

Energy of graphs and signed digraphs



By

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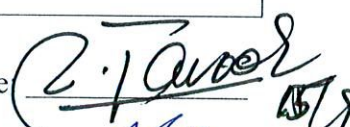
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Dedicated
to my
Parents and Teachers

Whose prayers always help me in every step of life and has been a source of inspiration for me

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Abstract

The energy of a graph is given by $\sum_{q=1}^n |\theta_q|$, where $\theta_{q's}$ are the adjacency eigenvalues of the graph. A graph has real eigenvalues because its adjacency matrix is always symmetric. The energy of a sidigraph is defined by $\sum_{q=1}^n |\operatorname{Re}(\xi_q)|$, where $\operatorname{Re}(\xi_q)$ represents the real part of eigenvalue ξ_q of the sidigraph. A sidigraph has complex eigenvalues because its adjacency matrix is not necessarily symmetric. A topological index is recognized as molecular descriptor that is a conversion of a molecular structure into some real number.

In our disquisition, we first focused on the extremal energy of sidigraphs. We investigate the bicyclic sidigraphs having largest energy in the set of all bicyclic sidigraphs with fixed order. We construct some non-cospectral bicyclic sidigraphs having equal energy. We also investigate the energy ordering of signed digraphs in the class of all vertex-disjoint bicyclic sidigraphs. Our second focus is on the energy of graphs based on the inverse sum indeg matrix and generalized inverse sum indeg matrix. These matrices are defined by using definition of respective indices. We give inverse sum indeg energy formula of some graphs. Bounds on inverse sum indeg energy of graphs are obtained. Some non-cospectral equienergetic graphs with respect to inverse sum indeg energy are also obtained. In the end, we introduce generalized inverse sum indeg index and generalized inverse sum indeg energy of graphs. We study the generalized inverse sum indeg index and energy from an algebraic point of view. Extremal values of this index for some graph classes are determined. Some spectral properties of generalized inverse sum indeg matrix are studied. We also find Nordhaus-Gaddum-type results for generalized sum indeg energy and spectral radius of generalized inverse sum indeg matrix.

List of publications

- (1) Sumaira Hafeez, Rashid Farooq, Mehtab Khan,
Bicyclic signed digraphs with maximal energy, *Appl. Math. Comput.*, **347** (2019), 702–711.
- (2) Sumaira Hafeez, Rashid Farooq,
Inverse sum indeg energy of graphs, *IEEE Access*, **7** (2019), 100860–100866.
- (3) Sumaira Hafeez, Rashid Farooq,
On energy ordering of vertex-disjoint bicyclic sidigraphs, *AIMS Mathematics*, **5** (6) (2020), 6693–6713.
- (4) Sumaira Hafeez, Rashid Farooq,
On generalized inverse sum indeg index and energy of graphs, *AIMS Mathematics*, **5** (3) (2020), 2388–2411.

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Chapter 1

Introduction to Graph Theory

In the first section of current chapter, a brief history review of graph theory is given. Some terminologies of graph theory that we have used in our whole disquisition is given in Section 1.2. In next sections, a short review on spectral graph theory is given and some special types of graphs are discussed. In the end, we give plan of the whole disquisition.

1.1 Background

A Swiss mathematician Leonhard Euler introduced the notion of graphs in the 18th century. His attempt of solution to the eminent “Königsberg bridge” problem given below is the origin of graph theory: On the Pregel river, the Königsberg city (now Kaliningrad, Russia) is situated. The river divides city into four parts of land connected by seven bridges. A question arose that whether there is the possibility of a walk over the city such that every bridge is crossed exactly once? The visual representation of this problem is given in Figure 1.1.

In 1736, Euler solved the problem using graph theory and proved that such type of walk is not possible. In the graph given by Euler (see Figure 1.2), he represented the lands by vertices and bridges by edges.

For further study on the historical aspects and Königsberg bridge problem solution given by Euler, see [5, 42]. In 1936, the first known graph theory book titled “Theorie der endlichen

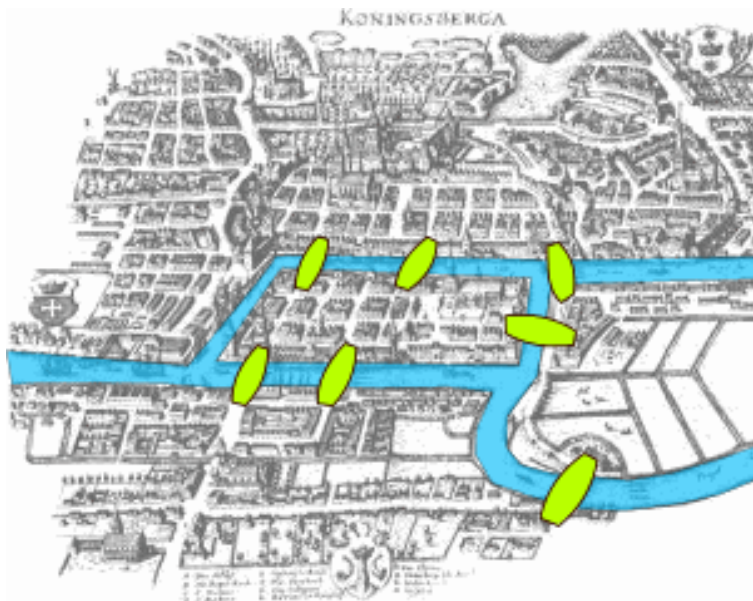


Figure 1.1: Königsberg bridge problem

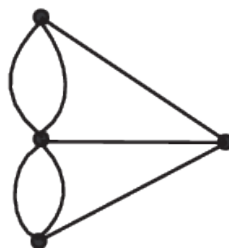


Figure 1.2: The Königsberg bridge problem graph

und unendlichen Graphen” was given by König. Graph theory has remarkable applications in almost every branch of science such as applied mathematics, chemistry, engineering, computer science, biology and a lot more.

1.2 Graph terminologies

An m -vertex graph $\mathcal{G} = (\mathbb{V}_{\mathcal{G}}, \mathbb{E}_{\mathcal{G}})$, consists of $\mathbb{V}_{\mathcal{G}}$, a set of m vertices and $\mathbb{E}_{\mathcal{G}}$, a set of edges. If $w, z \in \mathbb{V}_{\mathcal{G}}$ are joined by an edge then they are called adjacent, denoted by wz (or zw) and an edge wz is an incident edge on w and z . Two edges are called adjacent if their some of end vertices are common. For a graph \mathcal{G} , the size $e_{\mathcal{G}}$ and order $n_{\mathcal{G}}$ are given by $e_{\mathcal{G}} = |\mathbb{E}_{\mathcal{G}}|$ and $n_{\mathcal{G}} = |\mathbb{V}_{\mathcal{G}}|$, respectively. For any $w \in \mathbb{V}_{\mathcal{G}}$, the neighbourhood $N_{\mathcal{G}}(w)$ of w is given as $N_{\mathcal{G}}(w) = \{z \mid wz \in \mathbb{E}_{\mathcal{G}}\}$. Parallel edges are the edges that have same end vertices. An edge $wz \in \mathbb{E}_{\mathcal{G}}$ is said to be a loop if $w = z$. A graph is simple whenever it contains no loop or parallel edges. For vertex $w \in \mathbb{V}_{\mathcal{G}}$, the degree of w is the cardinality $|N_{\mathcal{G}}(w)|$, denoted by $d_{\mathcal{G}}(w)$ or $d(w)$ or $d_{\mathcal{G}}^{(w)}$. For any vertex w , if $|N_{\mathcal{G}}(w)| = 0$, then w is recognized as an isolated vertex and if $|N_{\mathcal{G}}(w)| = 1$, then w is a leaf. A graph formed from \mathcal{G} by eliminating $w \in \mathbb{V}_{\mathcal{G}}$ and each edge incident on w is expressed as $\mathcal{G} \setminus \{w\}$. For any $wz \in \mathbb{E}_{\mathcal{G}}$, the term $\mathcal{G} \setminus \{wz\}$ is defined similarly.

The largest (respectively, smallest) degree of \mathcal{G} is the largest (respectively, smallest) vertex degree in \mathcal{G} , represented as $\nabla_{\mathcal{G}}$ (respectively, $\delta_{\mathcal{G}}$). A graph of order $n_{\mathcal{G}}$, size $e_{\mathcal{G}}$, largest degree $\nabla_{\mathcal{G}}$ and smallest degree $\delta_{\mathcal{G}}$ is represented by $\mathcal{G}(n_{\mathcal{G}}, e_{\mathcal{G}}, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ and a graph of order $n_{\mathcal{G}}$ and size $e_{\mathcal{G}}$ is represented by $\mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$. A graph with $d_{\mathcal{G}}^{(w)} = b$ for every $w \in \mathbb{V}_{\mathcal{G}}$, is a b -regular graph.

The complement of a simple graph \mathcal{G} is a graph represented by $\overline{\mathcal{G}}$ with the property that $\mathbb{V}_{\mathcal{G}} = \mathbb{V}_{\overline{\mathcal{G}}}$ and $wz \in \mathbb{E}_{\mathcal{G}}$ if and only if $wz \notin \mathbb{E}_{\overline{\mathcal{G}}}$. Therefore $n_{\mathcal{G}} = n_{\overline{\mathcal{G}}}$, $e_{\overline{\mathcal{G}}} = \frac{1}{2}(n_{\mathcal{G}}^2 - n_{\mathcal{G}}) - e_{\mathcal{G}}$, $\nabla_{\overline{\mathcal{G}}} = n_{\mathcal{G}} - 1 - \delta_{\mathcal{G}}$ and $\delta_{\overline{\mathcal{G}}} = n_{\mathcal{G}} - 1 - \nabla_{\mathcal{G}}$.

Suppose \mathcal{G} is a graph with $\mathbb{V}_{\mathcal{G}} = \{w_0, \dots, w_m\}$ and $\mathbb{E}_{\mathcal{G}} = \{s_1, \dots, s_m\}$. Then a terminable sequence $w_0, s_1, w_1, s_2, w_2, s_3, \dots, w_{m-1}, s_m, w_m$, where $s_q = w_{q-1}w_q$, $q = 1, \dots, m$ is said to be a walk between w_0 and w_m . An m -vertex path \mathcal{P}_m , ($m \geq 1$), is a simple graph with $\mathbb{V}_{\mathcal{P}_m} = \{w_1, \dots, w_m\}$ and $\mathbb{E}_{\mathcal{P}_m} = \{w_q w_{q+1} \mid q = 1, 2, \dots, m-1\}$. An m -vertex cycle C_m ($m \geq 3$) is a simple graph with $\mathbb{V}_{C_m} = \{w_1, \dots, w_m\}$ and $\mathbb{E}_{C_m} = \{w_q w_{q+1} \mid q = 1, 2, \dots, m-1\} \cup \{w_m w_1\}$. A graph not containing any cycle is an acyclic graph. If for every pair $w, z \in \mathbb{V}_{\mathcal{G}}$ of \mathcal{G} , a path exists between w and z , then \mathcal{G} is a connected graph; otherwise disconnected.

A connected and acyclic graph of order m is a tree represented by \mathcal{T}_m . A star graph \mathcal{S}_m is a

tree with $n_{S_m} = m$, in which one vertex is adjacent to $m - 1$ leaves. For $w, z \in \mathbb{V}_{\mathcal{G}}$, the distance between w and z is the length of the smallest path between w and z . The largest distance between a vertex w of a graph \mathcal{G} to every other vertex of \mathcal{G} is called the eccentricity of w . The diameter of \mathcal{G} is the largest eccentricity of a vertex in \mathcal{G} .

An m -vertex simple graph whose every vertex is adjacent to other $m - 1$ vertices is termed as a complete graph represented by \mathcal{K}_m . If we can split vertex set $\mathbb{V}_{\mathcal{G}}$ of a graph \mathcal{G} into two disjoint sets X_1 and X_2 with the property that vertices of the same set are pairwise nonadjacent then \mathcal{G} is termed as a bipartite graph. The sets X_1 and X_2 are called partite sets of a bipartite graph \mathcal{G} . A complete bipartite graph $\mathcal{K}_{r,s}$ is a bipartite graph with partite sets X_1 and X_2 such that $|X_1| = r$, $|X_2| = s$ and each vertex in X_1 is adjacent to each vertex in X_2 .

Suppose \mathcal{H}_1 and \mathcal{H}_2 are two simple graphs with $\mathbb{V}_{\mathcal{H}_1} \cap \mathbb{V}_{\mathcal{H}_2} = \phi$. The disjoint graph union $\mathcal{H}_1 \cup \mathcal{H}_2$ is a graph with $\mathbb{V}_{\mathcal{H}_1 \cup \mathcal{H}_2} = \mathbb{V}_{\mathcal{H}_1} \cup \mathbb{V}_{\mathcal{H}_2}$ and $\mathbb{E}_{\mathcal{H}_1 \cup \mathcal{H}_2} = \mathbb{E}_{\mathcal{H}_1} \cup \mathbb{E}_{\mathcal{H}_2}$. For any vertex $w \in \mathbb{V}_{\mathcal{H}_1 \cup \mathcal{H}_2}$, $d_{\mathcal{H}_1 \cup \mathcal{H}_2}^{(w)} = d_{\mathcal{H}_q}^{(w)}$, $q = 1, 2$. The join $\mathcal{H}_1 \wedge \mathcal{H}_2$ is formed by adding $wz \in \mathbb{E}_{\mathcal{H}_1 \wedge \mathcal{H}_2}$ for each $w \in \mathbb{V}_{\mathcal{H}_1}$ and $z \in \mathbb{V}_{\mathcal{H}_2}$. Two graphs \mathcal{H}_1 and \mathcal{H}_2 are said to be isomorphic if there exists a bijection ψ among $\mathbb{V}_{\mathcal{H}_1}$ and $\mathbb{V}_{\mathcal{H}_2}$ with the property that $wz \in \mathbb{E}_{\mathcal{H}_1}$ if and only if $\psi(w)\psi(z) \in \mathbb{E}_{\mathcal{H}_2}$, represented as $\mathcal{H}_1 \cong \mathcal{H}_2$.

A subgraph \mathcal{G}_1 of \mathcal{G} is the graph with $\mathbb{V}_{\mathcal{G}_1} \subseteq \mathbb{V}_{\mathcal{G}}$ and $\mathbb{E}_{\mathcal{G}_1} \subseteq \mathbb{E}_{\mathcal{G}}$. A largest connected subgraph of \mathcal{G} is a component of \mathcal{G} . A graph \mathcal{G} is said to be an elementary figure if $\mathcal{G} \cong \mathcal{K}_2$ or $\mathcal{G} \cong C_m$, $m \geq 3$. A basic figure is a graph with elementary figures as components.

Any subset of non-adjacent vertices of \mathcal{G} forms an independent set of \mathcal{G} . An independence number of a graph \mathcal{G} is the largest size of its independent set. The line graph $\mathcal{L}_{\mathcal{G}}$ of \mathcal{G} is the graph with $\mathbb{V}_{\mathcal{L}_{\mathcal{G}}} = \mathbb{E}_{\mathcal{G}}$ and two vertices of $\mathcal{L}_{\mathcal{G}}$ are adjacent if and only if their corresponding edges in \mathcal{G} have a common end vertex.

1.3 Spectral graph theory

Spectral graph theory is a field of graph theory that study the graph properties through some properties of a matrix related to it, that is, eigenvalues and characteristic polynomial. It is used

to find the solutions of some chemical problems. Spectral graph theory appears in 1950. At that time two major researches were going on: a technique suggested by Erich Hückel in 1930 called Hückel molecular orbital (HMO) method and a connection among spectral and structural properties of graphs.

In 1980, Cvetković et al. [16] study the connection between these directions. The authors compiled approximately whole research till date in aforementioned area. The authors revised the survey in 1988 [14]. In 1995, Cvetkovic et al. [15] give the third edition of the book.

