi).$$

The applications of wiener index can be seen in [1].

Zagreb index

There are many indices introduced on connectivity and Zagreb index is one of them. There are two terms, represented by $M_1(\mathcal{G})$ and $M_2(\mathcal{G})$, involved in Zagreb index which are treated as separate indices known as Zagreb first

index and Zagreb second index ([17, 21]), respectively. It is given as:

$$M_1(\mathcal{G}) = \sum_{x\mathfrak{z} \in \mathcal{E}(\mathcal{G})} d_{\mathcal{G}}(x) + d_{\mathcal{G}}(\mathfrak{z}),$$

$$M_2(\mathcal{G}) = \sum_{x\mathfrak{z} \in \mathcal{E}(\mathcal{G})} d_{\mathcal{G}}(x)d_{\mathcal{G}}(\mathfrak{z}).$$

Randić index

Another connectivity based index is Randić index, represented by $\mathcal{R}(\mathcal{G})$. It is calculated as:

$$\mathcal{R}(\mathcal{G}) = \sum_{x\mathfrak{z} \in \mathcal{E}(\mathcal{G})} \sqrt{\frac{1}{d_{\mathcal{G}}(x)d_{\mathcal{G}}(\mathfrak{z})}}$$

Inverse sum indeg index

Inverse sum indeg index, represented by $ISI(\mathcal{G})$ for a graph \mathcal{G} , was introduced in 2010 by Vukičević [8] and it is defined as

$$ISI(\mathcal{G}) = \sum_{x\mathfrak{z} \in \mathcal{E}(\mathcal{G})} \frac{d_{\mathcal{G}}(x)d_{\mathcal{G}}(\mathfrak{z})}{d_{\mathcal{G}}(x) + d_{\mathcal{G}}(\mathfrak{z})}.$$

Variable sum exdeg index

The variable sum exdeg index was first introduced by Vukičević in 2011 [9]. The purpose of establishing this index was to study the octanol-water partition coefficient, physiochemical property, of certain molecules. For a graph \mathcal{G} , the variable sum exdeg index is defined as:

$$SEI_{\nu}(\mathcal{G}) = \sum_{u\mathfrak{w} \in \mathcal{E}(\mathcal{G})} (\nu^{d_{\mathcal{G}}(u)} + \nu^{d_{\mathcal{G}}(\mathfrak{w})}),$$

where $\nu \in (0, 1) \cup (1, +\infty)$.

There are several other indices, see [18].

Topological index of a graph \mathcal{G} , represented by $TI(\mathcal{G})$, can be expressed in

the form

$$TI(\mathcal{G}) = \sum_{uw \in \mathcal{E}(\mathcal{G})} \mathcal{F}(u, w),$$

where \mathcal{F} is suitably chosen function for topological index and $\mathcal{F}(u, w) = \mathcal{F}(w, u)$.

If \mathcal{G} is a graph with vertex set of size n then a matrix $T = [d_{ij}]_{n \times n}$ can be associated to $TI(\mathcal{G})$ defined as:

$$d_{ij} = \begin{cases} \mathcal{F}(u, w) & \text{if } uw \in \mathcal{E}(\mathcal{G}), \\ 0 & \text{otherwise.} \end{cases}$$

If the eigenvalues of $T = [d_{ij}]_{n \times n}$ be $\tau_1, \tau_2, \dots, \tau_n$, then topological index energy of a graph can be defined as:

$$\xi_{TI}(\mathcal{G}) = \sum_{k=1}^n |\tau_k|.$$

The topic of Randić energy is the most widely studied topic in graph energy. It was introduced in 2010, by Bozkurt et al. ([38], [39]). Later in 2014, Gutman et al. proved few properties of Randic energy and Randic matrix. In 2017 Gutman [31] studied Zagreb energy and established bounds on this graph invariant. The idea of inverse sum indeg energy [40] and generalized inverse sum indeg energy [41] of a graph is established recently.

Let a matrix $\mathcal{I}(\mathcal{G})$ be associated to inverse sum indeg index of a graph \mathcal{G} . The following result shows the relationship between trace of inverse sum indeg matrix of graph and complete graph.

Theorem 2.3.1 (S. Hafeez [40]). *Consider a graph \mathcal{G} with vertex set of size n . Then,*

$$tr(\mathcal{I}^2(\mathcal{G})) \leq tr(\mathcal{I}^2(\mathcal{K}_n)).$$

The equality above is obtained for a complete graph. The lemma stated next tells that for a graph the sum of eigenvalues of inverse

sum indeg matrix is zero.

Lemma 2.3.1 (Zangi et al. [46]). *Consider a graph \mathcal{G} with vertex set of n and let s_1, s_2, \dots, s_n be the eigenvalues of $\mathcal{I}(\mathcal{G})$. Then,*

$$\sum_{k=1}^n s_k = 0.$$

Next theorem gives a result about the *ISI* energy of components of a graph.

Theorem 2.3.2 (S. Hafeez [40]). *Let the components of a graph \mathcal{G} be $\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_s$. Then,*

$$\xi_{ISI}(\mathcal{G}) = \sum_{k=1}^s \xi_{ISI}(\mathcal{X}_k).$$

In recent past study on geometric-arithmetic energy [27] of a graph is introduced. Various forms of graph energies are summarized by Das et al. [29] in 2018 studied several forms of energy of graphs and also calculated some bounds for these graph energies. For some new results on graph energies we refer to [33, 31, 10, 27].

Vukićević in [9] gave the properties and mathematical studies of variable sum exdeg index. The author also finds the maximal and minimal graphs among different classes of graphs with respect to SEI_v for $v > 1$. The polynomial form of this topological index was introduced by Yarahmadi and Ashrafi [47] and it has applications in nanoscience. Xiaoling Sun et al. [44] studied the minimum and maximum quasi-tree graphs and also for quasi-tree graphs with perfect matching with respect to variable sum exdeg index. The minimum and maximum unicyclic graphs along with given pendant vertices with respect to SEI_v and cycle length were also obtained.

Chapter 3

Variable Sum Exdeg Energy of graphs

In current chapter the idea of variable sum exdeg energy of a simple and undirected graph is introduced. Some algebraic properties of variable sum exdeg index are discussed. The variable sum exdeg energy of some particular graphs is computed. Moreover, the bounds for variable sum exdeg energy are calculated. Lastly, some results about noncospectral graphs with same variable sum exdeg energy are established.

Here we introduce the variable sum exdeg matrix associated to a graph \mathcal{G} with set vertices of size n , represented by $\mathcal{A}_v(\mathcal{G}) = [a_{ij}]_{n \times n}$ and define it as:

$$a_{ij} = \begin{cases} v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)} & \text{if } u_i u_j \in \mathcal{E}(\mathcal{G}), \\ 0 & \text{otherwise.} \end{cases}$$