The adjacency matrix $\mathcal{A}(\mathcal{G}) = [a_{rs}]_{m \times m}$ of a simple graph \mathcal{G} with $n_{\mathcal{G}} = m$ is an $m \times m$ matrix, where

$$a_{rs} = \begin{cases} 1 & \text{if } w_r, w_s \in \mathbb{E}_{\mathcal{G}} \\ 0 & \text{otherwise.} \end{cases}$$

The \mathcal{A} -characteristic polynomial of \mathcal{G} is given by:

$$\begin{aligned} \Psi_{\mathcal{G}}(\theta) &= \det(\mathcal{A}(\mathcal{G}) - \theta I_m) \\ &= \theta^m + \sum_{q=1}^m a_q \theta^{m-q}, \end{aligned} \quad (1.1)$$

where I_m is an $m \times m$ identity matrix. The \mathcal{A} -eigenvalues of \mathcal{G} are the roots of $\Psi_{\mathcal{G}}(\theta)$ given in Equation (1.1). The \mathcal{A} -spectrum, $\text{spec}_{\mathcal{A}}(\mathcal{G})$, is the collection of all \mathcal{A} -eigenvalues of \mathcal{G} together with multiplicities.

Graph energy is one of the strongest area in spectral graph theory. This concept of graph energy is given by Hückel. The equation $(P - \mathcal{E})\varphi = 0$ with P as the energy operator and \mathcal{E} as the energy of electron is the Schrodinger wave equation. The solution of this equation is φ (also called wave function). To get the result for the molecules, a very important role is played by Hückel. Hückel normalizes the system in such a way that P becomes $\mathcal{A}(\mathcal{G})$ of the respective graph \mathcal{G} . The solution φ becomes the roots of $\Psi_{\mathcal{G}}(\theta)$.

One can study about Hückel theory and its relation with spectral graph theory in [16]. In chemistry, the levels of energy of many classes of conjugated hydrocarbons can be determined by knowing about the energy levels of general class of graphs. A significant amount of research has been done by Hückel [46] till date.

If a graph \mathcal{G} represents a structural formula of some chemical compound, then \mathcal{G} is called a molecular graph or chemical graph. In this graph, hydrogen atoms are not considered, see [26]. The edges and vertices of such graph corresponds to the chemical bond and atom of the compound, respectively.

The graph energy determines the π -electron energy of a conjugated carbon molecule. The energy of a graph \mathcal{G} is given by:

$$\mathcal{E}(\mathcal{G}) = \sum_{q=1}^m |\theta_q|,$$

where $\theta_{q's}$ are the \mathcal{A} -eigenvalues of \mathcal{G} .

Gutman [27] gave the concept of graph energy in 1978. Till now, a significant amount of research has been done in this direction.

1.3.1 Spectra and graph energy

In the current section, a brief introduction to graph energy is given. Next theorem is used to find the coefficients of the \mathcal{A} -characteristic polynomial of a graph.

Theorem 1.1 (Cvetković et al. [16]). *Suppose \mathcal{G} is a graph with $n_{\mathcal{G}} = m$ and \mathcal{A} -characteristic polynomial of the form*

$$\Psi_{\mathcal{G}}(\theta) = \theta^m + \sum_{q=1}^m a_q \theta^{m-q}.$$

Then for each $q = 1, \dots, m$,

$$a_q = \sum_{Y \in \mathbb{L}_q} (-1)^{p(Y)2^{c(Y)}},$$

where \mathbb{L}_p is the collection of every basic figure Y of \mathcal{G} of order q , $p(Y)$ represents the number of components of Y and $c(Y)$ represents the collection of each cycle of Y .

Coulson's integral formula is one of the most important formula that calculates the graph energy without finding the eigenvalues. It finds the energy by using the characteristic polynomial. The term $p.v. \int_{-\infty}^{\infty} F(z)dz$ represents the principal value of $\int_{-\infty}^{\infty} F(z)dz$.

Theorem 1.2 (Coulson [13]). *Suppose \mathcal{G} is a graph with $n_{\mathcal{G}} = m$ and \mathcal{A} -characteristic polynomial $\Psi_{\mathcal{G}}(\theta)$. Then*

$$\mathcal{E}(\mathcal{G}) = \frac{1}{\pi} p.v \int_{-\infty}^{+\infty} \left(m - \frac{i\theta \Psi'_{\mathcal{G}}(i\theta)}{\Psi_{\mathcal{G}}(i\theta)} \right) d\theta,$$

where $\Psi'_{\mathcal{G}}(i\theta) = \frac{d}{d(i\theta)} \Psi_{\mathcal{G}}(i\theta)$.

An alternative form of Coulson integral formula is given by Gutman [27].

Theorem 1.3 (Gutman [27]). *Suppose \mathcal{G} is a graph with $n_{\mathcal{G}} = m$ and \mathcal{A} -characteristic polynomial $\Psi_{\mathcal{G}}(\theta) = \theta^m + \sum_{q=1}^m b_q \theta^{m-q}$. Then*

$$\mathcal{E}(\mathcal{G}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\theta^2} \log \left[\left(\sum_{q=0}^{\lfloor \frac{m}{2} \rfloor} (-1)^q b_{2q} \theta^{2q} \right)^2 + \left(\sum_{q=0}^{\lfloor \frac{m}{2} \rfloor} (-1)^q b_{2q+1} \theta^{2q+1} \right)^2 \right] d\theta.$$

Many bounds for the graph energy are known. We here give some of the bounds. The following theorem gives bounds on graph energy.

Theorem 1.4 (McClelland [55]). *Suppose $\mathcal{H} = \mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$ is a graph. Then*

$$\sqrt{2e_{\mathcal{G}} + n_{\mathcal{G}}(n_{\mathcal{G}} - 1)|\mathcal{A}(\mathcal{H})|^{\frac{n_{\mathcal{G}}}{2}}} \leq \mathcal{E}(\mathcal{H}) \leq \sqrt{2e_{\mathcal{H}}n_{\mathcal{H}}}. \quad (1.2)$$

A graph is nonsingular if it has nonsingular adjacency matrix. Das and Gutman [19] gave the following lower bound.

Theorem 1.5 (Das and Gutman [19]). *Suppose $\mathcal{H} = \mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$ is a nonsingular graph with $n_{\mathcal{H}} \geq 1$.*

Also let $W = \frac{4}{(n_{\mathcal{H}}+1)(n_{\mathcal{H}}-2)} \left[\sqrt{\frac{2e_{\mathcal{H}}}{n_{\mathcal{H}}}} - \left(\frac{2e_{\mathcal{H}}}{n_{\mathcal{H}}} \right)^{\frac{1}{4}} \right]^2$. Then

$$\mathcal{E}(\mathcal{H}) \geq \sqrt{2e_{\mathcal{H}} + n_{\mathcal{H}}(n_{\mathcal{H}} - 1)|\det \mathcal{A}(\mathcal{H})|^{\frac{2}{n_{\mathcal{H}}}} + W},$$

where the inequality becomes equality for $\mathcal{H} \cong \overline{\mathcal{K}}_{n_{\mathcal{G}}}$ or \mathcal{H} is isomorphic to $\frac{n_{\mathcal{G}}}{2}$ copies of \mathcal{K}_2 (when $n_{\mathcal{G}}$ is even).

Next theorem gives bounds on graph energy with respect to its size and order.

Theorem 1.6 (Koolen and Moulton [52]). *Suppose $\mathcal{H} = \mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$ is a graph with $2e_{\mathcal{H}} \geq n_{\mathcal{H}}$. Also suppose \mathcal{G}_1 is a graph which is connected and has exactly two non trivial \mathcal{A} -eigenvalues with absolute value $\sqrt{\frac{2e_{\mathcal{H}} - \frac{4e_{\mathcal{H}}^2}{n_{\mathcal{H}}}}{n_{\mathcal{H}} - 1}}$. Then*

$$\mathcal{E}(\mathcal{H}) \leq \frac{2e_{\mathcal{H}}}{n_{\mathcal{H}}} + \sqrt{(n_{\mathcal{H}} - 1) \left(2e_{\mathcal{H}} - \frac{4e_{\mathcal{H}}^2}{n_{\mathcal{H}}} \right)},$$

where the inequality becomes equality for $\mathcal{H} \cong \mathcal{G}_1$ or $\mathcal{H} \cong \mathcal{K}_{n_{\mathcal{H}}}$ or \mathcal{H} is isomorphic to $\frac{n_{\mathcal{H}}}{2}$ copies of \mathcal{K}_2 .

Following two theorems give some information about the energy of a graph \mathcal{G} .

Theorem 1.7 (Bapat and Pati [3]). *For an odd integer b , $\mathcal{E}(\mathcal{G}) \neq b$.*

Theorem 1.8 (Pirzada and Gutman [63]). *For an odd integer b , $\mathcal{E}(\mathcal{G}) \neq \sqrt{b}$.*

Next result is about the bounds on graph spectra.

Theorem 1.9 (Brigham and Dutton [6]). *Suppose $\mathcal{H} = \mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$ is a graph with \mathcal{A} -eigenvalues $\theta_1 \geq \dots \geq \theta_{n_{\mathcal{H}}}$. Then for each integer $f \in [1, n_{\mathcal{H}}]$*

$$-\sqrt{\frac{2(f-1)e_{\mathcal{H}}}{(n_{\mathcal{H}}+1-f)}} \leq \sqrt{n_{\mathcal{H}}} \theta_f \leq \sqrt{\frac{2(-f+n_{\mathcal{H}})e_{\mathcal{H}}}{f}}.$$

Nikiforov [59] proved the following conjecture given by Koolen and Moulton [51]: For some $\varepsilon > 0$, a graph $\mathcal{H} = \mathcal{G}_{n_{\mathcal{G}}}^{e_{\mathcal{G}}}$ exists with

$$\mathcal{E}(\mathcal{H}) \geq (\sqrt{n_{\mathcal{H}}} + 1)(1 - \varepsilon) \frac{n_{\mathcal{H}}}{2},$$

for almost every $n_{\mathcal{H}} \geq 1$.

1.4 Weighted graphs

A wighted graph is a pair $\mathcal{W} = (\mathcal{G}, \varpi)$, where $\mathcal{G} = (\mathbb{V}_{\mathcal{G}}, \mathbb{E}_{\mathcal{G}})$ is the underlying graph and $\varpi : \mathbb{E}_{\mathcal{G}} \rightarrow \mathbb{R} \setminus \{0\}$ is the corresponding weight function. For any edge $e \in \mathbb{E}_{\mathcal{W}}$, the weight of e

is denoted by $\varpi(e)$. If $\varpi(e) = 1$ for each $e \in \mathbb{E}_{\mathcal{W}}$, then \mathcal{W} is considered as a graph. Therefore graphs are subclass of weighted graphs. The weight of \mathcal{W} , represented by $\varpi(\mathcal{W})$ is defined as $\varpi(\mathcal{W}) = \prod_{wz \in \mathbb{E}_{\mathcal{W}}} \varpi(wz)$. If $\varpi(\mathcal{W}) > 0$ (respectively, $\varpi(\mathcal{W}) < 0$), then \mathcal{W} is called positive (respectively, negative) weighted graph. If every cycle of weighted graph \mathcal{W} is positive, then \mathcal{W} is called balanced; otherwise unbalanced. Note that if the conjugated molecule has atoms that are not carbon or hydrogen, then its respective graph has weighted edges. Hence there is chemical significance of results on the energy of weighted graphs.

The adjacency matrix $\mathcal{A}(\mathcal{W}) = [a_{pq}]_{m \times m}$ of a weighted graph \mathcal{W} with $n_{\mathcal{W}} = m$, is an $m \times m$ matrix, where

$$a_{pq} = \begin{cases} \varpi(w_p w_q) & \text{if } w_p w_q \in \mathbb{E}_{\mathcal{W}} \\ 0 & \text{otherwise.} \end{cases}$$

The \mathcal{A} -characteristic polynomial of \mathcal{W} is given by:

$$\begin{aligned} \Psi_{\mathcal{W}}(\theta) &= \det(\mathcal{A}(\mathcal{W}) - \theta I_m) \\ &= \theta^m + \sum_{q=1}^m c_q \theta^{m-q}, \end{aligned}$$

where I_m is an $m \times m$ identity matrix. The \mathcal{A} -eigenvalues of \mathcal{W} are the roots of $\Psi_{\mathcal{W}}(\theta)$.

The recursive formula for characteristic polynomial of \mathcal{W} is given in next theorem.

Theorem 1.10 (Gutman and Shao [32]). *Suppose $\mathcal{W} = (G, \varpi)$ be a weighted graph and $wz \in \mathbb{E}_{\mathcal{W}}$. Then,*

$$\Psi_{\mathcal{W}}(\theta) = \Psi_{\mathcal{W} \setminus \{wz\}}(\theta) - \varpi^2(wz) \Psi_{\mathcal{W} \setminus \{w\} \setminus \{z\}}(\theta) - 2 \sum_C \omega(C) \Psi_{\mathcal{W} \setminus C}(\theta),$$

where the summation is taken on each cycle C containing wz .

Now if $\varpi : \mathbb{E}_{\mathcal{W}} \rightarrow \{1, -1\}$, then \mathcal{W} is called a signed graph. Thus weighted graphs are the generalization of signed graphs.

Gutman and Shao [32] defined the energy of weighted graphs as

$$\mathcal{E}(\mathcal{W}) = \sum_{q=1}^m |\theta_q|,$$

where θ_q denotes the \mathcal{A} -eigenvalues of \mathcal{W} . For the study about eigenvalues of weighted graphs and chemical theories related to it, see [12, 24]

1.5 Weighted digraphs

A directed graph (for short, digraph) $\mathcal{D} = (\mathbb{V}_{\mathcal{D}}, \mathbb{A}_{\mathcal{D}})$ consists of $\mathbb{V}_{\mathcal{D}}$, a set of nodes (vertices) and $\mathbb{A}_{\mathcal{D}}$, a set of arcs. A weighted digraph $\mathbb{W} = (\mathcal{D}, \psi)$ is a pair, where $\mathcal{D} = (\mathbb{V}_{\mathbb{W}}, \mathbb{A}_{\mathbb{W}})$ is the underlying digraph of \mathbb{W} and $\psi : \mathbb{A}_{\mathbb{W}} \rightarrow \mathbb{R} \setminus \{0\}$ is the corresponding weight function. For any $w, z \in \mathbb{W}$, if there is an arc from w to z then they are called adjacent, represented by (w, z) . A weighted arc is an arc with a given weight. The weight of (w, z) is denoted by $\psi(w, z)$. The sign of a weighted arc is the sign of its weight. The weight of \mathbb{W} , represented by $\psi(\mathbb{W})$, is defined as $\psi(\mathbb{W}) = \prod_{wz \in \mathbb{A}_{\mathbb{W}}} \psi(w, z)$. The weighted digraph \mathbb{W} is said to be positive if $\psi(\mathbb{W}) > 0$ and negative if $\psi(\mathbb{W}) < 0$. The order $n_{\mathbb{W}}$ and size $e_{\mathbb{W}}$ of \mathbb{W} are the cardinalities $n_{\mathbb{W}} = |\mathbb{V}_{\mathbb{W}}|$ and $e_{\mathbb{W}} = |\mathbb{A}_{\mathbb{W}}|$, respectively.

An m -vertex directed weighted path \mathcal{P}_m is a weighted digraph with $\mathbb{V}_{\mathcal{P}_m} = \{w_1, w_2, \dots, w_m\}$ and weighted arcs $\mathbb{A}_{\mathcal{P}_m} = \{(w_q, w_{q+1}) \mid q = 1, 2, \dots, m-1\}$. An m -vertex weighted directed cycle C_m , ($m \geq 2$), is a weighted digraph with $\mathbb{V}_{C_m} = \{w_1, w_2, \dots, w_m\}$ and weighted arcs $\mathbb{A}_{C_m} = \{(w_q, w_{q+1}) \cup (w_m, w_1), q = 1, 2, \dots, m-1\}$. For every cycle C_m of \mathbb{W} , if $\psi(C_m) > 0$ (respectively, $\psi(C_m) < 0$), then \mathbb{W} is called cycle-balanced (respectively, cycle unbalanced) weighted digraph. A linear weighted digraph is a digraph whose all components are cycles. If for every pair $w, z \in \mathbb{V}_{\mathbb{W}}$, a weighted directed path from a vertex w to a vertex z and from a vertex z to a vertex w exists, then \mathbb{W} is said to be a strongly connected weighted digraph. The maximal connected subdigraphs of \mathbb{W} are the strong components of \mathbb{W} .