The SEI_v -characteristic polynomial is determined as:

$$\begin{aligned} \phi_v(\mathcal{G}, \lambda) &= \det(\mathcal{A}_v(\mathcal{G}) - \lambda \mathcal{I}_n) \\ &= \lambda^n + \sum_{k=1}^n a_k \lambda^{n-k}, \end{aligned}$$

where \mathcal{I}_n is identity matrix. The zeros of the SEI_v -characteristic polynomial $\phi_v(\mathcal{G}, \lambda)$ are termed as \mathcal{A}_v -eigenvalues of $\mathcal{A}_v(\mathcal{G})$. The \mathcal{A}_v -eigenvalues are always real as $\mathcal{A}_v(\mathcal{G})$ is symmetric and real matrix. The set containing \mathcal{A}_v -eigenvalues along with their algebraic multiplicities is known as \mathcal{A}_v -spectrum, denoted by $\text{spec}_{\mathcal{A}_v}(\mathcal{G})$, of graph \mathcal{G} . Let the distinct \mathcal{A}_v -eigenvalues of graph \mathcal{G} and their respective multiplicities be $\lambda_1, \lambda_2, \dots, \lambda_\ell$ and $\tau_1, \tau_2, \dots, \tau_\ell$, respectively, then the \mathcal{A}_v -spectrum of is given by: $\text{spec}_{\mathcal{A}_v}(\mathcal{G}) = \{\lambda_1^{(\tau_1)}, \lambda_2^{(\tau_2)}, \dots, \lambda_\ell^{(\tau_\ell)}\}$. Variable sum exdeg energy of an n -order graph \mathcal{G} (represented by $\xi_v(\mathcal{G})$), $\lambda_1, \lambda_2, \dots, \lambda_n$ be its \mathcal{A}_v -eigenvalues, is defined as:

$$\xi_v(\mathcal{G}) = \sum_{k=1}^n |\lambda_k|. \quad (3.1)$$

3.1 Auxiliary Results

For our convenience, let us define some notations. For a graph \mathcal{G} with $\mathcal{V}(\mathcal{G})$ of size n , we represent the determinant of $\mathcal{A}_v(\mathcal{G})$ by $\det(\mathcal{A}_v(\mathcal{G}))$ and the trace of the matrix $\mathcal{A}_v(\mathcal{G})$ is represented by $\text{tr}(\mathcal{A}_v(\mathcal{G}))$ and $\text{tr}(\mathcal{A}_v(\mathcal{G})) = \sum_{k=1}^n (a_{kk})$.

Let

$$\Theta = \sum_{1 \leq i < j \leq n} (v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)})^2, \quad \chi = \det(\mathcal{A}_v(\mathcal{G})).$$

Let $(\mathcal{A}_v(\mathcal{G}))_{ij}$ be the (i, j) -entry of $\mathcal{A}_v(\mathcal{G})$. Now we prove the lemma stated below.

Lemma 3.1.1. *Consider a graph \mathcal{G} with $\mathcal{V}(\mathcal{G})$ of size n . Suppose that its \mathcal{A}_v -eigenvalues be $\lambda_1, \lambda_2, \dots, \lambda_n$. Then we prove following results.*

$$(1) \sum_{k=1}^n \lambda_k = 0,$$

$$(2) \text{tr}(\mathcal{A}_v^2(\mathcal{G})) = \sum_{k=1}^n \lambda_k^2 = 2\Theta.$$

Proof. (1). The diagonal elements of a simple graph are zero. Hence the diagonal entries of $\mathcal{A}_\nu(\mathcal{G}) = [a_{ij}]_{n \times n}$ are zero, which gives $\sum_{k=1}^n (a_{kk}) = 0$ and thus $\text{tr}(\mathcal{A}_\nu(\mathcal{G})) = 0$. Moreover, $\text{tr}(\mathcal{A}_\nu(\mathcal{G})) = \sum_{k=1}^n \lambda_k$. Therefore,

$$\sum_{k=1}^n \lambda_k = 0.$$

(2). Let $i = j$, then it is given as:

$$\begin{aligned} (\mathcal{A}_\nu^2(\mathcal{G}))_{jj} &= \sum_{k=1}^n (\mathcal{A}_\nu(\mathcal{G}))_{jk} (\mathcal{A}_\nu(\mathcal{G}))_{kj} = \sum_{k=1}^n (\mathcal{A}_\nu(\mathcal{G}))_{jk}^2 \\ &= \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (\mathcal{A}_\nu(\mathcal{G}))_{ij}^2 = 2 \sum_{1 \leq i < j \leq n} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)})^2 = 2\Theta \end{aligned}$$

□

Next theorem represents the relation between the trace of SEI_ν matrix of a general graph \mathcal{G} and trace of SEI_ν matrix of a complete graph.

Theorem 3.1.1. *Consider a simple connected n -vertex graph \mathcal{G} . Then for a real number $\nu > 1$ we have,*

$$\text{tr}(\mathcal{A}_\nu^2(\mathcal{G})) \leq \text{tr}(\mathcal{A}_\nu^2(\mathcal{K}_n)).$$

Proof. Suppose that $\mathcal{G} \neq \mathcal{K}_n$, then for $i = 1, \dots, n$, $d_{\mathcal{G}}(u_i) \leq n - 1$ for every vertex u_i of \mathcal{G} . Therefore, we have

$$\begin{aligned} \nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)} &\leq \nu^{n-1} + \nu^{n-1} = 2\nu^{n-1}. \\ \text{tr}(\mathcal{A}_\nu^2(\mathcal{G})) &= 2 \sum_{1 \leq i < j \leq n} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)})^2. \end{aligned}$$

The summation involved in equation above represents the total number of

edges in $\mathcal{E}(\mathcal{G})$, that is m . Then, we have

$$\text{tr}(\mathcal{A}_v^2(\mathcal{G})) = 2m(v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)})^2 \leq 2m(2v^{n-1})^2.$$

Note that $m < \frac{n(n-1)}{2}$ for $\mathcal{G} \neq \mathcal{K}_n$. Thus

$$\begin{aligned} \text{tr}(\mathcal{A}_v^2(\mathcal{G})) &\leq 8mv^{2n-2} < \frac{8n(n-1)}{2}(v^{2n-2}), \\ \text{tr}(\mathcal{A}_v^2(\mathcal{G})) &< 4n(n-1)v^{2n-2}. \end{aligned}$$

Now we suppose that $\mathcal{G} \cong \mathcal{K}_n$, then for every vertex u_i of \mathcal{G} , $d_{\mathcal{G}}(u_i) = n-1$, where $i = 1, \dots, n$. Hence,

$$\begin{aligned} v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)} &= v^{n-1} + v^{n-1} = 2v^{n-1}. \\ \text{tr}(\mathcal{A}_v^2(\mathcal{K}_n)) &= 2m(v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)})^2 = 2m(2v^{n-1})^2. \end{aligned}$$

Also for \mathcal{K}_n , $m = \frac{n(n-1)}{2}$, therefore,

$$\begin{aligned} \text{tr}(\mathcal{A}_v^2(\mathcal{K}_n)) &= 8mv^{2n-2} = \frac{8n(n-1)}{2}(v^{2n-2}), \\ \text{tr}(\mathcal{A}_v^2(\mathcal{K}_n)) &= 4n(n-1)v^{2n-2}. \end{aligned}$$

Consequently, $\text{tr}(\mathcal{A}_v^2(\mathcal{G})) \leq \text{tr}(\mathcal{A}_v^2(\mathcal{K}_n))$. □

A block diagonal matrix is a square and diagonal matrix and its diagonal entries are block matrices and all other entries are zero.

The spectrum of variable sum exdeg matrix of any graph is equal to union of spectrum of its all components and which is proved in the theorem stated below.

Theorem 3.1.2. *For a graph \mathcal{G} and its components $\Gamma_1, \Gamma_2, \dots, \Gamma_s$ we have,*

$$\xi_v(\mathcal{G}) = \sum_{k=1}^s \xi_v(\Gamma_k).$$

Proof. Since $\Gamma_1, \Gamma_2, \dots, \Gamma_s$ are components of \mathcal{G} , hence it can be written as $\mathcal{G} = \Gamma_1 \cup \Gamma_2 \cup \dots \cup \Gamma_s$. Then the SEI_v matrix of \mathcal{G} is a block diagonal matrix and $\mathcal{A}_v(\Gamma_1), \mathcal{A}_v(\Gamma_2), \dots, \mathcal{A}_v(\Gamma_s)$ are its diagonal entries. Therefore, the spectrum of $\mathcal{A}_v(\mathcal{G})$ is given as:

$$spec_{\mathcal{A}_v}(\mathcal{G}) = spec_{\mathcal{A}_v}(\Gamma_1) \cup spec_{\mathcal{A}_v}(\Gamma_2) \cup \dots \cup spec_{\mathcal{A}_v}(\Gamma_s).$$

Consequently,

$$\xi_v(\mathcal{G}) = \sum_{k=1}^s \xi_v(\Gamma_k).$$

□

An interesting result about variable sum exdeg energy of a non-trivial graph is stated in the next theorem and its proof is not included because it is similar to theorem 2.5 [40] proof.

Theorem 3.1.3. *The variable sum exdeg energy of a graph must be an even positive integer if it is an integer.*

3.2 Variable sum exdeg energy of various graphs

In current section SEI_v energy of few particular graphs is calculated and proved. The formula for the SEI_v energy of a cycle, an δ -regular graph, complete graph and complete bipartite graph is obtained. Moreover, the variable sum exdeg energy for duplicate graphs is included.

The formula for energy of a cycle was given by Bhat and Pirzada as:

$$\xi(C_n) = \begin{cases} 4 \csc \frac{\pi}{n} & \text{if } n \equiv 2(\text{mod}4) \\ 4 \cot \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}4) \\ 2 \csc \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (3.2)$$

The theorem given next proves the variable sum exdeg energy of an δ -regular

graph.

Theorem 3.2.1. *Consider an s -regular graph \mathcal{G} with vertex set of size n . Then*

$$\xi_v(\mathcal{G}) = 2v^s \xi(\mathcal{G}).$$

Proof. Let the \mathcal{A}_v -eigenvalues of \mathcal{G} be $\lambda_1, \lambda_2, \dots, \lambda_n$. The non-zero entries of variable sum exdeg matrix of an s -regular graph are $2v^s$. Then it can be written as: $\mathcal{A}_v(\mathcal{G}) = 2v^s \mathcal{A}(\mathcal{G})$. Therefore, $\lambda_j = 2v^s \sigma_j$, where $j = 1, 2, \dots, n$. This implies

$$\begin{aligned} \xi_v(\mathcal{G}) &= \sum_{j=1}^n |\lambda_j| = \sum_{j=1}^n |2v^s \sigma_j| \\ &= 2v^s \sum_{j=1}^n |\sigma_j| = 2v^s \xi(\mathcal{G}). \end{aligned}$$

Hence statement is proved. \square

Using the theorem stated above we can establish the following results for cycle and complete graph.

Corollary 3.2.1. *For a cycle of order n , $\xi_v(C_n) = 2v^2 \xi(C_n)$.*

As cycle is a 2-regular graph, then $s=2$ for cycle. Substituting $s=2$ in the formula proved in theorem 3.2.1 gives the formula for C_n stated in corollary above.

Corollary 3.2.2. *For an n -vertex complete graph, $\xi_v(\mathcal{K}_n) = 4(n-1)v^{n-1}$*

Proof. As complete graph is regular for $s = n - 1$, hence $\xi_v(\mathcal{K}_n) = 2v^{n-1} \xi(\mathcal{K}_n)$. Given that, $\text{spec}(\mathcal{K}_n) = \{(n-1), (-1)^{n-1}\}$, therefore it is calculated that $\xi(\mathcal{K}_n) = 2(n-1)$. Hence $\xi_v(\mathcal{K}_n) = 4(n-1)v^{n-1}$. \square

Remark 3.2.3. *Let $n \equiv 2 \pmod{4}$. Then using equation (3.2) it is obtained that $\xi_v(C_n) = 2 \xi_v(C_{\frac{n}{2}})$.*

The next theorem gives the formula for variable sum exdeg energy of a complete bipartite graph $\mathcal{K}_{\mathfrak{s},\mathfrak{z}}$.

Theorem 3.2.2. *For a complete bipartite graph $\mathcal{K}_{\mathfrak{s},\mathfrak{z}}$, we have*

$$\xi_v(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = 2(\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}})\sqrt{\mathfrak{s}\mathfrak{z}}$$

Proof. The entries of a variable sum exdeg matrix of $\mathcal{K}_{\mathfrak{s},\mathfrak{z}}$ are either $\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}}$ or 0. Let us denote $\mathfrak{s} \times \mathfrak{z}$ and $\mathfrak{z} \times \mathfrak{s}$ matrices by \mathcal{A} and \mathcal{B} , whose each entry is $\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}}$, respectively. Suppose \mathcal{O} be a \mathfrak{s} -square matrix and \mathcal{O}' be a \mathfrak{z} -matrix, whose each entry is zero. Then we have,

$$\mathcal{A}_v(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = \begin{bmatrix} \mathcal{O} & \mathcal{A} \\ \mathcal{B} & \mathcal{O}' \end{bmatrix}.$$

This implies that

$$\mathcal{A}_v(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = (\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}}).$$

Hence,

$$\text{spec}_{\mathcal{A}_v}(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = (\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}}) \text{spec}_{\mathcal{A}}(\mathcal{K}_{\mathfrak{s},\mathfrak{z}})$$

From equation (1.1) we have

$$\text{spec}_{\mathcal{A}}(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = \{0^{(\mathfrak{s}+\mathfrak{z}-2)}, \pm\sqrt{\mathfrak{s}\mathfrak{z}}\}$$

Therefore,

$$\text{spec}_{\mathcal{A}_v}(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) = \{0^{(\mathfrak{s}+\mathfrak{z}-2)}, \pm(\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}})\sqrt{\mathfrak{s}\mathfrak{z}}\}$$

So,

$$\begin{aligned} \xi_v(\mathcal{K}_{\mathfrak{s},\mathfrak{z}}) &= \sum_{k=1}^{\mathfrak{s}+\mathfrak{z}} |\lambda_k| \\ &= |(\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}})\sqrt{\mathfrak{s}\mathfrak{z}}| + |-(\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}})\sqrt{\mathfrak{s}\mathfrak{z}}| \\ &= 2(\mathfrak{v}^{\mathfrak{s}} + \mathfrak{v}^{\mathfrak{z}})\sqrt{\mathfrak{s}\mathfrak{z}} \end{aligned}$$

Hence, statement is proved. \square

Using the formula proved in theorem 3.2.2 following result is obtained.

Corollary 3.2.4. *For a star graph of n vertices, $\xi_v(\mathcal{S}_n) = 2(v + v^{n-1})\sqrt{n-1}$.*

In the next remark, variable sum exdeg energy of complement of complete bipartite graph is studied.

Remark 3.2.5. *Note that $\overline{\mathcal{K}_{s,\tau}}$ is a disconnected graph with components \mathcal{K}_s and \mathcal{K}_τ . Hence by using theorem 3.1.2,*

$$\xi_v(\overline{\mathcal{K}_{s,\tau}}) = \xi_v(\mathcal{K}_s) + \xi_v(\mathcal{K}_\tau)$$

Now by corollary 3.2.2,

$$\begin{aligned} \xi_v(\overline{\mathcal{K}_{s,\tau}}) &= 4(s-1)v^{s-1} + 4(\tau-1)v^{\tau-1} \\ &= \frac{4}{v} [(s-1)v^s + (\tau-1)v^\tau]. \end{aligned}$$

Let $\mathcal{A} = (a_{ij})_{n \times n}$ be an n -square and $\mathcal{B} = (b_{ij})_{m \times m}$ be a m -square matrix and their eigenvalues be η_ℓ , $\ell = 1, 2, \dots, n$ and μ_k , $k = 1, 2, \dots, m$, respectively. Then the tensor product of \mathcal{A} and \mathcal{B} is another matrix which is constructed by substituting every entry of \mathcal{A} by $a_{ij}\mathcal{B}$. It is denoted by $\mathcal{A} \otimes \mathcal{B}$ and its eigenvalues are obtained by $\eta_\ell \mu_k$.

The next two theorems give the relation between the SEI_v energy of a graph \mathcal{G} and the variable sum exdeg energy of its duplicate graph.