If all arcs of a weighted digraph \mathbb{W} are replaced by undirected edges then the corresponding graph is called the underlying weighted graph of \mathbb{W} . A weighted digraph in which $n_{\mathbb{W}} = e_{\mathbb{W}}$ and has a unique cycle is a unicyclic weighted digraph. A weighted digraph whose underlying weighted graph is connected and that has exactly two weighted directed cycles is called a bicyclic weighted digraph.

A symmetric weighted digraph $\overleftrightarrow{\mathbb{W}}$ is a weighted digraph with the property that if $(w, z) \in \mathbb{A}_{\overleftrightarrow{\mathbb{W}}}$ with $\psi(w, z) = p$, then $(z, w) \in \mathbb{A}_{\overleftrightarrow{\mathbb{W}}}$ with $\psi(z, w) = p$. A one to one correspondence between \mathcal{W} and $\overleftrightarrow{\mathbb{W}}$ is given by $\mathcal{W} \rightsquigarrow \overleftrightarrow{\mathbb{W}}$, where $\mathbb{V}_{\overleftrightarrow{\mathbb{W}}} = \mathbb{V}_{\mathcal{W}}$ and each $wz \in \mathbb{E}_{\mathcal{W}}$ with $\varpi(wz) = p$ is

replaced by two arcs $(w, z), (z, w)$ with $\psi(w, z) = \psi(z, w) = p$.

The adjacency matrix $\mathcal{A}(\mathbb{W}) = [a_{pq}]_{m \times m}$ of a weighted digraph \mathbb{W} with $n_{\mathbb{W}} = m$ is defined by

$$a_{pq} = \begin{cases} \psi(w_p, w_q) & \text{if } (w_p, w_q) \in \mathbb{A}_{\mathbb{W}}, \\ 0 & \text{otherwise.} \end{cases}$$

The \mathcal{A} -characteristic polynomial of \mathbb{W} is given by:

$$\Psi_{\mathbb{W}}(\xi) = \det(\mathcal{A}(\mathbb{W}) - \xi I_m),$$

where I_m is an $m \times m$ identity matrix. The \mathcal{A} -eigenvalues of \mathbb{W} are the roots of $\Psi_{\mathbb{W}}(\xi)$. The \mathcal{A} -spectrum, $\text{spec}_{\mathcal{A}}(\mathbb{W})$, is the collection of all \mathcal{A} -eigenvalues of \mathbb{W} together with their multiplicities. Next theorem is used to find the coefficients of the \mathcal{A} -characteristic polynomial of weighted digraph.

Theorem 1.11 (Achariya [1]). *Suppose \mathbb{W} is a weighted digraph with \mathcal{A} -characteristic polynomial*

$$\Psi_{\mathbb{W}}(\xi) = \xi^m + \sum_{q=1}^m b_q \xi^{m-q}.$$

Then for each $q = 1, 2, \dots, m$

$$b_q = \sum_{Y \in \mathcal{L}_q} (-1)^{p(Y)} |\omega(Y)| s(Y),$$

where \mathcal{L}_q represents the collection of each linear weighted subdigraph Y of \mathbb{W} of order q , $p(Y)$ represents the number of components of Y , $\omega(Y)$ is the weight of linear weighted subdigraph Y and $s(Y)$ denotes the sign of Y .

Now if $\psi(w, z) = 1$ for each arc $(w, z) \in \mathbb{A}_{\mathbb{W}}$, then \mathbb{W} is called a digraph. Also if in weighted digraph $\mathbb{W} = (\mathcal{D}, \psi)$, we take $\psi : \mathbb{A}_{\mathbb{W}} \rightarrow \{1, -1\}$, then \mathbb{W} is called a signed digraph or sidigraph. Hence weighted digraphs are generalizations of digraphs and sidigraphs.

1.6 Overview

We give here whole plan of our disquisition. In second chapter, some results related to energy of sidigraphs and degree based energies of graphs are given. In third chapter, we find extremal energy over a set of all bicyclic sidigraphs. At the end of this chapter, we find some noncospectral equienergetic sidigraphs. For this chapter, see the paper by Hafeez et al. [36]. In fourth chapter, we investigate the ordering of all vertex-disjoint bicyclic sidigraphs with respect to energy. In fifth chapter, we give some properties of inverse sum indeg matrix and energy. This matrix is defined using definition of inverse sum indeg index. We give energy formula for some graphs with respect to ISI matrix and also find bounds for ISI energy. We also give some non-cospectral graphs having same ISI energy. For this chapter, see the paper by Hafeez and Farooq [37]. In sixth chapter, we define generalized inverse sum indeg index and energy. We determine the largest and smallest value of this index in some graph classes. We study the spectral properties of generalized ISI matrix. Some bounds on generalized ISI spectral radius and energy are calculated and finds the Nordhaus-Gaddum type inequalities for them. For this chapter, see the paper by Hafeez and Farooq [38]

Chapter 2

Graphs and sidigraphs energy

In first section of the current chapter, we give a review of energy of sidigraphs. This concept was introduced by Pirzada and Bhat [62]. In second section, we discuss about the energy of graphs based on degree of vertices and give some basic results. This concept of the adjacency matrix related to topological indices was introduced in [67]. Later, many types of graph energies related to topological indices are introduced and some of them have applications in chemistry.

2.1 Energy of sidigraphs

Suppose ξ_1, \dots, ξ_m are the eigenvalues of a sidigraph \mathcal{S} . The energy of \mathcal{S} is given by

$$\mathcal{E}(\mathcal{S}) = \sum_{q=1}^m |\operatorname{Re}(\xi_q)|, \quad (2.1)$$

where $\operatorname{Re}(\xi_q)$ represents the real part of ξ_q , see [60].

The \mathcal{A} -characteristic polynomials of a positive directed signed cycle C_m and a negative directed signed cycle C_m computed through Theorem 1.11 are:

$$\Psi_{C_m}(\xi) = \xi^m - 1,$$

$$\Psi_{C_m}(\xi) = \xi^m + 1.$$

Therefore, the energy of C_m and \mathbf{C}_m are, respectively, computed as:

$$\begin{aligned}\mathcal{E}(C_m) &= \sum_{q=0}^{m-1} \left| \cos \frac{2q\pi}{m} \right|, \\ \mathcal{E}(\mathbf{C}_m) &= \sum_{q=0}^{m-1} \left| \cos \frac{(2q+1)\pi}{m} \right|.\end{aligned}$$

Pirzada and Bhat [62] computed the following formulas for energy of C_m and \mathbf{C}_m :

$$\mathcal{E}(C_m) = \begin{cases} 2 \cot \frac{\pi}{m} & \text{if } m \equiv 0 \pmod{4} \\ 2 \csc \frac{\pi}{m} & \text{if } m \equiv 2 \pmod{4} \\ \csc \frac{\pi}{2m} & \text{if } m \equiv 1 \pmod{2}, \end{cases} \quad (2.2)$$

$$\mathcal{E}(\mathbf{C}_m) = \begin{cases} 2 \csc \frac{\pi}{m} & \text{if } m \equiv 0 \pmod{4} \\ 2 \cot \frac{\pi}{m} & \text{if } m \equiv 2 \pmod{4} \\ \csc \frac{\pi}{2m} & \text{if } m \equiv 1 \pmod{2}. \end{cases} \quad (2.3)$$

We denote a signed cycle of order m by C'_m with either a positive sign or negative sign.

Next two theorems give extremal energy among m -vertex unicyclic cycle-balanced and cycle unbalanced sidigraphs, $m \geq 2$.

Theorem 2.1 (Peña and Rada [60]). *In the class of all m -vertex unicyclic cycle balanced sidigraphs, the sidigraphs containing C_2 , C_3 or C_4 has the smallest energy and the sidigraphs containing C_m has the largest energy.*

Theorem 2.2 (Pirzada and Bhat [62]). *For each $q \geq 2$, $\mathcal{E}(C_q) < \mathcal{E}(C_{q+1})$. In addition, in the set of all m -vertex unicyclic cycle unbalanced sidigraphs, the sidigraphs containing C_2 has smallest energy and the sidigraphs containing C_m has the largest energy.*

Pirzada and Bhat [62] proved the following relation between energy of a sidigraph and its strong components.

Theorem 2.3 (Pirzada and Bhat [62]). *Suppose \mathcal{S} is a sidigraph and $\mathcal{H}_1, \dots, \mathcal{H}_s$ be its strong components. Then $\mathcal{E}(\mathcal{S}) = \sum_{q=1}^s \mathcal{E}(\mathcal{H}_q)$.*

Integral representation of energy is very useful as one can find the sidigraph energy without knowing the eigenvalues of the sidigraph.

Theorem 2.4 (Pirzada and Bhat [62]). *Suppose \mathcal{S} is a sidigraph with $n_{\mathcal{S}} = m$ and \mathcal{A} -characteristic polynomial $\Psi_{\mathcal{S}}(\xi)$. Then*

$$\mathcal{E}(\mathcal{S}) = \frac{1}{\pi} p.v. \int_{-\infty}^{+\infty} \left(m - \frac{i\xi \Psi'_{\mathcal{S}}(i\xi)}{\Psi_{\mathcal{S}}(i\xi)} \right) d\xi.$$

Next corollary is obtained from Theorem 2.4.

Corollary 2.5 (Pirzada and Bhat [62]). *Let Ψ be a monic polynomial of degree m with roots ξ_1, \dots, ξ_m and define $\gamma_{\mathcal{S}}(y) = y^m \Psi(\frac{i}{y})$. Then*

$$\mathcal{E}(\mathcal{S}) = \frac{1}{\pi} p.v. \int_{-\infty}^{+\infty} \ln |\gamma_{\mathcal{S}}(y)| \frac{dy}{y^2}.$$

The sidigraph energy also satisfies the following integral formula [56, 62]:

$$\mathcal{E}(\mathcal{S}) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{y^2} \ln |\gamma_{\mathcal{S}}(y)| dy. \quad (2.4)$$

Now we give some bounds on sidigraph energy. In next theorem, Pirzada and Bhat [62] give the McClland inequality for sidigraphs.

Theorem 2.6 (Pirzada and Bhat [62]). *Suppose \mathcal{S} is a sidigraph of order $n_{\mathcal{S}}$ and size $e_{\mathcal{S}}$. Then*

$$\mathcal{E}(\mathcal{S}) \leq \sqrt{\frac{n_{\mathcal{S}}}{2} (e_{\mathcal{S}} + c_2 - c_2)},$$

where c_2 and c_2 are the number of positive and negative closed walks of size 2, respectively. The inequality becomes equality when \mathcal{S} is isomorphic to $\frac{n_{\mathcal{S}}}{2}$ copies of $\vec{\mathcal{K}}_2$.

Next theorem gives another upper bound on sidigraph energy.

Theorem 2.7 (Pirzada and Bhat [62]). *Suppose \mathcal{S} is a sidigraph of order $n_{\mathcal{S}}$ and size $e_{\mathcal{S}}$. Then $\mathcal{E}(\mathcal{S}) \leq e_{\mathcal{S}}$, where the inequality becomes equality when \mathcal{S} is isomorphic to $\frac{n_{\mathcal{S}}}{2}$ copies of $\vec{\mathcal{K}}_2$.*

Following theorem gives some further information about energy of a sidigraph.

Theorem 2.8 (Pirzada and Bhat [62]). *Suppose \mathcal{S} be a sidigraph. Then*

- (1). $\mathcal{E}(\mathcal{S}) \neq (2^p b)^{\frac{1}{r}}$, where b is an odd integer, $0 \leq p < r$ and $r \geq 1$.
- (2). $\mathcal{E}(\mathcal{S}) \neq \left(\frac{k}{s}\right)^{\frac{1}{t}}$, where $\frac{k}{s}$ is a rational number, $\frac{k}{s} \notin \mathbb{Z}$ and $t \geq 1$.

2.2 Energy of graphs based on degree

In current section, we discuss about the graph energy which is based on vertex degree. These types of energies are related to the topological index of a graph.

A topological index $TI(\mathcal{G})$ of a graph \mathcal{G} is recognized as a molecular descriptor which is a conversion of a molecular structure into some real numbers. In computational chemistry, topological indices are of vital importance. Numerous types of topological indices are found in literature which include indices based on vertex degree, indices based on distance of vertices, indices that are based on eccentricities of vertices, etc.

A topological index of a graph \mathcal{G} which is based on vertex degree is given as

$$TI(\mathcal{G}) = \sum_{w_p w_q \in \mathbb{E}_{\mathcal{G}}} \mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}),$$

where \mathcal{F} is a function satisfying $\mathcal{F}(w, z) = \mathcal{F}(z, w)$.

To every $TI(\mathcal{G})$, an m -square adjacency matrix $\mathcal{A}_{TI}(\mathcal{G}) = [a_{pq}]$ is defined and given as

$$a_{pq} = \begin{cases} \mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) & \text{if } w_p w_q \in \mathbb{E}_{\mathcal{G}} \\ 0 & \text{otherwise.} \end{cases}$$

The \mathcal{A}_{TI} -characteristic polynomial of \mathcal{G} is

$$\Psi_{\mathcal{G}}(\tilde{\theta}) = \det(\mathcal{A}_{TI}(\mathcal{G}) - \tilde{\theta}I_m),$$

where I_m is an $m \times m$ identity matrix. The \mathcal{A}_{TI} -eigenvalues of \mathcal{G} are the roots of $\Psi_{\mathcal{G}}(\tilde{\theta})$. The \mathcal{A}_{TI} -spectrum, $\text{spec}_{TI}(\mathcal{G})$ of \mathcal{G} is the collection of all \mathcal{A}_{TI} -eigenvalues \mathcal{G} together with their multiplicities. A graph has real \mathcal{A}_{TI} -eigenvalues because $\mathcal{A}_{TI}(\mathcal{G})$ is always symmetric. If \mathcal{G} is a graph with distinct \mathcal{A}_{TI} -eigenvalues θ_i and respective multiplicities are p_i , the \mathcal{A}_{TI} -spectrum of \mathcal{G} is represented as $\text{spec}_{TI}(\mathcal{G}) = \{\theta_i^{(p_i)} \mid i = 1, 2, \dots, k\}$.

Let $\theta_1, \dots, \theta_m$ be the eigenvalues of $\mathcal{A}_{TI}(\mathcal{G})$. Then graph energy related to $\mathcal{A}_{TI}(\mathcal{G})$ is defined by

$$\mathcal{E}_{TI}(\mathcal{G}) = \sum_{q=1}^m |\theta_q|.$$

After the remarkable success of the graph energy concept, the energies that are based on eigenvalues of degree-based graph matrices are introduced. Recently, a significant amount of research has been done in this direction. We list here some of the topological indices of graphs based on vertex degree and energies related to it.

1. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}$, then $TI(\mathcal{G})$ is the first Zagreb index [35], represented by $M_1(\mathcal{G})$. The first Zagreb energy $\mathcal{E}_{M_1}(\mathcal{G})$ was introduced in [64].
2. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = (d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{-1/2}$, then $TI(\mathcal{G})$ is the sum connectivity index [78], denoted by $\chi(\mathcal{G})$. The sum-connectivity energy $\mathcal{E}_{\chi}(\mathcal{G})$ was defined in [80].
3. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = (d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{\alpha}$, where $\alpha \in \mathbb{R}$, then $TI(\mathcal{G})$ is the general sum connectivity index [79], represented by $\chi_{\alpha}(\mathcal{G})$. The general sum-connectivity energy $\mathcal{E}_{\chi_{\alpha}}(\mathcal{G})$ could also be defined by using this function in $\mathcal{A}_{\chi_{\alpha}}(\mathcal{G})$.
4. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = (d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)})^{-1/2}$, then $TI(\mathcal{G})$ is the Randić index [66], denoted by $R(\mathcal{G})$. The Randić energy $\mathcal{E}_R(\mathcal{G})$ was defined in [9, 10].
5. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = (d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)})^{\alpha}$, then $TI(\mathcal{G})$, where $\alpha \in \mathbb{R}$, is the generalized form of Randić index [8], represented by $R_{\alpha}(\mathcal{G})$. The general Randić energy $\mathcal{E}_{R_{\alpha}}(\mathcal{G})$ was introduced in [30].
6. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = 2(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)})^{1/2} (d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{-1}$, then $TI(\mathcal{G})$ is the geometric-arithmetic index [73], denoted by $GA(\mathcal{G})$. The geometric-arithmetic energy $\mathcal{E}_{GA}(\mathcal{G})$ was defined in [68].
7. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = (d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}) (d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{-1}$, then $TI(\mathcal{G})$ is the inverse sum indeg index [74], denoted by $ISI(\mathcal{G})$. The inverse sum indeg energy $\mathcal{E}_{ISI}(\mathcal{G})$ was defined in [77].
8. If $\mathcal{F}(d_{\mathcal{G}}^{(w_p)}, d_{\mathcal{G}}^{(w_q)}) = 2 (d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{-1}$, then $TI(\mathcal{G})$ is the harmonic index [22], represented by $H(\mathcal{G})$. The Harmonic energy $\mathcal{E}_H(\mathcal{G})$ was defined in [45].