Theorem 3.2.3. *Let \mathcal{G} be an n -vertex graph. Then we have*

$$\xi_v(\mathcal{G}^*) = 2 \xi_v(\mathcal{G}).$$

Proof. Observe that $\mathcal{A}_v(\mathcal{G}^*)$ is a block matrix and its diagonal elements are n -square blocks of all entries zero and the non-diagonal blocks are $\mathcal{A}_v(\mathcal{G})$. Let us represent zero matrix of order n by \mathcal{O} and 2-square matrix of diagonal

entries are zero and non-diagonal entries 1 by \mathcal{Q} . Then it can be expressed as:

$$\begin{aligned}\mathcal{A}_v(\mathcal{G}^*) &= \begin{bmatrix} \mathcal{O} & \mathcal{A}_v(\mathcal{G}) \\ \mathcal{A}_v(\mathcal{G}) & \mathcal{O} \end{bmatrix} = \mathcal{A}_v(\mathcal{G}) \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= \mathcal{A}_v(\mathcal{G}) \otimes \mathcal{Q}\end{aligned}$$

The eigenvalues of $\mathcal{A}_v(\mathcal{G})$ are λ_j and the eigenvalues of \mathcal{Q} are $\{\pm 1\}$. Consequently, $\text{spec}_{\mathcal{A}_v}(\mathcal{G}^*) = \{\pm \lambda_k \mid k = 1, 2, \dots, n\}$. Consequently,

$$\xi_v(\mathcal{G}^*) = \sum_{k=1}^n |\lambda_k| + \sum_{k=1}^n |-\lambda_k|$$

This implies that

$$\xi_v(\mathcal{G}^*) = 2 \xi_v(\mathcal{G}).$$

□

3.3 Spectral radius and spread of the variable sum exdeg matrix

In this section, the bounds on spectral radius and spread of variable sum exdeg matrix are obtained.

The spectral radius of a variable sum exdeg matrix is the largest absolute value of its eigenvalues. For any complex $n \times n$ matrix \mathcal{P} with eigenvalues μ_1, \dots, μ_n , the spread $s(\mathcal{P})$ of \mathcal{P} is defined as $s(\mathcal{P}) = \max_{k,\ell} |\mu_k - \mu_\ell|$. Let $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_\ell$ be the distinct \mathcal{A}_v -eigenvalues of a simple graph, such that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_\ell$ are all real. Then the spread of the matrix $\mathcal{A}_v(\mathcal{G})$, represented by $s(\mathcal{A}_v(\mathcal{G}))$, is defined as $s(\mathcal{A}_v(\mathcal{G})) = \lambda_1 - \lambda_\ell$. Now we prove the bounds for the largest eigenvalue of variable sum exdeg matrix.

Theorem 3.3.1. *Let $n \geq 2$. Consider a simple and connected graph \mathcal{G} with $\mathcal{V}(\mathcal{G})$ of size n . Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be its \mathcal{A}_ν -eigenvalues and let $\nu > 1$ is a real number. Then*

$$\frac{2m\nu^{\delta(\mathcal{G})}}{n} \leq \lambda_1 \leq 2\nu^{n-1}\sqrt{2m-n+1}.$$

Proof. Let $x \in \mathbb{R}^n$ and $x = (x_1, x_2, \dots, x_n)^T$. Then

$$\begin{aligned} x^T \mathcal{A}_\nu(\mathcal{G}) x &= \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)}) x_i x_j \geq \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (\nu^{\delta(\mathcal{G})} + \nu^{\delta(\mathcal{G})}) x_i x_j \\ &= 2 \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} \nu^{\delta(\mathcal{G})} x_i x_j. \end{aligned}$$

The summation $\sum_{u_i u_j \in \mathcal{E}(\mathcal{G})}$ represents the total number of edges, that is m .

Hence

$$x^T \mathcal{A}_\nu(\mathcal{G}) x \geq 2m\nu^{\delta(\mathcal{G})} x_i x_j$$

Taking $x = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots, \frac{1}{\sqrt{n}})^T$ we get $x_i x_j = \frac{1}{n}$. Hence, $x^T \mathcal{A}_\nu(\mathcal{G}) x \geq \frac{2m}{n} \nu^{\delta(\mathcal{G})}$.

Now by Lemma 2.1.1 which states,

$$x^T \mathcal{A}_\nu(\mathcal{G}) x \leq \lambda_1 x^T x$$

Here $x^T x = 1$, which gives $x^T \mathcal{A}_\nu(\mathcal{G}) x \leq \lambda_1$. Therefore, $\lambda_1 \geq \frac{2m}{n} \nu^{\delta(\mathcal{G})}$.

Now for any vertex $u_j \in \mathcal{V}(\mathcal{G})$, $j = 1, 2, \dots, n$, we have $1 \leq \delta(\mathcal{G}) \leq d_{\mathcal{G}}(u_j) \leq \Delta(\mathcal{G}) \leq (n-1)$. Therefore

$$\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)} \leq \nu^{\Delta(\mathcal{G})} + \nu^{\Delta(\mathcal{G})} = 2\nu^{\Delta(\mathcal{G})} \leq 2\nu^{n-1}.$$

Now, as $\mathcal{A}_\nu(\mathcal{G}) = (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)}) \mathcal{A}(\mathcal{G}) \leq 2\nu^{n-1} \mathcal{A}(\mathcal{G})$. Therefore by lemma 2.1.2 we obtain $\lambda_1 \leq \omega_1 2\nu^{n-1}$, where ω_1 is the spectral radius of $2\nu^{n-1}(\mathcal{A}(\mathcal{G}))$.

By theorem 2.1.1 it implies that

$$\lambda_1 \leq 2v^{n-1} \sigma_1 \leq 2v^{n-1} \sqrt{2m - n + 1},$$

where σ_1 is the spectral radius of $\mathcal{A}(\mathcal{G})$. \square

Next theorem gives bounds on the smallest \mathcal{A}_v -eigenvalue of a graph \mathcal{G} . The proof of next theorem is omitted it is same as the proof of Theorem 4.7 [41].

Theorem 3.3.2. *Consider a graph \mathcal{G} and its \mathcal{A}_v -eigenvalues be $\lambda_1 \geq \dots \geq \lambda_n$. Then*

$$\sqrt{\frac{2\Theta + (n-2)(n-1)\chi^{2/n-1}}{2}} \leq \lambda_n \leq \sqrt{\frac{2(n-1)\Theta}{n}},$$

where $v \neq 1$ is a positive real number.

In the following result, we give bounds on spread of the variable sum exdeg matrix $\mathcal{A}(\mathcal{G})$.

Theorem 3.3.3. *Consider a connected graph \mathcal{G} with \mathcal{A}_v -eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Then*

$$\begin{aligned} s(\mathcal{A}_v(\mathcal{G})) &\geq 2 \left(\frac{mv}{n} - v^{n-1} \sqrt{\frac{2(n-1)m}{n}} \right), \\ s(\mathcal{A}_v(\mathcal{G})) &\leq 2v^{n-1} \sqrt{2m+1-n} - \frac{1}{\sqrt{2}} \sqrt{8mv^2 + (n-1)(n-2)\chi^{\frac{2}{n-1}}}, \end{aligned}$$

where $v > 1$ is a real number.

Proof. For any $u_j \in \mathcal{V}(\mathcal{G})$, $j = 1, \dots, n$, we have $1 \leq \delta(\mathcal{G}) \leq d_{\mathcal{G}}(u_j) \leq \Delta(\mathcal{G}) \leq (n-1)$. Therefore

$$2\Theta = 2 \sum_{1 \leq i < j \leq n} (v^{d_{\mathcal{G}}(u_i)} + v^{d_{\mathcal{G}}(u_j)})^2 \geq 2 \sum_{1 \leq i < j \leq n} (v^{\delta(\mathcal{G})} + v^{\delta(\mathcal{G})})^2 \geq 8mv^2. \quad (3.3)$$

Also

$$2\Theta = 2 \sum_{1 \leq i < j \leq n} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)})^2 \leq 2 \sum_{1 \leq i < j \leq n} (\nu^{\Delta(\mathcal{G})} + \nu^{\Delta(\mathcal{G})})^2 \leq 8m\nu^{2n-2}. \quad (3.4)$$

Hence using Theorem 3.3.1, Theorem 3.3.2 and Equations (3.3) and (3.4), we get

$$\begin{aligned} \delta(\mathcal{A}_\nu(\mathcal{G})) &= \lambda_1 - \lambda_n \\ &\leq 2\nu^{n-1}\sqrt{2m-n+1} - \sqrt{\frac{2\Theta + (n-2)(n-1)\chi^{2/n-1}}{2}} \\ &\leq 2\nu^{n-1}\sqrt{2m+1-n} - \sqrt{\frac{8m\nu^2 + (n-2)(n-1)\chi^{2/n-1}}{2}} \\ &= 2\nu^{n-1}\sqrt{2m+1-n} - \frac{1}{\sqrt{2}}\sqrt{8m\nu^2 + (n-1)(n-2)\chi^{2/n-1}} \end{aligned}$$

Since $\delta(\mathcal{G}) \geq 1$, we have

$$\begin{aligned} \delta(\mathcal{A}_\nu(\mathcal{G})) &= \lambda_1 - \lambda_n \geq \frac{2m\nu^{\delta(\mathcal{G})}}{n} - \sqrt{\frac{2(n-1)\chi}{n}} \geq \frac{2m\nu}{n} - \sqrt{\frac{8m\nu^{2n-2}(n-1)}{n}} \\ &= \left(\frac{m\nu}{n} - \nu^{n-1}\sqrt{\frac{2m(n-1)}{n}} \right) 2. \end{aligned}$$

The proof is complete. \square

3.4 Bounds on variable sum exdeg energy

In this section, the bounds are obtained and proved for variable sum exdeg energy of a simple and connected graph.

Theorem 3.4.1. *Consider a graph \mathcal{G} with \mathcal{A}_ν -eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and let $\nu > 1$, then we have*

$$\frac{2m\nu}{n} \leq \xi_\nu(\mathcal{G}) \leq \nu^{n-1}\sqrt{8mn}.$$

Proof. Suppose that without any loss of generality $\lambda_1, \dots, \lambda_t$ are positive and $\lambda_{t+1}, \dots, \lambda_n$ are negative. Using Theorem 3.3.1, we get

$$\xi_v(\mathcal{G}) = \sum_{j=1}^n |\lambda_j| = 2 \sum_{j=1}^t \lambda_j \geq 2\lambda_1 \geq \frac{2m\vartheta^{\delta(\mathcal{G})}}{n} \geq \frac{2m\vartheta}{n}.$$

By applying Cauchy-Schwartz inequality, $(\sum_{i=1}^n x_i y_i)^2 \leq (\sum_{i=1}^n x_i^2)(\sum_{i=1}^n y_i^2)$, we have

$$\xi_v(\mathcal{G}) = \sum_{k=1}^n |\lambda_k| \leq \left(\sum_{k=1}^n |\lambda_k| \right)^{1/2} \left(\sum_{k=1}^n 1 \right)^{1/2} = \sqrt{\sum_{k=1}^n \lambda_k^2 n}$$

Now using lemma 1.1 part (2) and equation (1.3), we have

$$\xi_v(\mathcal{G}) \leq \sqrt{\sum_{k=1}^n \lambda_k^2 n} = \sqrt{2n \Theta} \leq \sqrt{8mn\vartheta^{2n-2}} = \vartheta^{n-1} \sqrt{8mn}.$$

Hence proved. □

Theorem 3.4.2. Consider a graph \mathcal{G} with \mathcal{A}_v -eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Then

$$4\vartheta\sqrt{m} \leq \xi_v(\mathcal{G}) \leq \vartheta^{n-1} \left(2\sqrt{2m - n + 1} + \sqrt{\frac{8mn^2(n-1) - 4m^2(n-1)\vartheta^{4-2n}}{n^2}} \right),$$

where $\vartheta \neq 1$ is a positive real number.

Proof. By Part (1) of Lemma 2.1, $\sum_{k=1}^n \lambda_k = 0$, we have

$$\begin{aligned} \left(\sum_{k=1}^n \lambda_k\right)^2 &= \sum_{k=1}^n \lambda_k^2 + 2 \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j, \\ \sum_{k=1}^n \lambda_k^2 &= -2 \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j \end{aligned}$$

Also,

$$(\xi_v(\mathcal{G}))^2 = \left(\sum_{k=1}^n |\lambda_k|\right)^2 = \sum_{k=1}^n \lambda_k^2 + 2 \sum_{1 \leq i < j \leq n} |\lambda_i \lambda_j|$$

Using part (2) of lemma 2.1, we obtain

$$(\xi_v(\mathcal{G}))^2 \geq 2\Theta + 2 \left| \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j \right| = 4\Theta.$$

Now,

$$\begin{aligned} 4\Theta &= 4 \sum_{1 \leq i < j \leq n} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)})^2 \geq 4 \sum_{1 \leq i < j \leq n} (\nu^{\delta(\mathcal{G})} + \nu^{\delta(\mathcal{G})})^2 \\ &= 4 \sum_{1 \leq i < j \leq n} 4(\nu^{\delta(\mathcal{G})})^2 \geq 16m\nu^2. \end{aligned}$$

Therefore, $\xi_v(\mathcal{G}) \geq 4\nu\sqrt{m}$.

Now we prove the right side of inequality. We have,

$$\begin{aligned} \xi_v(\mathcal{G}) &= \sum_{k=1}^n |\lambda_k| = \sum_{k=2}^n |\lambda_k| + |\lambda_1|, \\ (\xi_v(\mathcal{G}) - \lambda_1)^2 &= \left(\sum_{k=2}^n |\lambda_k|\right)^2 \end{aligned}$$

Now using Cauchy-Schwartz inequality to obtain, $\left(\sum_{k=2}^n |\lambda_k|\right)^2 \leq (n-1) \sum_{k=2}^n \lambda_k^2$.

Hence,

$$(\xi_v(\mathcal{G}) - \lambda_1)^2 \leq (n-1) \sum_{k=2}^n \lambda_k^2 \quad (3.5)$$

By part (2) of lemma 2.1, $\sum_{k=1}^n \lambda_k^2 = 2\Theta$, therefore

$$2\Theta = \sum_{k=2}^n \lambda_k^2 + \lambda_1^2; \quad 2\Theta - \lambda_1^2 = \sum_{k=2}^n \lambda_k^2$$

Consequently, equation (3.5) becomes $(\xi_v(\mathcal{G}) - \lambda_1)^2 \leq (n-1)(2\Theta - \lambda_1^2)$. Hence by Theorem 3.3.1, we get

$$\begin{aligned} \xi_v(\mathcal{G}) &\leq \lambda_1 + \sqrt{(n-1)(2\Theta - \lambda_1^2)} \\ &\leq 2v^{n-1}\sqrt{2m+1-n} + \sqrt{(n-1)\left(8mv^{2n-2} - \frac{4m^2v^2}{n^2}\right)} \\ &= 2v^{n-1}\sqrt{2m+1-n} + \sqrt{(n-1)\left(\frac{8mn^2v^{2n-2} - 4m^2v^2}{n^2}\right)} \\ &= v^{n-1}\left(2\sqrt{2m+1-n} + \sqrt{\frac{8mn^2(n-1) - 4m^2(n-1)v^{4-2n}}{n^2}}\right) \end{aligned}$$

This gives the required result. \square

3.5 Nordhaus–Gaddum-type results for variable sum exdeg spectral radius and energy

In this section bounds are obtained for spectral radius of SEI_v matrix of a simple graph and its complement. Also bounds for variable sum exdeg energy of \mathcal{G} and $\overline{\mathcal{G}}$ are proved. Let $\bar{n}, \bar{m}, \delta(\overline{\mathcal{G}}) = \bar{\delta}$ and $\Delta(\overline{\mathcal{G}}) = \bar{\Delta}$ be the order,

size, minimum and maximum degree of the complement of graph. From the definition of complement of a graph it follows that $\bar{n} = n$, $\bar{m} = \frac{n^2-n}{2} - m$, $\bar{\delta} = n - 1 - \Delta(\mathcal{G})$ and $\bar{\Delta} = n - 1 - \delta(\mathcal{G})$. The \mathcal{A}_ν - eigenvalues of $\bar{\mathcal{G}}$ are given by $\bar{\lambda}_k$, $k = 1, 2, \dots, n$. A subgraph of a graph \mathcal{G} which is maximal and also connected is called component of \mathcal{G} . If a maximal subgraph has a path between every pair vertices of \mathcal{G} , then it is termed as component of \mathcal{G} .