The first well known graph energy based on vertex degree is the Randić energy. The adjacency matrix related to Randić index is called Randić matrix. For detailed study on Randić energy, see [9, 10, 29, 30, 41, 53, 69] and references therein.

2.2.1 Some known results

In this section, we discuss some valuable results about degree based energies of graphs. By $\det(M)$, we meant determinant of a matrix M .

The most studied degree based graph energy is Randić energy. First, we give result about the Randić energy.

Theorem 2.9 (Gutman et al. [29]). *Let \mathcal{P}_m be an m -vertex path. Then $\mathcal{E}_R(\mathcal{P}_m) = 2 + \frac{1}{2}\mathcal{E}(\mathcal{P}_{m-2})$.*

Note that for a b -regular graph \mathcal{G} , $\mathcal{E}_R(\mathcal{G}) = \frac{1}{b}\mathcal{E}(\mathcal{G})$.

Next theorem is about the Randić spectral radius.

Theorem 2.10 (Liu et al. [53]). *The Randić spectral radius of a graph is equal to 1.*

In the following theorem, we give bounds on Randić energy.

Theorem 2.11 (He et al. [41]). *Suppose \mathcal{G} is a graph of order $n_{\mathcal{G}}$. Also suppose $\Gamma = \det(\mathcal{A}_R(\mathcal{G}))$.*

Then

$$\begin{aligned}\mathcal{E}_R(\mathcal{G}) &\geq 1 + \sqrt{\sum_{wz \in \mathbb{E}_{\mathcal{G}}} \frac{2}{d_{\mathcal{G}}^{(w)} d_{\mathcal{G}}^{(z)}} - 1 + (n_{\mathcal{G}} - 1)(n_{\mathcal{G}} - 2)\Gamma^{n_{\mathcal{G}}^{-2}}}, \\ \mathcal{E}_R(\mathcal{G}) &\leq 1 + \sqrt{(n_{\mathcal{G}} - 2) \left(\sum_{wz \in \mathbb{E}_{\mathcal{G}}} \frac{2}{d_{\mathcal{G}}^{(w)} d_{\mathcal{G}}^{(z)}} - 1 \right) + (n_{\mathcal{G}} - 1)\Gamma^{n_{\mathcal{G}}^{-2}}}.\end{aligned}$$

The concept of Randić energy was further extended to general Randić energy by Gu et al. [30]. The authors obtained bounds for general Randić energy and general Randić spectral radius. In the following two theorems, Gu et al. [30] give some property of general Randić matrix.

Theorem 2.12 (Gu et al. [30]). *The $\mathcal{A}_{R_{\alpha}}$ -eigenvalues of a simple and connected m -vertex graph \mathcal{G} are exactly two if and only if $\mathcal{G} \cong \mathcal{K}_m$.*

Theorem 2.13 (Gu et al. [30]). *Suppose \mathcal{G} is a graph that has no isolated vertex and $\mathbb{V}_{\mathcal{G}} = \{w_1, \dots, w_m\}$. Then $\det(\mathcal{A}_{R_\alpha}(\mathcal{G})) = (d_{\mathcal{G}}^{(w_1)} d_{\mathcal{G}}^{(w_2)} \dots d_{\mathcal{G}}^{(w_m)})^\alpha \det(\mathcal{A}(\mathcal{G}))$.*

This concept was also extended to Hermitian Randić energy by Lu et al. [54]. For detailed study about general Randić energy and Hermitian Randić energy, we refer to [30, 54].

Zhou and Trinajstić [80] put forward the concept of sum connectivity energy. The authors studied the algebraic properties of eigenvalues of sum connectivity matrix and energy. Later, this concept was extended to distance sum connectivity matrix [25] but we here discuss only about sum connectivity matrix and energy.

In the following result, Zhou and Trinajstić [80] obtained bounds for sum-connectivity energy.

Theorem 2.14 (Zhou and Trinajstić [80]). *Suppose \mathcal{G} is a graph of order $n_{\mathcal{G}}$. Then*

$$2 \sqrt{\sum_{wz \in \mathbb{E}_{\mathcal{G}}} \frac{1}{d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)}}} \leq \mathcal{E}_{\chi}(\mathcal{G}) \leq \sqrt{2n_{\mathcal{G}} \sum_{wz \in \mathbb{E}_{\mathcal{G}}} \frac{1}{d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)}}},$$

where the left inequality becomes equality for a null graph or a 1-regular graph and right inequality becomes equality for a null graph or a complete bipartite graph possibly having isolated vertices.

Note that for a b -regular graph \mathcal{G} , $\mathcal{E}_{\chi}(\mathcal{G}) = \frac{1}{\sqrt{2b}} \mathcal{E}(\mathcal{G})$. For sum-connectivity energy formulas of some specific graphs, study [61].

Next theorem gives bounds on largest eigenvalue of $\mathcal{A}_{\chi}(\mathcal{G})$.

Theorem 2.15 (Zhou and Trinajstić [80]). *Suppose \mathcal{G} be a graph of order $n_{\mathcal{G}}$ and $\theta_1 \geq \dots \geq \theta_{n_{\mathcal{G}}}$ be its \mathcal{A}_{χ} -eigenvalues. Then*

$$\frac{2\mathcal{A}_{\chi}(\mathcal{G})}{n_{\mathcal{G}}} \leq \theta_1 \leq \sqrt{\frac{2(n_{\mathcal{G}} - 1)}{n_{\mathcal{G}}} \sum_{wz \in \mathbb{E}_{\mathcal{G}}} \frac{1}{d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)}}},$$

where left inequality becomes equality for $\mathcal{A}_{\chi}(\mathcal{G})$ having equal row sums and right inequality becomes equality for an empty graph or a complete graph.

Recently, Zangi et al. [77] put forward the concept of inverse sum indeg energy of graphs. The authors have not studied the ISI energy in detail. This detailed study was done by Hafeez and Farooq [37]. They discuss the properties of ISI matrix and obtained several results about ISI energy bounds (see Chapter 5).

The trace of the ISI matrix $\mathcal{A}_{\text{ISI}}(\mathcal{G}) = [a_{pq}]_{m \times m}$ is defined by $\sum_{q=1}^m a_{qq}$ and is denoted by $\text{tr}(\mathcal{A}_{\text{ISI}}(\mathcal{G}))$. Zangi et al. [77] prove the following lemma.

Lemma 2.16 (Zangi et al. [77]). *Suppose \mathcal{G} be a graph with $n_{\mathcal{G}} = m$ and let $\theta_1, \dots, \theta_m$ be its \mathcal{A}_{ISI} -eigenvalues. Then*

$$(1) \sum_{q=1}^m \theta_q = 0,$$

$$(2) \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{G})) = \sum_{q=1}^m \theta_q^2 = 2 \sum_{wz \in \mathbb{E}_{\mathcal{G}}} \left(\frac{d_{\mathcal{G}}^{(w)} d_{\mathcal{G}}^{(z)}}{d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)}} \right)^2.$$

Zangi et al. [77] prove the following result for b -regular graphs.

Theorem 2.17 (Zangi et al. [77]). *For a b -regular graph \mathcal{G} , it holds that $\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \frac{b}{2} \mathcal{E}(\mathcal{G})$.*

For more information about degree-based energies of graphs, study [21] and references therein.

Chapter 3

Bicyclic signed digraphs with maximal energy

Finding sidigraphs with extremal energy over a certain set of sidigraphs is one of the fundamental concept in the theory of sidigraph energy. In 2015, Khan et al. [49] studied the problem to find the smallest and largest energy in the set of all vertex-disjoint bicyclic digraphs with m vertices. In 2017, Khan and Farooq [50] considered the problem to find the extremal energy over the set of all vertex-disjoint bicyclic sidigraphs with m vertices. Monslave and Rada [58] determined the bicyclic digraphs with largest energy over the set of all bicyclic digraphs. In this chapter, we determine the largest energy of bicyclic sidigraphs in the set of all bicyclic sidigraphs.

3.1 Known results and notations

In this section, we will give some notations and familiar results. Let \mathcal{D}_m represents the collection of m -vertex-disjoint bicyclic digraphs and \mathcal{D}_m^s represents the collection of m -vertex-disjoint bicyclic sidigraphs. Suppose \mathcal{B}_m represents the set of all m -vertex bicyclic digraphs and \mathcal{B}_m^s represents the set of all m -vertex bicyclic sidigraphs. Sidigraphs in \mathcal{B}_m^s are classified in three categories: the sidigraphs whose cycles are vertex-disjoint; the sidigraphs whose cycles share

exactly one vertex and the sidigraphs whose cycles share atleast one edge.

Let $q, s \geq 2$ and let $D_m^s[q, s] = C_q \cup C_s$ and $D_m^s[\mathbf{q}, \mathbf{s}] = \mathbf{C}_q \cup \mathbf{C}_s$. Also suppose $D_m^s[\mathbf{q}, \mathbf{s}] = C_q \cup C_s$ and $D_m^s[q, \mathbf{s}] = C_q \cup C_s$. Let $\mathcal{D}_m^s[q, s] = \{D_m^s[q, s], D_m^s[\mathbf{q}, \mathbf{s}], D_m^s[\mathbf{q}, s], D_m^s[q, \mathbf{s}]\}$. Note that $n_S = q + s$ for any $S \in \mathcal{D}_m^s[q, s]$.

Let g, r, t are positive integers with $g \geq r$ and $(g, r) \neq (1, 1)$. A ϑ -sidigraph with parameters g, r, t is made up of three directed signed paths $\mathcal{P}_{g+1}, \mathcal{P}_{r+1}$ and \mathcal{P}_{t+1} so that the end vertex of \mathcal{P}_{t+1} is the starting vertex of \mathcal{P}_{g+1} and \mathcal{P}_{r+1} and the starting vertex of \mathcal{P}_{t+1} is the end vertex of \mathcal{P}_{g+1} and \mathcal{P}_{r+1} . Note that the paths \mathcal{P}_{g+1} and \mathcal{P}_{t+1} constitute a signed cycle of size $g + t$ in a ϑ -sidigraph. Similarly, the paths \mathcal{P}_{r+1} and \mathcal{P}_{t+1} constitute a signed cycle of size $r + t$ in a ϑ -sidigraph. Both cycles in a ϑ -sidigraph share at least one common edge. We denote a ϑ -sidigraph with parameters g, r and t by $\vartheta[g, r, t]$ when both of its cycles are positive. Similarly a ϑ -sidigraph with parameters g, r and t is denoted by $\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]$ when both of its cycles are negative. A ϑ -sidigraph whose cycle constituted by paths \mathcal{P}_{g+1} and \mathcal{P}_{t+1} is positive and the cycle constituted by paths \mathcal{P}_{r+1} and \mathcal{P}_{t+1} is negative is denoted by $\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]$. Similarly, a ϑ -sidigraph whose cycle constituted by paths \mathcal{P}_{g+1} and \mathcal{P}_{t+1} is negative and the cycle constituted by paths \mathcal{P}_{r+1} and \mathcal{P}_{t+1} is positive is denoted by $\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]$. Let $\tilde{\vartheta}[g, r, t] = \{\vartheta[g, r, t], \vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}], \vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}], \vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]\}$. Note that a ϑ -sidigraph has $g + r + t - 1$ vertices.

Let q, s be two positive integers with $q \geq s \geq 2$. A Θ -sidigraph with parameters q, s is made up of two directed signed cycles of sizes q and s , which share only one vertex. A Θ -sidigraph in which both cycles are positive is denoted by $\Theta[q, s]$ and a Θ -sidigraph in which both cycles are negative is denoted by $\Theta[\mathbf{q}, \mathbf{s}]$. Let $\Theta[\mathbf{q}, \mathbf{s}]$ be the Θ -sidigraph whose q -cycle is negative and s -cycle is positive and $\Theta[q, \mathbf{s}]$ be the Θ -sidigraph whose q -cycle is positive and s -cycle is negative. Let $\tilde{\Theta}[q, s] = \{\Theta[q, s], \Theta[\mathbf{q}, \mathbf{s}], \Theta[\mathbf{q}, \mathbf{s}], \Theta[q, \mathbf{s}]\}$. Note that a Θ -sidigraph has $q + s - 1$ vertices.

By Theorem 2.3, to find the sidigraph energy, it is enough to find the energy of its strong components. Using this fact, following two theorems give extremal energy in \mathcal{D}_m and \mathcal{B}_m .

Theorem 3.1 (Khan et al. [49]). *For each $\mathcal{D} \in \mathcal{D}_m$, $\mathcal{E}(\mathcal{D}) \leq \mathcal{E}(D_m^s[m - 2, 2])$.*

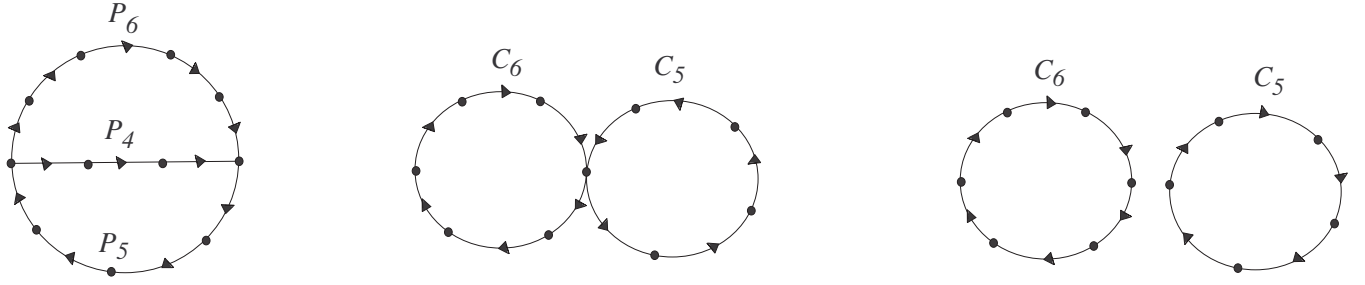


Figure 3.1: On left, a ϑ -sidigraph with parameters $g = 6, r = 4$ and $t = 5$. In middle, a Θ -sidigraph with parameters $q = 6$ and $s = 5$. On right is $D_m^s[6, 5]$.

Theorem 3.2 (Monslave and Rada [58]). *If $m \geq 19$, then for each $\mathcal{D} \in \mathcal{B}_m$, $\mathcal{E}(\mathcal{D}) \leq \mathcal{E}(D_m^s[m - 2, 2])$.*

In the following theorem, Khan et al. [50] give extremal energy among m -vertex bicyclic sidigraphs in \mathcal{D}_m^s .

Theorem 3.3 (Khan et al. [50]). *Let $\mathcal{S} \in \mathcal{D}_m^s$. Then we have*

- (i) $\mathcal{E}(\mathcal{S}) \geq \mathcal{E}(D_m^s[2, 2])$.
- (ii) For each $m \equiv 0 \pmod{4}$, $\mathcal{E}(\mathcal{S}) \leq \mathcal{E}(D_m^s[m - 2, 2])$.
- (iii) For each $m \equiv 2 \pmod{4}$, $\mathcal{E}(\mathcal{S}) \leq \mathcal{E}(D_m^s[m - 2, 2])$.
- (iv) For each $m \equiv 1 \pmod{2}$, $\mathcal{E}(\mathcal{S}) \leq \mathcal{E}(D_m^s[m - 2, 2]) = \mathcal{E}(m - 2, 2)$.

3.2 Maximal energy

In this section, we find those sidigraphs in \mathcal{B}_m^s which have largest energy. Recall that the polynomial $\gamma_{\mathcal{S}}(y)$ is defined by $\gamma_{\mathcal{S}}(y) = y^m \Psi_{\mathcal{S}}(\frac{1}{y})$, where \mathcal{S} is a sidigraph (see (2.4)). Following lemma will be used to compare energies of sidigraphs. The proof is analogous to the proof of Lemma 2.1 [58] and thus neglected.

Lemma 3.4. *Suppose $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3$ and \mathcal{S}_4 are sidigraphs. Then*

(1.) For each $0 \leq y < \infty$, if $|\gamma_{S_1}(y)| \leq |\gamma_{S_2}(y)|$, then $\mathcal{E}(S_1) \leq \mathcal{E}(S_2)$;

(2.) For each $0 \leq y < \infty$, if $|\gamma_{S_2}(y)| \cdot |\gamma_{S_3}(y)| \leq |\gamma_{S_1}(y)| \cdot |\gamma_{S_4}(y)|$, then

$$\mathcal{E}(S_3) - \mathcal{E}(S_4) \leq \mathcal{E}(S_1) - \mathcal{E}(S_2).$$

Let $\mathcal{H} \in \mathcal{D}_m^s[q, s] \cup \widetilde{\Theta}[q, s] \cup \widetilde{\vartheta}[g, r, t]$.

1. When $\mathcal{H} \in \mathcal{D}_m^s[q, s]$.

$$\Psi_{\mathcal{H}}(\xi) = \begin{cases} \xi^{q+s} - \xi^q - \xi^s + 1 & \text{if } \mathcal{H} = D_m^s[q, s] \\ \xi^{q+s} + \xi^q + \xi^s + 1 & \text{if } \mathcal{H} = D_m^s[q, s] \\ \xi^{q+s} + \xi^q - \xi^s - 1 & \text{if } \mathcal{H} = D_m^s[q, s] \\ \xi^{q+s} - \xi^q + \xi^s - 1 & \text{if } \mathcal{H} = D_m^s[q, s]. \end{cases} \quad (3.1)$$

2. When $\mathcal{H} \in \widetilde{\Theta}[q, s]$.

$$\Psi_{\mathcal{H}}(\xi) = \begin{cases} \xi^{q+s-1} - \xi^{q-1} - \xi^{s-1} & \text{if } \mathcal{H} = \Theta[q, s] \\ \xi^{q+s-1} + \xi^{q-1} + \xi^{s-1} & \text{if } \mathcal{H} = \Theta[q, s] \\ \xi^{q+s-1} + \xi^{q-1} - \xi^{s-1} & \text{if } \mathcal{H} = \Theta[q, s] \\ \xi^{q+s-1} - \xi^{q-1} + \xi^{s-1} & \text{if } \mathcal{H} = \Theta[q, s]. \end{cases} \quad (3.2)$$

3. When $\mathcal{H} \in \widetilde{\vartheta}[g, r, t]$.

$$\Psi_{\mathcal{H}}(\xi) = \begin{cases} \xi^{g+r+t-1} - \xi^{g-1} - \xi^{r-1} & \text{if } \mathcal{H} = \vartheta[g, r, t] \\ \xi^{g+r+t-1} + \xi^{g-1} + \xi^{r-1} & \text{if } \mathcal{H} = \vartheta[g, r, t] \\ \xi^{g+r+t-1} + \xi^{g-1} - \xi^{r-1}, & \text{if } \mathcal{H} = \vartheta[g, r, t] \\ \xi^{g+r+t-1} - \xi^{g-1} + \xi^{r-1} & \text{if } \mathcal{H} = \vartheta[g, r, t]. \end{cases} \quad (3.3)$$

The strong components of any sidigraph $\mathcal{S} \in \mathcal{B}_m^s$ are: some isolated vertices and a sidigraph either belong to the set $\mathcal{D}_m^s[q, s]$ or $\widetilde{\Theta}[q, s]$ or $\vartheta\Theta[g, r, t]$. Hence by using Theorem 2.3, it is enough to compute the energy of sidigraphs in the sets $\mathcal{D}_m^s[q, s]$, $\widetilde{\Theta}[q, s]$ and $\widetilde{\vartheta}[g, r, t]$.

Next lemma determines the relationship between a ϑ -sidigraph energy and a Θ -sidigraph energy.

Lemma 3.5. *The following equations hold true:*

- (1). $\mathcal{E}(\vartheta[g, r, t]) = \mathcal{E}(\Theta[g + t, r + t]).$
- (2). $\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) = \mathcal{E}(\Theta[\mathbf{g} + \mathbf{t}, \mathbf{r} + \mathbf{t}]).$
- (3). $\mathcal{E}(\vartheta[g, \mathbf{r}, \mathbf{t}]) = \mathcal{E}(\Theta[g + \mathbf{t}, \mathbf{r} + \mathbf{t}]).$
- (4). $\mathcal{E}(\vartheta[\mathbf{g}, r, \mathbf{t}]) = \mathcal{E}(\Theta[\mathbf{g} + \mathbf{t}, r + \mathbf{t}]).$

Proof. (1). It follows from Lemma 2.2 [58].

(2). From Equation (3.2), we have

$$\begin{aligned} \Psi_{\Theta[g+t, r+t]}(\xi) &= \xi^{g+r+2t-1} + \xi^{g+t-1} + \xi^{r+t-1} \\ &= \xi^t (\xi^{g+r+t-1} + \xi^{g-1} + \xi^{r-1}) \\ &= \xi^t \Psi_{\vartheta[g, r, t]}(\xi). \end{aligned}$$

(3). From Equation (3.3), we obtain

$$\begin{aligned} \Psi_{\Theta[g+t, r+t]}(\xi) &= \xi^{g+r+2t-1} + \xi^{g+t-1} - \xi^{r+t-1} \\ &= \xi^t (\xi^{g+r+t-1} + \xi^{g-1} - \xi^{r-1}) \\ &= \xi^t \Psi_{\vartheta[g, r, t]}(\xi). \end{aligned}$$

(4). From Equation (3.3), we get

$$\begin{aligned} \Psi_{\Theta[g+t, r+t]}(\xi) &= \xi^{g+r+2t-1} - \xi^{g+t-1} + \xi^{r+t-1} \\ &= \xi^t (\xi^{g+r+t-1} - \xi^{g-1} + \xi^{r-1}) \\ &= \xi^t \Psi_{\vartheta[g, r, t]}(\xi). \end{aligned}$$

This completes the proof. □

Thus by Lemma 3.5, it is enough to deal with the energies of sidigraphs belonging to the sets $\mathcal{D}_m^s[q, s]$ and $\widetilde{\Theta}[q, s]$. For finding sidigraphs with maximal energy in \mathcal{B}_m^s , we compute the polynomials $\gamma_{\Theta[q, s]}$, $\gamma_{\widetilde{\Theta}[q, s]}$ and $\gamma_{\Theta[q, s]}$. See Tables 3.1 ~ 3.5.

In the next two propositions, we will show that $\mathcal{E}(\Theta[q, \mathbf{q}]) \leq \mathcal{E}(D_m^s[q-1, 2])$ and $\mathcal{E}(\Theta[\mathbf{q}, q]) \leq \mathcal{E}(D_m^s[q-1, 2])$.

Table 3.1: The polynomials $\gamma_{\Theta[q,s]}(y)$ (see [58])

	$q \equiv 0(\text{mod } 4)$	$q \equiv 1(\text{mod } 4)$	$q \equiv 2(\text{mod } 4)$	$q \equiv 3(\text{mod } 4)$
$s \equiv 0(\text{mod } 4)$	$iy^q + iy^s - i$	$iy^q - y^s + 1$	$iy^q - iy^s + i$	$iy^q + y^s - 1$
$s \equiv 1(\text{mod } 4)$	$-y^q + iy^s + 1$	$-y^q - y^s + i$	$-y^q - iy^s - 1$	$-y^q + y^s - i$
$s \equiv 2(\text{mod } 4)$	$-iy^q + iy^s + i$	$-iy^q - y^s - 1$	$-iy^q - iy^s - i$	$-iy^q + y^s + 1$
$s \equiv 3(\text{mod } 4)$	$y^q + iy^s - 1$	$y^q - y^s - i$	$y^q - iy^s + 1$	$y^q + y^s + i$

Table 3.2: The polynomials $\gamma_{\Theta[q,s]}(y)$

	$q \equiv 0(\text{mod } 4)$	$q \equiv 1(\text{mod } 4)$	$q \equiv 2(\text{mod } 4)$	$q \equiv 3(\text{mod } 4)$
$s \equiv 0(\text{mod } 4)$	$-iy^q - iy^s - i$	$-iy^q + y^s + 1$	$-iy^q + iy^s + i$	$-iy^q - y^s - 1$
$s \equiv 1(\text{mod } 4)$	$y^q - iy^s + 1$	$y^q + y^s + i$	$y^q + iy^s - 1$	$y^q - y^s - i$
$s \equiv 2(\text{mod } 4)$	$iy^q - iy^s + i$	$iy^q + y^s - 1$	$iy^q + iy^s - i$	$iy^q - y^s + 1$
$s \equiv 3(\text{mod } 4)$	$-y^q - iy^s - 1$	$-y^q + y^s - i$	$-y^q + iy^s + 1$	$-y^q - y^s + i$

Table 3.3: The polynomials $\gamma_{D_m^s[q,2]}(y)$ (see [58])

$q \equiv 0(\text{mod } 4)$	$q \equiv 1(\text{mod } 4)$	$q \equiv 2(\text{mod } 4)$	$q \equiv 3(\text{mod } 4)$
$y^{q+2} + y^q - y^2 - 1$	$y^{q+2} + y^q - i(y^2 + 1)$	$y^{q+2} + y^q + y^2 + 1$	$y^{q+2} + y^q + i(y^2 + 1)$

Table 3.4: The polynomials $\gamma_{\Theta[q,s]}(y)$

	$q \equiv 0(\text{mod } 4)$	$q \equiv 1(\text{mod } 4)$	$q \equiv 2(\text{mod } 4)$	$q \equiv 3(\text{mod } 4)$
$s \equiv 0(\text{mod } 4)$	$iy^q - iy^s - i$	$iy^q + y^s + 1$	$iy^q + iy^s + i$	$iy^q - y^s - 1$
$s \equiv 1(\text{mod } 4)$	$-y^q - iy^s + 1$	$-y^q + y^s + i$	$-y^q + iy^s - 1$	$-y^q - y^s - i$
$s \equiv 2(\text{mod } 4)$	$-iy^q - iy^s + i$	$-iy^q + y^s - 1$	$-iy^q + iy^s - i$	$-iy^q - y^s + 1$
$s \equiv 3(\text{mod } 4)$	$y^q - iy^s - 1$	$y^q + y^s - i$	$y^q + iy^s + 1$	$y^q - y^s + i$

Proposition 3.6. For each $q \geq 3$, $\mathcal{E}(\Theta[q, q]) \leq \mathcal{E}(D_m^s[q - 1, 2])$.

Proof. We consider four cases for all values of q to prove the result.

Table 3.5: The polynomials $\gamma_{\Theta[q,s]}(y)$

	$q \equiv 0(\text{mod } 4)$	$q \equiv 1(\text{mod } 4)$	$q \equiv 2(\text{mod } 4)$	$q \equiv 3(\text{mod } 4)$
$s \equiv 0(\text{mod } 4)$	$-iy^q + iy^s - i$	$-iy^q - y^s + 1$	$-iy^q - iy^s + i$	$-iy^q + y^s - 1$
$s \equiv 1(\text{mod } 4)$	$y^q + iy^s + 1$	$y^q - y^s + i$	$y^q - iy^s - 1$	$y^q + y^s - i$
$s \equiv 2(\text{mod } 4)$	$iy^q + iy^s + i$	$iy^q - y^s - 1$	$iy^q - iy^s - i$	$iy^q + y^s + 1$
$s \equiv 3(\text{mod } 4)$	$-y^q + iy^s - 1$	$-y^q - y^s - i$	$-y^q - iy^s + 1$	$-y^q + y^s + i$

(1). If $q \equiv 2(\text{mod } 4)$ or $q \equiv 0(\text{mod } 4)$, then

$$|\gamma_{D_m^s[q-1,2]}|^2 - |\gamma_{\Theta[q,q]}|^2 = y^{2q-2} (y^2 + 1)^2 + y^4 + 2y^2 \geq 0,$$

for each $0 \leq y < \infty$. Hence Part 1 of Lemma 3.4 implies $\mathcal{E}(\Theta[q, \mathbf{q}]) \leq \mathcal{E}(D_m^s[q-1, 2])$ for every $q \geq 4$.

(2). If $q \equiv 3(\text{mod } 4)$, then

$$|\gamma_{D_m^s[q-1,2]}|^2 - |\gamma_{\Theta[q,q]}|^2 = y^{2q-2}(y^2 + 1)^2 + y^2(y^2 + 2) + 2y^{q-1}(y^4 + 2y^2 + 1) \geq 0,$$

for each $0 \leq y < \infty$. Therefore Part 1 of Lemma 3.4 implies that $\mathcal{E}(\Theta[q, \mathbf{q}]) \leq \mathcal{E}(D_m^s[q-1, 2])$ for every $q \geq 3$.

(3). If $q \equiv 1(\text{mod } 4)$ then

$$|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,q]}|^2 = (y^q + y^{q-2})^2 + y^4 + 2y^2 \geq 0,$$

for each $0 \leq y < \infty$. Thus by Theorem 2.1 and Part 1 of Lemma 3.4, we obtain $\mathcal{E}(\Theta[q, \mathbf{q}]) \leq \mathcal{E}(D_m^s[q-2, 2]) \leq \mathcal{E}(D_m^s[q-1, 2])$ for all $q \geq 5$. \square

Proposition 3.7. For each $q \geq 3$, $\mathcal{E}(\Theta[\mathbf{q}, q]) \leq \mathcal{E}(D_m^s[q-1, 2])$.

Proof. Since $|\gamma_{\Theta[q,q]}|^2 - |\gamma_{\Theta[q,q]}|^2 = 0$, for every $0 \leq y < \infty$. Hence by using Proposition 3.6 and Part 1 of Lemma 3.4, we get $\mathcal{E}(\Theta[\mathbf{q}, q]) \leq \mathcal{E}(D_m^s[q-1, 2])$. \square

In next two propositions, we prove that $\mathcal{E}(\Theta[\mathbf{q}, s]) \leq \mathcal{E}(D_m^s[q-2, 2])$ and $\mathcal{E}(\Theta[q, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$ for all $q > s$. We would like to mention that the idea of proofs are taken from the proof of Proposition 2.5 [58].

Proposition 3.8. *Suppose $q > s$ and $q \geq 22$. Then $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$.*

Proof. We will prove this result by considering different cases for q and s .

(1). If $q \equiv 2(\pmod{4})$ and $s \equiv 2(\pmod{4})$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,s]}|^2 = -4(y^q + y^s) \leq 0,$$

for each $0 \leq y < \infty$. Thus Part 1 of Lemma 3.4 implies that $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(\Theta[q, s])$ and by Proposition 2.5 [58], we have $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q-2, 2])$. Hence $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$ for $s \geq 2$.

(2). If $q \equiv 2(\pmod{4})$ and $s \equiv 3(\pmod{4})$ or $s \equiv 1(\pmod{4})$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,s]}|^2 = -4y^q \leq 0,$$

for each $0 \leq y < \infty$. Therefore by Part 1 of Lemma 3.4 and Proposition 2.5 [58], we have $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$ for $s \geq 3$.