Firstly, the bounds on $\lambda_1 + \bar{\lambda}_1$ are obtained.

Theorem 3.5.1. *Consider a graph \mathcal{G} and its vertex set be of size n . Then we have*

$$\lambda_1 + \bar{\lambda}_1 \geq \frac{1}{n}(2m(\nu - 1) + n^2 - n),$$

where $\nu > 1$ is a real number.

Proof. Let $x \in \mathbb{R}^n$ such that $x = (x_1, x_2, \dots, x_n)^T$. Then

$$\begin{aligned} x^T [\mathcal{A}_\nu(\mathcal{G}) + \mathcal{A}_\nu(\bar{\mathcal{G}})] x &= \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (\nu^{d_{\mathcal{G}}(u_i)} + \nu^{d_{\mathcal{G}}(u_j)}) x_i x_j + \sum_{u_i u_j \in \mathcal{E}(\bar{\mathcal{G}})} (\nu^{d_{\bar{\mathcal{G}}}(u_i)} + \nu^{d_{\bar{\mathcal{G}}}(u_j)}) x_i x_j \\ &\geq \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (\nu^{\delta(\mathcal{G})} + \nu^{\delta(\mathcal{G})}) x_i x_j + \sum_{u_i u_j \in \mathcal{E}(\bar{\mathcal{G}})} (\nu^{\bar{\delta}} + \nu^{\bar{\delta}}) x_i x_j \\ &= \sum_{u_i u_j \in \mathcal{E}(\mathcal{G})} (2\nu^{\delta(\mathcal{G})}) x_i x_j + \sum_{u_i u_j \in \mathcal{E}(\bar{\mathcal{G}})} (2\nu^{\bar{\delta}}) x_i x_j \end{aligned}$$

Let $x = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots, \frac{1}{\sqrt{n}})^T$, then by using lemma 2.1.1, it is obtained

$$x^T [\mathcal{A}_\nu(\mathcal{G}) + \mathcal{A}_\nu(\bar{\mathcal{G}})] x \leq x^T x (\lambda_1 + \bar{\lambda}_1) = \bar{\lambda}_1 + \lambda_1.$$

Now using $\bar{\delta} = n - 1 - \Delta(\mathcal{G})$, $\Delta(\mathcal{G}) \leq n - 1$ and $\delta(\mathcal{G}) \geq 1$ and replacing

$\sum_{u_i u_j \in \mathcal{E}(\mathcal{G})}$ and $\sum_{u_i u_i \in \mathcal{E}(\overline{\mathcal{G}})}$ by m and \overline{m} , we obtain

$$\begin{aligned} \lambda_1 + \overline{\lambda}_1 &\geq \frac{2\upsilon m}{n} + \frac{2\overline{m}}{n}(\upsilon^{n-1} - \Delta(\mathcal{G})) \\ &\geq \frac{2}{n}(\upsilon m + \overline{m} \upsilon^{n-1} - (n-1)) \\ &= \frac{2}{n} \left(\frac{2m\upsilon - n - 2m + n^2}{2} \right) = \frac{1}{n} ((\upsilon - 1)2m + n^2 - n). \end{aligned}$$

Hence proved. \square

Theorem 3.5.2. *Consider a connected graph \mathcal{G} and \mathcal{G}_1 be component of $\overline{\mathcal{G}}$ with largest eigenvalue λ_1 and $\overline{\lambda}_1 = \lambda_1(\mathcal{G}_1)$. Let m_1 and n_1 be the size and order of \mathcal{G}_1 respectively.*

(a). *If $\Delta(\mathcal{G}) = n - 1$ or $\overline{\Delta} = n - 1$, then*

$$\lambda_1 + \overline{\lambda}_1 \leq 2(\upsilon^{n-1} \sqrt{2m - n + 1} + \upsilon^{n_1-1} \sqrt{2m_1 - n_1 + 1})$$

(b). *For $\Delta(\mathcal{G}) \leq n - 2$ and $\overline{\Delta} \leq n - 2$, we have*

$$\lambda_1 + \overline{\lambda}_1 \leq 2\upsilon^{n-1} (\sqrt{2m - n + 1} + \sqrt{n^2 - 2n - 2m + 1})$$

Proof. (a). If $\Delta(\mathcal{G}) = n - 1$ or $\overline{\Delta} = n - 1$, then Theorem 3.3.1 gives

$$\lambda_1 \leq 2\upsilon^{n-1} \sqrt{2m - n + 1}. \quad (3.6)$$

Let the components of $\overline{\mathcal{G}}$ are $\mathcal{G}_1, \mathcal{G}_2, \dots, \mathcal{G}_t$. Suppose that, without loss of generality, $\lambda_1(\mathcal{G}_1) \geq \lambda_1(\mathcal{G}_2) \geq \dots \geq \lambda_1(\mathcal{G}_t)$ and $\overline{\lambda}_1 = \lambda_1(\mathcal{G}_1)$. Thus using Theorem 3.3.1, we obtain

$$\overline{\lambda}_1 \leq 2\upsilon^{(n_1-1)} \sqrt{2m_1 - n_1 + 1}. \quad (3.7)$$

From Equations (3.6) and (3.7), we have

$$\lambda_1 + \bar{\lambda}_1 \leq 2(v^{n-1}\sqrt{2m-n+1} + v^{n_1-1}\sqrt{2m_1-n_1+1}).$$

(b). If $\bar{\Delta} \leq n-2$ also $\Delta_{\mathcal{G}} \leq n-2$, and $\bar{\delta} \geq 1$. From Theorem 3.3.1, we have

$$\lambda_1 \leq 2v^{n-2}\sqrt{2m-n+1}. \quad (3.8)$$

Now using $\bar{\delta} = n-1-\Delta_{\mathcal{G}}$ and $\bar{\Delta} \leq n-2$, Theorem 2.1.2 and proof of Theorem 3.3.1, we obtain

$$\begin{aligned} \bar{\lambda}_1 &\leq 2v^{n-2}\sqrt{2\frac{n(n-1)}{2} - 2m + (\bar{\delta}-1)\bar{\Delta} - \bar{\delta}(n-1)} \\ &= 2v^{n-2}\sqrt{(n^2+1-2m-2n) + \delta(\mathcal{G})(2+\Delta(\mathcal{G})-n)} \\ &\leq 2v^{n-2}\sqrt{(n^2+1-2m-2n) + \Delta(\mathcal{G})(2+(n-2)-n)} \\ &= 2v^{n-2}\sqrt{(n^2+1-2m-2n)} \end{aligned} \quad (3.9)$$

From Equations (3.8) and (3.9), we get

$$\lambda_1 + \bar{\lambda}_1 \leq 2v^{n-2}(\sqrt{2m-n+1} + \sqrt{(n^2-2n-2m+1)}). \quad (3.10)$$

□

Theorem 3.5.3. *Suppose \mathcal{G} be a connected and simple graph and \mathcal{G}_1 be a*

connected component of its complement $\overline{\mathcal{G}}$ with $\overline{\lambda}_1 = \lambda_1(\mathcal{G}_1)$. Let

$$U_1 = \sqrt{8mn^2(n-1) - 4m^2(n-1)v^{4-2n}},$$

$$U'_1 = \sqrt{\frac{4n^2(n-1)}{v^{2\delta(\mathcal{G})}} - \frac{(n^2 - n - 2m)(n-1)}{v^{2\Delta(\mathcal{G})}}},$$

$$U_2 = \sqrt{\frac{8mn^2(n-1) - 4m^2(n-1)v^{6-2n}}{n^2}},$$

$$U'_2 = 2\sqrt{1 + \frac{1-n}{n^2 - n - 2m}} + \sqrt{4(n-1) - \frac{(n-1)(n^2 - n - 2m)v^{6-2n}}{n^2}}.$$