(3). If $q \equiv 2(\pmod{4})$ and $s \equiv 0(\pmod{4})$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,2]}|^2 = -(y^2 + 2y^q - y^s) \times (2 + y^2 + y^s).$$

Let

$$\begin{aligned} q_1(y) &= y^2 + 2y^q - y^s \\ &= (y^2 - y^s) + 2y^q \end{aligned} \tag{3.4}$$

$$= (y^q - y^s) + y^2 + y^q. \tag{3.5}$$

Take $p_1(y) = -(2 + y^2 + y^s) q_1(y)$. When $0 \leq y < 1$, then by Equation (3.4), it is clear that $q_1(y) \geq 0$ and by Equation (3.5), clearly $q_1(y) \geq 0$ if $y \geq 1$. So $p_1(y) \leq 0$ for each $0 \leq y < \infty$. Therefore Part 1 of Lemma 3.4 implies $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(\Theta[q, 2])$, and by Proposition 2.5 [58], we have $\mathcal{E}(\Theta[q, 2]) \leq \mathcal{E}(D_m^s[q-2, 2])$. Therefore $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$ for $s \geq 4$ and we are done.

(4). If $q \equiv 3 \pmod{4}$ and $s \equiv 2 \pmod{4}$ then

$$\begin{aligned} |\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 &= y^{2q-4} + 2y^{2q-2} + y^4 + 2y^2 - y^{2s} + 2y^s \\ &= (y^4 - y^{2s}) + y^{2q-4} + 2y^{2q-2} + 2y^2 + 2y^s \end{aligned} \quad (3.6)$$

$$= (y^{2q-2} - y^{2s}) + y^{2q-4} + y^{2q-2} + y^4 + 2y^2 + 2y^s. \quad (3.7)$$

Since $s \leq q - 1$, therefore from Equations (3.6) and (3.7), clearly $|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 \geq 0$ for each $0 \leq y < \infty$. Hence by Part 1 of Lemma 3.4, we have $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 2$.

(5). If $q \equiv 3 \pmod{4}$ and $s \equiv 3 \pmod{4}$ then we have

$$\begin{aligned} |\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 &= y^{2q-4} + 2y^{2q-2} + y^4 + 2y^2 - y^{2s} - 2y^{q+s} \\ &= (y^4 - y^{2s}) + (2y^2 - 2y^{q+s}) + y^{2q-4} + 2y^{2q-2} \end{aligned} \quad (3.8)$$

$$= (y^{2q-4} - y^{2s}) + (2y^{2q-2} - 2y^{q+s}) + y^4 + 2y^2. \quad (3.9)$$

From Equations (3.8) and (3.9), it is clear that $|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 \geq 0$ for each $0 \leq y < \infty$, since $s \leq q - 4$. Therefore Part 1 of Lemma 3.4 implies that $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 3$.

(6). If $q \equiv 3 \pmod{4}$ and $s \equiv 1 \pmod{4}$ then

$$\begin{aligned} |\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 &= y^{2q-4} + 2y^{2q-2} + y^4 + 2y^2 - y^{2s} + 2y^{q+s} \\ &= (y^4 - y^{2s}) + y^{2q-4} + 2y^{2q-2} + 2y^2 + 2y^{q+s} \end{aligned} \quad (3.10)$$

$$= (y^{2q-2} - y^{2s}) + y^{2q-4} + y^{2q-2} + y^4 + 2y^2 + 2y^{q+s}. \quad (3.11)$$

Since $s \leq q - 2$, therefore from Equations (3.10) and (3.11), clearly $|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 \geq 0$ for each $0 \leq y < \infty$. Thus by Part 1 of Lemma 3.4, we get $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 5$.

(7). If $q \equiv 3 \pmod{4}$ and $s \equiv 0 \pmod{4}$ then

$$\begin{aligned} |\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 &= y^{2q-4} + 2y^{2q-2} + y^4 + 2y^2 - y^{2s} - 2y^s \\ &= (y^4 - y^{2s}) + (2y^2 - 2y^s) + y^{2q-4} + 2y^{2q-2} \end{aligned} \quad (3.12)$$

$$= (y^{2q-4} - y^{2s}) + (2y^{2q-2} - 2y^s) + y^4 + 2y^2. \quad (3.13)$$

From Equations (3.12) and (3.13), we get $|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 \geq 0$ for each $0 \leq y < \infty$, since $s \leq q - 3$. Consequently by Part 1 of Lemma 3.4, we have $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 4$.

Analogously one can prove for $q \equiv 0(\text{mod } 4)$ and $q \equiv 1(\text{mod } 4)$. \square

Proposition 3.9. *Suppose $q > s$ and $q \geq 22$. Then $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$.*

Proof. For $q \not\equiv 2(\text{mod } 4)$ and $q > s$, one can easily check that $|\gamma_{D_m^s[q-2,2]}|^2 - |\gamma_{\Theta[q,s]}|^2 \geq 0$ for each $0 \leq y < \infty$. Therefore by Part 1 of Lemma 3.4, we obtain $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$.

To prove the assertion for all $s \geq 2$ when $q \equiv 2(\text{mod } 4)$, we consider four cases.

(1). If $q \equiv 2(\text{mod } 4)$ and $s \equiv 2(\text{mod } 4)$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,s]}|^2 = 4y^s (1 + y^q) \geq 0,$$

for each $0 \leq y < \infty$. Therefore by Part 1 of Lemma 3.4 and Proposition 2.5 [58], we have $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 2$.

(2). If $q \equiv 2(\text{mod } 4)$ and $s \equiv 3(\text{mod } 4)$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,s]}|^2 = 0, \tag{3.14}$$

for each $0 \leq y < \infty$. Therefore by Part 1 of Lemma 3.4 and Proposition 2.5 [58], we get $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q - 2, 2])$ for $s \geq 3$.

(3). If $q \equiv 2(\text{mod } 4)$ and $s \equiv 0(\text{mod } 4)$ then

$$\begin{aligned} & |\gamma_{D_m^s[q-2,2]}|^2 |\gamma_{\Theta[q+4,s]}|^2 - |\gamma_{D_m^s[q+2,2]}|^2 |\gamma_{\Theta[q,s]}|^2 \\ &= -(y^2 - 1) (y^2 + 1)^3 (y^2 + y^s + 1) y^{q-4} \\ & \quad \times (y^{q+s} + y^{q+s+4} - y^{q+2} + y^{q+4} - y^{q+6} + 2y^{2q+4} + y^q - 2y^{s+2} - 2y^2). \end{aligned}$$

Let

$$\begin{aligned} q_2(y) &= y^{q+s} + y^{q+s+4} - y^{q+2} + y^{q+4} - y^{q+6} + 2y^{2q+4} + y^q - 2y^{s+2} - 2y^2 \\ &= (y^{2q+4} - y^{q+2}) + (y^{2q+4} - y^{q+6}) + (y^{q+s} - y^2) + (y^{q+4} - y^{s+2}) \\ & \quad + (y^{q+s+4} - y^{s+2}) + (y^q - y^2). \end{aligned} \tag{3.15}$$

Take $p_2(y) = -(y^2 - 1)(y^2 + 1)^3(y^2 + y^s + 1)y^{q-4}q_2(y)$. By Equation (3.15), clearly $q_2(y) \leq 0$ for each $0 \leq y < 1$ and $q_2(y) \geq 0$ for $y \geq 1$. Hence $p_2(y) \leq 0$ for each $0 \leq y < \infty$. Consequently by Part 2 of Lemma 3.4, it holds that

$$\begin{aligned}
\mathcal{E}(D_m^s[q+2, 2]) - \mathcal{E}(\Theta[q+4, s]) &\geq \mathcal{E}(D_m^s[q-2, 2]) - \mathcal{E}(\Theta[q, s]) \\
&\geq \mathcal{E}(D_m^s[q-6, 2]) - \mathcal{E}(\Theta[q-4, s]) \\
&\geq \dots\dots\dots \\
&\geq \mathcal{E}(D_m^s[s, 2]) - \mathcal{E}(\Theta[s+2, s]).
\end{aligned} \tag{3.16}$$

Also

$$\begin{aligned}
&|\gamma_{D_m^s[q-2, 2]}|^2 |\gamma_{\Theta[q+4, q+2]}|^2 - |\gamma_{D_m^s[q+2, 2]}|^2 |\gamma_{\Theta[q, q-2]}|^2 \\
&= -(y^2 - 1)(y^2 + 1)^3(2 + y^2)y^{q-2} \times (-2 - y^q + 2y^{2q} - y^{q+4} + 2y^{2q+2}).
\end{aligned}$$

Let

$$\begin{aligned}
q_3(y) &= -2 - y^q + 2y^{2q} - y^{q+4} + 2y^{2q+2} \\
&= (y^{2q} - y^q) + (y^{2q} - y^{q+4}) + (2y^{2q+2} - 2)
\end{aligned} \tag{3.17}$$

$$= (2y^{2q} - 2) + (y^{2q+2} - y^{2q}) + (y^{2q+2} - y^{q+4}). \tag{3.18}$$

Take $p_3(y) = -(y^2 - 1)(y^2 + 1)^3(2 + y^2)y^{q-4}q_3(y)$. From Equations (3.17) and (3.18), we see that $q_3(y) \leq 0$ for each $0 \leq y < 1$ and $q_3(y) \geq 0$ for $y \geq 1$. Thus $p_3(y) \leq 0$ for each $0 \leq y < \infty$.

Now Part 2 of Lemma 3.4 with $q = s + 2$ gives

$$\begin{aligned}
\mathcal{E}(D_m^s[s+4, 2]) - \mathcal{E}(\Theta[s+6, s+4]) &\geq \mathcal{E}(D_m^s[s, 2]) - \mathcal{E}(\Theta[s+2, s]) \\
&\geq \mathcal{E}(D_m^s[s-4, 2]) - \mathcal{E}(\Theta[s-2, s-4]) \\
&\geq \dots\dots\dots \\
&\geq \mathcal{E}(D_m^s[8, 2]) - \mathcal{E}(\Theta[10, 8]) \\
&> 0,
\end{aligned}$$

for each $s \geq 8$. Therefore $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q-2, 2])$. As $\mathcal{E}(D_m^s[8, 2]) - \mathcal{E}(\Theta[10, 4]) > 0$, so the case $s = 4$ follows from Equation (3.16) and the result is proved.

(4). If $q \equiv 2 \pmod{4}$ and $s \equiv 1 \pmod{4}$ then

$$|\gamma_{\Theta[q,s]}|^2 - |\gamma_{\Theta[q,s]}|^2 = 0, \quad (3.19)$$

for each $0 \leq y < \infty$. Hence by Part 1 of Lemma 3.4 and Proposition 2.5 [58], we get $\mathcal{E}(\Theta[q, s]) \leq \mathcal{E}(D_m^s[q-2, 2])$. The proof is completed. \square

The proofs of next propositions are similar to the proofs of Propositions 3.6 ~ 3.9, Propositions 2.3 and 2.5 [58] and are thus omitted.

Proposition 3.10. *If $q \geq 3$, then $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{q}]) \leq \mathcal{E}(D_m^s[q-1, 2])$.*

Proposition 3.11. *Let $q \geq s, 22$. Then $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[q-2, 2])$.*

Now we will find the sidigraphs with maximal energy in \mathcal{B}_m^s and to do this, two results are required, which we compute using MATLAB.

Lemma 3.12. *The following inequalities hold:*

- (1). *If $q+s-1 < 43$ then $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[41, 2])$, $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[41, 2])$ and $\mathcal{E}(\Theta[\mathbf{q}, \mathbf{s}]) \leq \mathcal{E}(D_m^s[41, 2])$.*
- (2). *If $g+r+t-1 < 43$ then $\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) \leq \mathcal{E}(D_m^s[41, 2])$, $\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) \leq \mathcal{E}(D_m^s[41, 2])$ and $\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) \leq \mathcal{E}(D_m^s[41, 2])$.*

Theorem 3.13. *Let $m \geq 43$ and let $\mathcal{S} \in \mathcal{B}_m^s$.*

- (1). *For each $m \equiv 0 \pmod{4}$, \mathcal{S} has the largest energy if it has $D_m^s[m-2, 2]$ as its strong component.*
- (2). *For each $m \equiv 2 \pmod{4}$, \mathcal{S} has the largest energy if it has $D_m^s[\mathbf{m}-2, 2]$ as its strong component.*
- (3). *For each $m \equiv 1 \pmod{2}$, \mathcal{S} has the largest energy if it has $D_m^s[m-2, 2]$ or $D_m^s[\mathbf{m}-2, 2]$ as its strong component.*

Proof. We consider three possibilities:

(i). When \mathcal{S} has a strong component in the set $\mathcal{D}_m^s[q, s]$ with $q, s \geq 2$ and $q + s \leq m$. Let $\mathcal{H} \in \mathcal{D}_m^s[q, s]$. Then by Theorem 3.3, $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[m-2, 2])$ for $m \equiv 0(\text{mod } 4)$ or $m \equiv 1(\text{mod } 2)$ and $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[\mathbf{m}-2, 2])$ for each $m \equiv 2(\text{mod } 4)$.

(ii). When \mathcal{S} has a strong component in the set $\widetilde{\Theta}[q, s]$ with $q \geq s \geq 2$ and $q + s - 1 \leq m$. If $q + s - 1 < 43$ then by Part 1 of Lemma 3.12 and Theorem 3.2, we have

$$\begin{aligned} \mathcal{E}(\Theta[q, s]) &\leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\Theta[\mathbf{q}, s]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\Theta[\mathbf{q}, s]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\Theta[q, s]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]). \end{aligned} \tag{3.20}$$

Now assume that $q + s - 1 \geq 43$. Then $q \geq 22$ as $q \geq s$. Thus by Proposition 3.6 ~ 3.11 and Theorem 3.2, we have

$$\begin{aligned} \mathcal{E}(\mathcal{S}) = \mathcal{E}(\Theta[q, s]) &\leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\mathcal{S}) = \mathcal{E}(\Theta[\mathbf{q}, s]) &\leq \mathcal{E}(D_m^s[q-1, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\mathcal{S}) = \mathcal{E}(\Theta[\mathbf{q}, s]) &\leq \mathcal{E}(D_m^s[q-1, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\ \mathcal{E}(\mathcal{S}) = \mathcal{E}(\Theta[q, s]) &\leq \mathcal{E}(D_m^s[q-1, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \end{aligned} \tag{3.21}$$

by reason of $q-1 \leq m-s \leq m-2$.

Let $\mathcal{H} \in \widetilde{\Theta}[q, s]$. Now using Equations (3.20), (3.21) and Theorem 3.3, $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[m-2, 2])$ for each $m \equiv 0 \pmod{4}$ or $m \equiv 1 \pmod{2}$ and $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[\mathbf{m}-2, 2])$ for each $m \equiv 2(\text{mod } 4)$.

(iii). When \mathcal{S} has a strong component in the set $\widetilde{\vartheta}[g, r, t]$, where g, r and t are positive integers with $g \geq r$, $(g, r) \neq (1, 1)$ and $g + r + t - 1 \leq m$. Since $41 \leq m-2$, therefore if $g + r + t - 1 < 43$

then by Theorem 3.2 and Lemma 3.12 (2), it holds

$$\begin{aligned}
\vartheta[g, r, t] &\leq \mathcal{E}(D_m^s[m-2, 2]), \\
\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\
\mathcal{E}(\vartheta[\mathbf{g}, r, \mathbf{t}]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]), \\
\mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) &\leq \mathcal{E}(D_m^s[41, 2]) \leq \mathcal{E}(D_m^s[m-2, 2]).
\end{aligned}$$

Now suppose that $g + r + t - 1 \geq 43$. Then $g + t \geq 22$. Since $g \geq r$, therefore if $g + t < 22$ then $r - 1 > 21$. This implies $g < 22$ and $r > 21$, which is a contradiction. Therefore by Lemma 3.5, Proposition 3.6 ~ 3.11 and Theorem 3.2, we have

$$\begin{aligned}
\mathcal{E}(\mathcal{S}) = \mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) &\leq \begin{cases} \mathcal{E}(D_m^s[g+t-1, 2]) & \text{if } g = r \\ \mathcal{E}(D_m^s[g+t-2, 2]) & \text{if } g > r, \end{cases} \\
\mathcal{E}(\mathcal{S}) = \mathcal{E}(\vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}]) &\leq \begin{cases} \mathcal{E}(D_m^s[g+t-1, 2]) & \text{if } g = r \\ \mathcal{E}(D_m^s[g+t-2, 2]) & \text{if } g > r, \end{cases} \\
\mathcal{E}(\mathcal{S}) = \mathcal{E}(\vartheta[\mathbf{g}, r, \mathbf{t}]) &\leq \begin{cases} \mathcal{E}(D_m^s[g+t-1, 2]) & \text{if } g = r \\ \mathcal{E}(D_m^s[g+t-2, 2]) & \text{if } g > r, \end{cases}
\end{aligned}$$

$$\mathcal{E}(\mathcal{S}) = \mathcal{E}(\vartheta[\mathbf{g}, r, \mathbf{t}]) \leq \mathcal{E}(D_m^s[m-2, 2]).$$

Now if $g > r$ then $m \geq g + r + t - 1 \geq g + t$ and thus $g + t - 2 \leq m - 2$. Hence Theorem 2.1 implies $\mathcal{E}(D_m^s[g+t-2, 2]) \leq \mathcal{E}(D_m^s[m-2, 2])$.

If $g = r$ then $r \geq 2$. Thus $g+t-1 \leq m-r \leq m-2$. Again by Theorem 2.1, $\mathcal{E}(D_m^s[g+t-1, 2]) \leq \mathcal{E}(D_m^s[m-2, 2])$.

Let $\mathcal{H} \in \widetilde{\vartheta}[g, r, t]$. Using Theorem 3.3 and all above facts, it holds that $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[m-2, 2])$ for $m \equiv 0 \pmod{4}$ or $m \equiv 1 \pmod{2}$. If $m \equiv 2 \pmod{4}$ then $\mathcal{E}(\mathcal{S}) = \mathcal{E}(\mathcal{H}) \leq \mathcal{E}(D_m^s[m-2, 2])$ and we are done. \square

3.3 Equienergetic bicyclic sidigraphs

Two sidigraphs with same spectrum are called cospectral sidigraphs, otherwise non-cospectral. Two sidigraphs with equal energy are called equienergetic sidigraphs. Two isomorphic sidigraphs are always cospectral and thus are equienergetic. In this section, we will find few classes of non-cospectral equienergetic bicyclic sidigraphs.

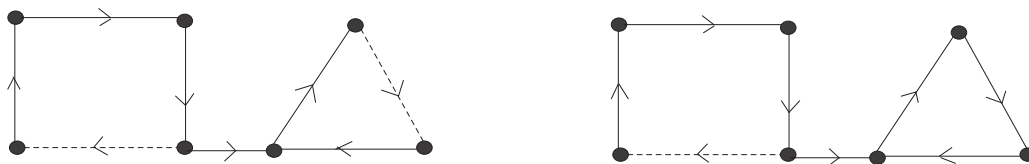


Figure 3.2: Equienergetic bicyclic sidigraphs.

Example 3.14. Let \mathcal{S} be the sidigraph on left side and \mathcal{H} be the sidigraph on right side of the Figure 3.2. The dotted lines represent negative arcs and solid ones represent positive arcs. Their \mathcal{A} -characteristic polynomials are:

$$\Psi_{\mathcal{S}}(\xi) = (\xi^4 + 1)(\xi^3 + 1),$$

$$\Psi_{\mathcal{H}}(\xi) = (\xi^4 + 1)(\xi^3 - 1).$$

Thus

$$\text{spec}_{\mathcal{A}}(\mathcal{S}) = \left\{ -1, \frac{1 \pm i}{\sqrt{2}}, \frac{-1 \pm i}{\sqrt{2}}, \frac{1 \pm \sqrt{3}i}{2} \right\}, \quad (3.22)$$

$$\text{spec}_{\mathcal{A}}(\mathcal{H}) = \left\{ 1, \frac{1 \pm i}{\sqrt{2}}, \frac{-1 \pm i}{\sqrt{2}}, \frac{-1 \pm \sqrt{3}i}{2} \right\}. \quad (3.23)$$

From (3.22) and (3.23), \mathcal{S} and \mathcal{H} are non-cospectral equienergetic bicyclic sidigraphs.

Theorem 3.15. Let $q \equiv 0 \pmod{2}$ and $s \equiv 1 \pmod{2}$. Let \mathcal{S}_1 and \mathcal{S}_2 be m -vertex bicyclic sidigraphs which contain $\Theta[q, s]$ and $\Theta[\mathbf{q}, s]$, respectively. Take m -vertex bicyclic sidigraphs \mathcal{H}_1 and \mathcal{H}_2 which contain $\Theta[q, s]$ and $\Theta[\mathbf{q}, s]$, respectively. Then \mathcal{S}_1 and \mathcal{H}_1 are non-cospectral equienergetic sidigraphs. Similarly, \mathcal{S}_2 and \mathcal{H}_2 are non-cospectral equienergetic sidigraphs.

Proof. By Theorem 1.11, \mathcal{A} -characteristic polynomials of \mathcal{S}_1 and \mathcal{H}_1 are, respectively, given by

$$\begin{aligned}\Psi_{\mathcal{S}_1}(\xi) &= \xi^m - \xi^{m-q} - \xi^{m-s}, \\ \Psi_{\mathcal{H}_1}(\xi) &= \xi^m - \xi^{m-q} + \xi^{m-s}.\end{aligned}$$

Similarly, \mathcal{A} -characteristic polynomials of \mathcal{S}_2 and \mathcal{H}_2 are, respectively, given by

$$\begin{aligned}\Phi_{\mathcal{S}_2}(\xi) &= \xi^m + \xi^{m-q} + \xi^{m-s}, \\ \Phi_{\mathcal{H}_2}(\xi) &= \xi^m + \xi^{m-q} - \xi^{m-s}.\end{aligned}$$

It is evident that the zeros of polynomials for \mathcal{S}_1 and \mathcal{H}_1 are not the same. Thus \mathcal{S}_1 and \mathcal{H}_1 are non-cospectral.

The strong components of \mathcal{S}_1 are $\Theta[q, s]$ and $m - (q + s - 1)$ isolated vertices and the strong components of \mathcal{H}_1 are $\Theta[q, s]$ and $m - (q + s - 1)$ isolated vertices. Therefore by Theorem 2.3, $\mathcal{E}(\mathcal{S}_1) = \mathcal{E}(\Theta[q, s])$ and $\mathcal{E}(\mathcal{H}_1) = \mathcal{E}(\Theta[q, s])$. The sidigraphs $\Theta[q, s]$ and $\Theta[q, s]$ are non-cospectral. Also

$$|\gamma_{\Theta[q, s]}|^2 - |\gamma_{\Theta[q, s]}|^2 = 0,$$

for each $0 \leq y < \infty$. Hence by Part 1 of Lemma 3.4, we have $\mathcal{E}(\Theta[q, s]) = \mathcal{E}(\Theta[q, s])$. Thus $\mathcal{E}(\mathcal{S}_1) = \mathcal{E}(\mathcal{H}_1)$.

Similarly, one can show that \mathcal{S}_2 and \mathcal{H}_2 are non-cospectral equienergetic sidigraphs. \square

In Theorems 3.16 ~ 3.19, we give few classes of pair of non-cospectral equienergetic bicyclic sidigraphs. The proofs of these theorems are same as the proof of Theorem 3.15 and are thus neglected.

Theorem 3.16. *Let $q \equiv 1 \pmod{2}$ and $s \equiv 1 \pmod{2}$. Let \mathcal{S}_3 and \mathcal{S}_4 be m -vertex bicyclic sidigraphs which contain $\Theta[q, s]$ and $\Theta[q, s]$, respectively. Take m -vertex bicyclic sidigraphs \mathcal{H}_3 and \mathcal{H}_4 which contain $\Theta[q, s]$ and $\Theta[q, s]$, respectively. Then \mathcal{S}_3 and \mathcal{H}_3 are non-cospectral equienergetic sidigraphs. Also, \mathcal{S}_4 and \mathcal{H}_4 are non-cospectral equienergetic sidigraphs.*

Theorem 3.17. *Let $q \equiv 0 \pmod{2}$ and $s \equiv 1 \pmod{2}$. Let $\mathcal{S}_5, \mathcal{S}_6, \mathcal{H}_5$ and \mathcal{H}_6 be m -vertex bicyclic sidigraphs which contain $D_m^s[q, s], D_m^s[\mathbf{q}, s], D_m^s[q, \mathbf{s}]$ and $D_m^s[\mathbf{q}, \mathbf{s}]$, respectively. Then $\mathcal{S}_5, \mathcal{H}_5$ and $\mathcal{S}_6, \mathcal{H}_6$ are non-cospectral equienergetic sidigraphs.*

Theorem 3.18. *Let $q \equiv 1 \pmod{2}$ and $s \equiv 0 \pmod{2}$. Let $\mathcal{S}_7, \mathcal{S}_8, \mathcal{H}_7$ and \mathcal{H}_8 be m -vertex bicyclic sidigraphs which contain $D_m^s[q, s], D_m^s[\mathbf{q}, s], D_m^s[\mathbf{q}, \mathbf{s}]$ and $D_m^s[q, \mathbf{s}]$, respectively. Then $\mathcal{S}_7, \mathcal{H}_7$ and $\mathcal{S}_8, \mathcal{H}_8$ are non-cospectral equienergetic sidigraphs.*

Theorem 3.19. *Let $q \equiv 1 \pmod{2}$ and $s \equiv 1 \pmod{2}$. Let $\mathcal{S}_9, \mathcal{S}_{10}, \mathcal{H}_9$ and \mathcal{H}_{10} be m -vertex bicyclic sidigraphs which contain $D_m^s[q, s], D_m^s[\mathbf{q}, s], D_m^s[q, \mathbf{s}]$ and $D_m^s[\mathbf{q}, \mathbf{s}]$, respectively. Then $\mathcal{S}_9, \mathcal{H}_9$ and $\mathcal{S}_{10}, \mathcal{H}_{10}$ and $\mathcal{S}_9, \mathcal{S}_{10}$ and $\mathcal{S}_9, \mathcal{H}_{10}$ and $\mathcal{S}_{10}, \mathcal{H}_9$ and $\mathcal{H}_9, \mathcal{H}_{10}$ are non-cospectral equienergetic sidigraphs.*

Using Theorem 3.16 and Lemma 3.5, one can easily prove the following two theorems.

Theorem 3.20. *Let $g + t \equiv 0 \pmod{2}$ and $r + t \equiv 1 \pmod{2}$ such that $g \geq r$ and $(g, r) \neq (1, 1)$. Let $\mathcal{S}_{11}, \mathcal{S}_{12}, \mathcal{H}_{11}$ and \mathcal{H}_{12} be m -vertex bicyclic sidigraphs which contain $\vartheta[g, r, t], \vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}], \vartheta[g, \mathbf{r}, \mathbf{t}]$ and $\vartheta[\mathbf{g}, \mathbf{r}, t]$, respectively. Then $\mathcal{S}_{11}, \mathcal{H}_{11}$ and $\mathcal{S}_{12}, \mathcal{H}_{12}$ are non-cospectral equienergetic sidigraphs.*

Theorem 3.21. *Let $g + t \equiv 1 \pmod{2}$ and $r + t \equiv 1 \pmod{2}$ such that $g \geq r$ and $(g, r) \neq (1, 1)$. Let $\mathcal{S}_{13}, \mathcal{S}_{14}, \mathcal{H}_{13}$ and \mathcal{H}_{14} be m -vertex bicyclic sidigraphs which contain $\vartheta[g, r, t], \vartheta[\mathbf{g}, \mathbf{r}, \mathbf{t}], \vartheta[g, \mathbf{r}, \mathbf{t}]$ and $\vartheta[\mathbf{g}, \mathbf{r}, t]$, respectively. Then $\mathcal{S}_{13}, \mathcal{H}_{13}$ and $\mathcal{S}_{14}, \mathcal{H}_{14}$ are non-cospectral equienergetic sidigraphs.*

3.4 Conclusion

In the current chapter, we determine the largest energy of sidigraphs in \mathcal{B}_m^s , where \mathcal{B}_m^s represents the set of m -vertex bicyclic sidigraphs with $m \geq 4$. We also construct few classes of non-cospectral equienergetic sidigraphs.

Chapter 4

On energy ordering of vertex-disjoint bicyclic sidigraphs

Recently, Yang and Wang [75] find the energy ordering of digraphs in \mathcal{D}_m and compute the maximal energy and iota energy. In the current chapter, we investigate the energy ordering of sidigraphs in the class of \mathcal{D}_m^s and find extremal energy.

4.1 Some results and notations

Let $q, s \geq 2$. For any $S \in \mathcal{D}_m^s$, its strong components are: a sidigraph from the set $\mathcal{D}_m^s[q, s]$ and few isolated vertices. Therefore using Theorem 2.3, we can only use the energy of strong components to find the energy ordering in \mathcal{D}_m^s .

Using Theorem 2.3, we give the following equations.

$$\mathcal{E}(D_m^s[q, s]) = \mathcal{E}(C_q) + \mathcal{E}(C_s),$$

$$\mathcal{E}(D_m^s[\mathbf{q}, s]) = \mathcal{E}(C_q) + \mathcal{E}(C_s),$$

$$\mathcal{E}(D_m^s[q, \mathbf{s}]) = \mathcal{E}(C_q) + \mathcal{E}(C_s),$$

$$\mathcal{E}(D_m^s[\mathbf{q}, \mathbf{s}]) = \mathcal{E}(C_q) + \mathcal{E}(C_s).$$

Let $m > 4$. In Lemmas 4.1~ 4.9, we gave some results about the monotonicity of some

functions which will be used to find the energy ordering of sidigraphs in \mathcal{D}_m^s .

Lemma 4.1 (Farooq et al. [23]). *Suppose $f(z) = 2\left(\cot \frac{\pi}{z} + \cot \frac{\pi}{m-z}\right)$. For $z \in \left[2, \frac{m}{2}\right]$, $f(z)$ is increasing and for $z \in \left[\frac{m}{2}, m-2\right]$, $f(z)$ is decreasing.*

Lemma 4.2 (Yang and Wang [75]). *Let $f(z) = 2\left(\csc \frac{\pi}{z} + \cot \frac{\pi}{m-z}\right)$. For $z \in [2, m-2]$, $f(z)$ is decreasing.*

Lemma 4.3 (Yang and Wang [75]). *Suppose $f(z) = 2\left(\csc \frac{\pi}{z} + \csc \frac{\pi}{m-z}\right)$. For $z \in \left[2, \frac{m}{2}\right]$, $f(z)$ is decreasing.*

Lemma 4.4 (Farooq et al. [23]). *Suppose $f(z) = z \sin \frac{\pi}{z}$. For $z \in [2, \infty)$, $f(z)$ is increasing.*

Lemma 4.5 (Yang and Wang [75]). *Suppose $f(z) = \frac{\pi}{z^2} \cos \frac{\pi}{z} \csc^2 \frac{\pi}{z}$. For $z \in [2, m-2]$, $f(z)$ is increasing.*

Next lemma has same proof as of Lemma 4.5 and is thus omitted.

Lemma 4.6. *Suppose $f(z) = \frac{\pi}{z^2} \cos \frac{\pi}{2z} \csc^2 \frac{\pi}{2z}$ and $g(z) = \frac{\pi}{z^2} \cos \frac{\pi}{z} \csc^2 \frac{\pi}{z}$. For $z \in [2, \infty)$, $f(z)$ and $g(z)$ are increasing.*

Now we prove the following results.

Lemma 4.7. *Suppose $f(z) = 2\left(\cot \frac{\pi}{z} + \csc \frac{\pi}{m-z}\right)$. For $z \in [2, m-2]$, $f(z)$ is increasing.*

Proof. To prove the result, we will show that for all $z \in [2, m-2]$, $f'(z) \geq 0$.