(a). If $\Delta(\mathcal{G}) = n-1$ or $\overline{\Delta} = n-1$, then

$$\begin{aligned} \xi_v(\mathcal{G}) + \xi_v(\overline{\mathcal{G}}) &\leq v^{n-1} \left(2\sqrt{2m-n+1} + \frac{1}{\sqrt{n}} U_1 \right) + 2v^{(n_1-1)} \sqrt{2m_1 - n_1 + 1} \\ &\quad + \frac{v^{n-1}}{n} \sqrt{n^2 - n - 2m} U'_1. \end{aligned}$$

(b). Let $\Delta(\mathcal{G}) \leq n-2$ or $\overline{\Delta} \leq n-2$, then

$$\xi_v(\mathcal{G}) + \xi_v(\overline{\mathcal{G}}) \leq v^{n-2} (2\sqrt{2m-n+1} + U_2 + \sqrt{n^2 - n - 2m} U'_2).$$

Proof. Using Part (2) of Lemma 3.1.1 on $\overline{\mathcal{G}}$ with $\overline{\Delta} = n-1 - \delta(\mathcal{G})$ and $\overline{\delta} = n-1 - \Delta(\mathcal{G})$, we have

$$2\Theta = 2 \sum_{1 \leq i < j \leq n} (v^{d_{\overline{\mathcal{G}}}(u_i)} + v^{d_{\overline{\mathcal{G}}}(u_j)})^2 \leq 2 \sum_{1 \leq i < j \leq n} (2v^{\overline{\Delta}})^2 = 4(n^2 - n - 2m)v^{2n-2-2\delta(\mathcal{G})}.$$

Same as in theorem 3.3.1 proof, we get

$$\overline{\lambda}_1 \geq \frac{2\overline{m}v^{\overline{\delta}}}{n} = \frac{(n^2 - n - 2m)v^{n-1-\Delta(\mathcal{G})}}{n}.$$

Applying Cauchy-Schwartz inequality to obtain $(\sum_{k=2}^n |\bar{\lambda}_k|)^2 \leq (n-1) \sum_{k=2}^n \bar{\lambda}_k^2$.
Therefore using Part (2) of Lemma 3.1.1, $(\xi_v(\bar{\mathcal{G}}) - \bar{\lambda}_1)^2 \leq (n-1) (2\Theta - \bar{\lambda}_1^2)$.

(a). Theorem 3.4.2 gives

$$\begin{aligned} \xi_v(\mathcal{G}) &\leq v^{n-1} \left(2\sqrt{2m+1-n} + \sqrt{\frac{8mn^2(n-1) - 2m(n-1)v^{4-2n}}{n}} \right) \\ &= v^{n-1} \left(2\sqrt{2m+1-n} + \frac{1}{\sqrt{n}} U_1 \right). \end{aligned} \tag{3.11}$$

Using inequality (3.7), we get

$$\begin{aligned} \xi_v(\bar{\mathcal{G}}) &\leq \bar{\lambda}_1 + \sqrt{(n-1) (2\Theta - \bar{\lambda}_1^2)} \\ &\leq 2v^{(n_1-1)} \sqrt{2m_1 - n_1 + 1} \\ &\quad + \sqrt{(n-1) \left(4(n^2 - n - 2m) v^{(2n-2-2\delta(\mathcal{G}))} - \frac{(n^2 - n - 2m)^2 v^{(2n-2-2\Delta(\mathcal{G}))}}{n^2} \right)} \\ &= 2v^{(n_1-1)} \sqrt{2m_1 - n_1 + 1} + \frac{v^{n-1}}{n} \sqrt{n^2 - n - 2m} U'_1 \end{aligned} \tag{3.12}$$

From Equations (3.11) and (3.12), we get

$$\begin{aligned} \xi_v(\mathcal{G}) + \xi_v(\bar{\mathcal{G}}) &\leq v^{n-1} \left(2\sqrt{2m-n+1} + \frac{1}{\sqrt{n}} U_1 \right) + 2v^{(n_1-1)} \sqrt{2m_1 - n_1 + 1} \\ &\quad + \frac{v^{n-1}}{n} \sqrt{n^2 - n - 2m} U'_1. \end{aligned}$$

(b). From proof of Theorem 3.4.2, we see that

$$\begin{aligned}
\xi_v(\mathcal{G}) &\leq v^{n-2} \left(2\sqrt{2m+1-n} + \sqrt{\frac{8mn^2(n-1) - 4m^2(n-1)v^{6-2n}}{n^2}} \right) \\
&= v^{n-2} \left(2\sqrt{2m-n+1} + U_2 \right).
\end{aligned} \tag{3.13}$$

Using Lemma 2.1.2, Equation (3.9) and proof of Theorem 3.3.1 it is obtained

$$\begin{aligned}
\xi_v(\overline{\mathcal{G}}) &\leq \overline{\lambda}_1 + \sqrt{(n-1)(2\Theta - \overline{\lambda}_1^2)} \\
&\leq 2v^{n-2}\sqrt{n^2 - 2n - 2m + 1} + \\
&\quad \sqrt{(n-1) \left(4(n^2 - 2m - n)v^{2n-2-2\delta(\mathcal{G})} - \frac{(n^2 - 2m - n)^2 v^{2n-2-2\Delta(\mathcal{G})}}{n^2} \right)} \\
&\leq 2v^{n-2}\sqrt{(n^2 - n - 2m)\left(1 + \frac{1-n}{n^2 - n - 2m}\right)} \\
&\quad + \sqrt{(n-1) \left(4(n^2 - n - 2m)v^{2n-4} - \frac{(n^2 - n - 2m)^2 v^2}{n^2} \right)} \\
&= v^{n-2}\sqrt{n^2 - n - 2m} \\
&\quad \times \left(2\sqrt{1 + \frac{-n+1}{n^2 - n - 2m}} + \sqrt{(n-1)4 - \frac{(n-1)(n^2 - n - 2m)v^{6-2n}}{n^2}} \right) \\
&= v^{n-2}\sqrt{n^2 - n - 2m} U'_2
\end{aligned} \tag{3.14}$$

From Equations (3.13) and (3.14), we get

$$\xi_v(\mathcal{G}) + \xi_v(\overline{\mathcal{G}}) \leq v^{n-2} (2\sqrt{2m-n+1} + U_2 + \sqrt{n^2 - n - 2m} U'_2).$$

The result is proved. \square

Theorem 3.5.4. *Suppose \mathcal{G} be a connected graph and $v > 1$. Then*

$$\xi_v(\mathcal{G}) + \xi_v(\overline{\mathcal{G}}) \geq 4v\sqrt{m} + 8(n^2 - n - 2m)v^{2n-2-2\Delta(\mathcal{G})}.$$

Proof. Theorem 3.4.2 gives

$$\xi_v(\mathcal{G}) \geq 4v\sqrt{m}. \quad (3.15)$$

By Part (1) of Lemma 3.1.1, we have $\sum_{k=1}^n \bar{\lambda}_k^2 = -2 \sum_{1 \leq i < j \leq n} \bar{\lambda}_i \bar{\lambda}_j$. Using Lemma 3.1.1 Part (2), we obtain

$$(\xi_v(\overline{\mathcal{G}}))^2 = \left(\sum_{k=1}^n |\bar{\lambda}_k| \right)^2 = \sum_{k=1}^n \lambda_k^2 + 2 \sum_{1 \leq i < j \leq n} |\bar{\lambda}_i \bar{\lambda}_j| \geq 2\Theta + 2 \sum_{1 \leq i < j \leq n} \bar{\lambda}_i \bar{\lambda}_j = 4\Theta.$$

We know that $\bar{\delta} = n - 1 - \Delta(\mathcal{G})$. Now

$$4\Theta = 4 \sum_{1 \leq i < j \leq n} (v^{d_{\overline{\mathcal{G}}}(u_i)} + v^{d_{\overline{\mathcal{G}}}(u_j)})^2 \geq 4 \sum_{1 \leq i < j \leq n} (2v^{\bar{\delta}})^2 = 8(n^2 - n - 2m)v^{2n-2-2\Delta(\mathcal{G})}.$$

Hence

$$\xi_v(\overline{\mathcal{G}}) \geq 8(n^2 - n - 2m)v^{2n-2-2\Delta(\mathcal{G})}. \quad (3.16)$$

From Equations (3.15) and (3.16), we have

$$\xi_v(\mathcal{G}) + \xi_v(\overline{\mathcal{G}}) \geq 4v\sqrt{m} + 8(n^2 - n - 2m)v^{2n-2-2\Delta(\mathcal{G})}.$$

□

3.6 V-equienergetic graphs

Graphs that have equal variable sum exdeg spectrum are called \mathcal{V} -cospectral, otherwise \mathcal{V} -noncospectral. The \mathcal{A}_v -spectrum of isomorphic graphs is equal and hence they have same variable sum exdeg energy. In current section,

we find certain classes of graphs that are \mathcal{V} -noncospectral but have same variable sum exdeg energy.

Let \mathcal{G} be a \mathcal{s} -regular graph. Suppose $\mathcal{L}_{\mathcal{G}}^1 = \mathcal{L}_{\mathcal{G}}$, $\mathcal{L}_{\mathcal{G}}^j = \mathcal{L}(\mathcal{L}_{\mathcal{G}}^{j-1})$ are repeated line graphs of \mathcal{G} , where $j = 1, 2, \dots$. Ramane et al. proved the formula given below for $\xi(\mathcal{L}_{\mathcal{G}}^2)$.

$$\xi(\mathcal{L}_{\mathcal{G}}^2) = 2n\mathcal{s}(\mathcal{s} - 2). \quad (3.17)$$

The idea of the proofs included in this section is taken from section 5 [40].

Theorem 3.6.1. *Consider two \mathcal{s} -regular graphs \mathcal{G}_1 and \mathcal{G}_2 with vertex set of size n . Also, let the graphs are \mathcal{A} -noncospectral. Then the line graphs $\mathcal{L}_{\mathcal{G}_1}^2$ and $\mathcal{L}_{\mathcal{G}_2}^2$ are \mathcal{V} -noncospectral with equal variable sum exdeg energy, that is $\xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_1}^2) = \xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_2}^2)$.*

Proof. As \mathcal{G} is an \mathcal{s} -regular and n -vertex graph, thus $\mathcal{L}_{\mathcal{G}}^2$ is $\frac{1}{2}n\mathcal{s}(\mathcal{s} - 1)$ -vertex and $(4\mathcal{s}-6)$ -regular graph. Now using theorem 3.1 we have,

$$\xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}}^2) = 2\mathcal{V}^{4\mathcal{s}-6}\xi(\mathcal{L}_{\mathcal{G}}^2)$$

Now using equation (3.17),

$$\xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}}^2) = 4n\mathcal{s}(\mathcal{s} - 2)\mathcal{V}^{4\mathcal{s}-6}$$

Hence $\xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_1}^2) = \xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_2}^2)$.

Since $\mathcal{A}_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}}^2) = 2\mathcal{V}^{4\mathcal{s}-6}\mathcal{A}(\mathcal{L}_{\mathcal{G}}^2)$ and $\mathcal{L}_{\mathcal{G}_1}^2$ and $\mathcal{L}_{\mathcal{G}_2}^2$ are \mathcal{A} -noncospectral graphs, therefore $\mathcal{L}_{\mathcal{G}_1}^2$ and $\mathcal{L}_{\mathcal{G}_2}^2$ are also \mathcal{V} -noncospectral graphs. \square

Corollary 3.6.1. *Consider two \mathcal{s} -regular and \mathcal{A} -noncospectral graphs \mathcal{G}_1 and \mathcal{G}_2 with vertex set of size n . Then for any $\mathcal{r} \geq 2$, the line graphs $\mathcal{L}_{\mathcal{G}_1}^{\mathcal{r}}$ and $\mathcal{L}_{\mathcal{G}_2}^{\mathcal{r}}$ are \mathcal{V} -noncospectral with $\xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_1}^{\mathcal{r}}) = \xi_{\mathcal{V}}(\mathcal{L}_{\mathcal{G}_2}^{\mathcal{r}})$.*

Theorem 3.6.2. *The graphs $\mathcal{G}_1 \cup \overline{\mathcal{K}}_t$ and $\mathcal{G}_2 \cup \overline{\mathcal{K}}_t$ are \mathcal{V} -noncospectral with $\xi_{\mathcal{V}}(\mathcal{G}_1 \cup \overline{\mathcal{K}}_t) = \xi_{\mathcal{V}}(\mathcal{G}_2 \cup \overline{\mathcal{K}}_t)$, where \mathcal{G}_1 and \mathcal{G}_2 are two n -vertex \mathcal{V} -noncospectral and \mathcal{V} -equienergetic graphs.*

Proof. Using theorem 3.3.2, we have

$$\xi_v(\mathcal{G}_1 \cup \overline{\mathcal{K}_t}) = \xi_v(\mathcal{G}_1) \cup \xi_v(\overline{\mathcal{K}_t})$$

As \mathcal{G}_1 and \mathcal{G}_2 are \mathcal{V} -equienergetic, $\xi_v(\mathcal{G}_1) = \xi_v(\mathcal{G}_2)$, hence

$$\begin{aligned} \xi_v(\mathcal{G}_1 \cup \overline{\mathcal{K}_t}) &= \xi_v(\mathcal{G}_2) \cup \xi_v(\overline{\mathcal{K}_t}) \\ &= \xi_v(\mathcal{G}_2 \cup \overline{\mathcal{K}_t}) \end{aligned}$$

Since \mathcal{G}_1 and \mathcal{G}_2 are \mathcal{V} -noncospectral, therefore $\mathcal{G}_1 \cup \overline{\mathcal{K}_t}$ and $\mathcal{G}_2 \cup \overline{\mathcal{K}_t}$ are \mathcal{V} -noncospectral. \square

Corollary 3.6.2. *For any $\tau \geq 2$, the graphs $\mathcal{L}^\tau_{\mathcal{G}_1} \cup \overline{\mathcal{K}_t}$ and $\mathcal{L}^\tau_{\mathcal{G}_2} \cup \overline{\mathcal{K}_t}$ are \mathcal{V} -noncospectral with $\xi_v(\mathcal{L}^\tau_{\mathcal{G}_1} \cup \overline{\mathcal{K}_t}) = \xi_v(\mathcal{L}^\tau_{\mathcal{G}_2} \cup \overline{\mathcal{K}_t})$, where \mathcal{G}_1 and \mathcal{G}_2 are both n -vertex, s -regular and \mathcal{V} -noncospectral graphs.*

Theorem 3.6.3. *Let \mathcal{G} be a graph with vertex set of size n . Let $q \equiv 0 \pmod{2}$. Suppose the disjoint union of $\frac{q}{2}$ copies of \mathcal{G}^* is the graph $\vec{\mathcal{G}}$. Then $\xi_v(\mathcal{G}^q) = \xi_v(\vec{\mathcal{G}})$.*

Theorem 3.6.4. *Consider a graph and let there is atleast one component of \mathcal{G} a cycle C_p . Also suppose $\check{\mathcal{G}}$ be another graph on n vertices having equal components as of \mathcal{G} excluding C_p . With respect to each cycle C_p in \mathcal{G} , the graph $\check{\mathcal{G}}$ has two corresponding cycles $C_{\frac{p}{2}}, C_{\frac{p}{2}}$. Then \mathcal{G} and $\check{\mathcal{G}}$ are \mathcal{V} -noncospectral graphs having equal variable sum exdeg energy.*

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