Now

$$f'(z) = 2\left(\frac{\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{(m-z)^2} \csc \frac{\pi}{m-z} \cot \frac{\pi}{m-z}\right). \quad (4.1)$$

Divide the interval in two parts. Firstly, let $z \in \left[\frac{m}{2}, m-2\right]$. Then $z \geq m-z$. By Lemma 4.5, we know that for $z \in [2, m-2]$, $\frac{\pi}{z^2} \cos \frac{\pi}{z} \csc^2 \frac{\pi}{z}$ is increasing. Therefore

$$\begin{aligned} \frac{\pi}{(m-z)^2} \csc \frac{\pi}{m-z} \cot \frac{\pi}{m-z} &= \frac{\pi}{(m-z)^2} \csc^2 \frac{\pi}{m-z} \cos \frac{\pi}{m-z} \\ &\leq \frac{\pi}{z^2} \csc^2 \frac{\pi}{z} \cos \frac{\pi}{z} \\ &< \frac{\pi}{z^2} \csc^2 \frac{\pi}{z}. \end{aligned}$$

Using Equation (4.1), $f'(z) \geq 0$ for $z \in \left[\frac{m}{2}, m-2\right]$.

Next, let $z \in \left[2, \frac{m}{2}\right]$. Then $z \leq m-z$. By Lemma 4.4, we know that $z \sin \frac{\pi}{z}$ is strictly increasing on $[2, \infty)$. We have $z \sin \frac{\pi}{z} \leq (m-z) \sin \frac{\pi}{m-z}$. From this, we get $\frac{1}{z} \csc \frac{\pi}{z} - \frac{1}{m-z} \csc \frac{\pi}{m-z} \geq 0$. Consider

$$\frac{\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{(m-z)^2} \csc^2 \frac{\pi}{m-z} = \pi \left(\frac{1}{z} \csc \frac{\pi}{z} + \frac{1}{m-z} \csc \frac{\pi}{m-z} \right) \left(\frac{1}{z} \csc \frac{\pi}{z} - \frac{1}{m-z} \csc \frac{\pi}{m-z} \right).$$

Clearly $\frac{1}{z} \csc \frac{\pi}{z} + \frac{1}{m-z} \csc \frac{\pi}{m-z} > 0$ and $\frac{1}{z} \csc \frac{\pi}{z} - \frac{1}{m-z} \csc \frac{\pi}{m-z} \geq 0$. Hence $\frac{\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{(m-z)^2} \csc^2 \frac{\pi}{m-z} \geq$

0. This implies that

$$\begin{aligned} \frac{\pi}{(m-z)^2} \csc \frac{\pi}{m-z} \cot \frac{\pi}{m-z} &= \frac{\pi}{(m-z)^2} \cos \frac{\pi}{m-z} \csc^2 \frac{\pi}{m-z} \\ &< \frac{\pi}{(m-z)^2} \csc^2 \frac{\pi}{m-z} \\ &< \frac{\pi}{z^2} \csc^2 \frac{\pi}{z}. \end{aligned} \tag{4.2}$$

Using Equations (4.1) and (4.2), $f'(z) \geq 0$ for $z \in \left[2, \frac{m}{2}\right]$. Thus $f'(z) \geq 0$ for $z \in [2, m-2]$. This proves the result. \square

Lemma 4.8. *Let $z \in [2, m-2]$. The following holds.*

- (1) *Suppose $f(z) = \csc \frac{\pi}{2z} + \csc \frac{\pi}{2(m-z)}$. For $z \in \left[2, \frac{m}{2}\right]$, $f(z)$ is decreasing and for $z \in \left[\frac{m}{2}, m-2\right]$, $f(z)$ is increasing.*
- (2) *Suppose $f(z) = 2 \csc \frac{\pi}{z} + \csc \frac{\pi}{2(m-z)}$. For $z \in \left[2, \frac{2m}{3}\right]$, $f(z)$ is decreasing and for $z \in \left[\frac{2m}{3}, m-2\right]$, $f(z)$ is increasing.*
- (3) *Suppose $f(z) = \csc \frac{\pi}{2z} + 2 \csc \frac{\pi}{(m-z)}$. For $z \in \left[2, \frac{m}{3}\right]$, $f(z)$ is decreasing and for $z \in \left[\frac{m}{3}, m-2\right]$, $f(z)$ is increasing.*

Proof. (1). To show that $f(z)$ is decreasing on $\left[2, \frac{m}{2}\right]$, it is sufficient to prove $f'(z) \leq 0$.

Since $z \leq (m-z)$ for $z \in \left[2, \frac{m}{2}\right]$, therefore using Lemma 4.6, we get

$$\begin{aligned} f'(z) &= \frac{\pi}{2z^2} \csc^2 \frac{\pi}{2z} \cos \frac{\pi}{2z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\leq \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} = 0 \end{aligned}$$

Hence $f(z)$ is decreasing on $\left[2, \frac{m}{2}\right]$.

Now we will show that $f'(z) \geq 0$. Since $z \geq (m - z)$ for $z \in \left[\frac{m}{2}, m - 2\right]$, therefore using Lemma 4.6, we obtain

$$\begin{aligned} f'(z) &= \frac{\pi}{2z^2} \csc^2 \frac{\pi}{2z} \cos \frac{\pi}{2z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\geq \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} = 0. \end{aligned}$$

Therefore $f(z)$ is increasing on $\left[\frac{m}{2}, m - 2\right]$.

(2). To show that $f(z)$ is decreasing on $\left[2, \frac{2m}{3}\right]$, we will prove that $f'(z) \leq 0$.

Since $z \leq 2(m - z)$ for $z \in \left[2, \frac{2m}{3}\right]$, therefore using Lemma 4.6, we get

$$\begin{aligned} f'(z) &= \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} \cos \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\leq \frac{2\pi}{4(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} = 0. \end{aligned}$$

Hence $f(z)$ is decreasing on $\left[2, \frac{2m}{3}\right]$.

Now we will show that $f'(z) \geq 0$. Since $z \geq 2(m - z)$ for $z \in \left[\frac{2m}{3}, m - 2\right]$, therefore using Lemma 4.6, we obtain

$$\begin{aligned} f'(z) &= \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} \cos \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\geq \frac{2\pi}{4(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} = 0. \end{aligned}$$

Hence $f(z)$ is increasing on $\left[\frac{2m}{3}, m - 2\right]$.

Analogously (3) can be proved. □

Lemma 4.9. Suppose $f(z) = 2 \cot \frac{\pi}{z} + \csc \frac{\pi}{2(m-z)}$. For $z \in [2, m - 2]$, $f(z)$ is increasing.

Proof. We will prove that $f'(z) \geq 0$ for $z \in [2, m - 2]$.

Since $\cos \frac{\pi}{z} \leq 1$ and $z \geq 2(m - z)$ for $z \in \left[2, \frac{2m}{3}, m - 2\right]$, therefore by Lemma 4.6, we have

$$\begin{aligned} f'(z) &= \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\geq \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} \cos \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\geq \frac{2\pi}{4(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} = 0 \end{aligned}$$

Also $-\cos \frac{\pi}{z} \geq -1$ and $z \leq 2(m-z)$ for $z \in [2, \frac{2m}{3}]$. Thus by proof of Lemma 2.4 [23], we see that

$$\begin{aligned} f'(z) &= \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \cos \frac{\pi}{2(m-z)} \\ &\geq \frac{2\pi}{z^2} \csc^2 \frac{\pi}{z} - \frac{\pi}{2(m-z)^2} \csc^2 \frac{\pi}{2(m-z)} \geq 0. \end{aligned}$$

Therefore $f(z)$ is increasing on $[2, m-2]$. □

Lemma 4.10 (Farooq et al. [23]). *For $0 < z \leq \frac{\pi}{2}$,*

$$\frac{1}{z} - 0.429z \leq \cot z \leq \frac{1}{z} - \frac{z}{3}.$$

For $0 < z < \frac{\pi}{2}$, we have

$$z - \frac{z^3}{3!} \leq \sin z \leq z. \tag{4.3}$$

Khan et al. [49] prove the following result.

Lemma 4.11 (Khan et al. [49]). *Suppose $z, d, e \in \mathbb{R}$ with $z \geq d > 0$ and $e > 0$. Then*

$$\frac{\pi z}{ez^2 - \pi^2} \leq \frac{\pi d}{ed^2 - \pi^2}.$$

4.2 Energy ordering

Sidigraphs in \mathcal{D}_m^s are classified into three categories: the sidigraphs whose cycles are of even length, the sidigraphs whose cycles are of odd length and the sidigraphs whose one cycle is of even length and one is of odd length. In the following section, we investigate separately energy ordering in all three categories and find maximal energy. Throughout this section, we take $b \in [2, m-2]$ and $m > 5$.

4.2.1 Both cycles are of even length

Yang and Wang [76] gave the following energy ordering of bicyclic sidigraphs in \mathcal{D}_m^s , where each cycle is of even length.

Theorem 4.12 (Yang and Wang [76]). *Let $m > 5$ and $b \in [2, m - 2]$. Also let the two directed even cycles are both positive or negative.*

(i) *If $m \equiv 2 \pmod{4}$ then we have the following energy ordering:*

(a) *When $\frac{m}{2} - 1 \equiv 0 \pmod{4}$.*

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) \\
> & \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[4, m-6]) \\
> & \mathcal{E}(D_m^s[6, m-8]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-2}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> & \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-2}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[4, m-8]) \\
> & \mathcal{E}(D_m^s[6, m-10]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> & \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> & \mathcal{E}(D_m^s[4, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-6}{2}\right]\right) \\
> & \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-6}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-10, 4]) \\
= & \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[4, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \dots \\
> & \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) \\
> & \dots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \dots > \mathcal{E}(D_m^s[4, 4]) \\
= & \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(b) When $\frac{m}{2} - 1 \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[\mathbf{4}, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[\mathbf{4}, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-2}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[\mathbf{4}, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-6}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-6}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[\mathbf{4}, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, 2]).
\end{aligned}$$

(ii) If $m \equiv 3 \pmod{4}$ then the following energy ordering holds:

(a) When $\frac{m-1}{2} - 1 \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[\mathbf{4}, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[\mathbf{4}, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-3}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[\mathbf{4}, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-7}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-7}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[\mathbf{4}, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, 2]).
\end{aligned}$$

(b) When $\frac{m-1}{2} - 1 \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[\mathbf{4}, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[\mathbf{4}, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-3}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[\mathbf{4}, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-7}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-7}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[\mathbf{4}, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[\mathbf{6}, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, 2]).
\end{aligned}$$

(iii) If $m \equiv 0 \pmod{4}$ then we have the following energy ordering:

(a) When $\frac{m}{2} \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[\mathbf{4}, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[\mathbf{4}, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[\mathbf{4}, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-4}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[\mathbf{4}, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-8}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-8}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, 2]).
\end{aligned}$$

(b) If $\frac{m}{2} \equiv 2 \pmod{2}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[\mathbf{4}, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[\mathbf{4}, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[\mathbf{4}, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-4}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[\mathbf{4}, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-8}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-8}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, 2]).
\end{aligned}$$

(iv) If $m \equiv 1 \pmod{4}$ then the following energy ordering holds:

(a) When $\frac{m-1}{2} \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[\mathbf{4}, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[\mathbf{4}, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[\mathbf{m}-3, \mathbf{2}]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[\mathbf{4}, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-5}{2}\right]\right) > \mathcal{E}(D_m^s[\mathbf{m}-5, \mathbf{2}]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[\mathbf{4}, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) \\
> \mathcal{E}(D_m^s[\mathbf{m}-7, \mathbf{2}]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[\mathbf{4}, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-9}{2}\right]\right) > \mathcal{E}(D_m^s[\mathbf{m}-9, \mathbf{2}]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-9}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{2}]).
\end{aligned}$$

(b) When $\frac{m-1}{2} \equiv 2 \pmod{2}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[4, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[4, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[4, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-5}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[4, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-9}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[4, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-9}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-9}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) = \mathcal{E}(D_m^s[2, 2]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

Theorem 4.13 (Yang and Wang [76]). *Let $m > 5$ and $b \in [2, m-2]$. Also let that one of the even cycle is positive and one of the even cycle is negative.*

(i) *If $m \equiv 2 \pmod{4}$ then we have the following energy ordering:*

(a) When $\frac{m}{2} - 1 \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[4, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m+2}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m+2}{2}, \frac{m-6}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[4, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[4, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-2}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[4, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m-6}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(b) When $\frac{m}{2} - 1 \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m+2}{2}, \frac{m-2}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m+2}{2}, \frac{m-2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[4, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m+2}{2}, \frac{m-6}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m+2}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[4, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-6}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-6}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[4, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-10}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m-10}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[4, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-10}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m-10}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(ii) If $m \equiv 3 \pmod{4}$ then the following energy ordering holds:

(a) When $\frac{m-1}{2} - 1 \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[4, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[4, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m+1}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m+1}{2}, \frac{m-7}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[4, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[4, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-3}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[4, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m-7}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(b) When $\frac{m-1}{2} - 1 \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[4, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m+1}{2}, \frac{m-3}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m+1}{2}, \frac{m-3}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[4, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m+1}{2}, \frac{m-7}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m+1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[4, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-7}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-7}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[4, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-11}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m-11}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[4, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-11}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m-11}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(iii) If $m \equiv 0 \pmod{4}$ then we have the following energy ordering:

(a) When $\frac{m}{2} \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m+4}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[4, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[4, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-8}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[4, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[4, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-12}{2}, \frac{m-4}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-12}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(b) If $\frac{m}{2} \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[6, m-6]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m+4}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-4, 4]) = \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[4, m-6]) \\
> \mathcal{E}(D_m^s[6, m-8]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-2, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-4}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-6, 4]) = \mathcal{E}(D_m^s[2, m-6]) > \mathcal{E}(D_m^s[4, m-8]) \\
> \mathcal{E}(D_m^s[6, m-10]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m}{2}\right]\right) > \mathcal{E}(D_m^s[m-4, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m-8}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-8, 4]) = \mathcal{E}(D_m^s[2, m-8]) \\
> \mathcal{E}(D_m^s[4, m-10]) > \mathcal{E}(D_m^s[6, m-12]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-6, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m-4}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-10, 4]) \\
= \mathcal{E}(D_m^s[2, m-10]) > \mathcal{E}(D_m^s[4, m-12]) > \mathcal{E}(D_m^s[6, m-14]) > \dots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-12}{2}, \frac{m-4}{2}\right]\right) > \mathcal{E}(D_m^s[m-8, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m-12}{2}\right]\right) \\
> \dots > \mathcal{E}(D_m^s[m-12, 4]) = \mathcal{E}(D_m^s[2, m-12]) > \dots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(iv) If $m \equiv 1 \pmod{4}$ then the following energy ordering holds:

(a) When $\frac{m-1}{2} \equiv 0 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[4, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m+3}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[4, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[4, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-9}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[4, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[4, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \cdots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-13}{2}, \frac{m-5}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-13}{2}\right]\right) \\
> \cdots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \cdots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(b) When $\frac{m-1}{2} \equiv 2 \pmod{4}$.

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-3]) > \mathcal{E}(D_m^s[4, m-5]) > \mathcal{E}(D_m^s[6, m-7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m+3}{2}\right]\right) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-5, 4]) = \mathcal{E}(D_m^s[2, m-5]) > \mathcal{E}(D_m^s[4, m-7]) \\
> \mathcal{E}(D_m^s[6, m-9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[m-3, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-5}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-7, 4]) = \mathcal{E}(D_m^s[2, m-7]) > \mathcal{E}(D_m^s[4, m-9]) \\
> \mathcal{E}(D_m^s[6, m-11]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}(D_m^s[m-5, 2]) \\
> \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-9}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-9, 4]) = \mathcal{E}(D_m^s[2, m-9]) \\
> \mathcal{E}(D_m^s[4, m-11]) > \mathcal{E}(D_m^s[6, m-13]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) \\
> \mathcal{E}(D_m^s[m-7, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-5}{2}\right]\right) > \dots > \mathcal{E}(D_m^s[m-11, 4]) \\
= \mathcal{E}(D_m^s[2, m-11]) > \mathcal{E}(D_m^s[4, m-13]) > \mathcal{E}(D_m^s[6, m-15]) > \dots \\
> \mathcal{E}\left(D_m^s\left[\frac{m-13}{2}, \frac{m-5}{2}\right]\right) > \mathcal{E}(D_m^s[m-9, 2]) > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-13}{2}\right]\right) \\
> \dots > \mathcal{E}(D_m^s[m-13, 4]) = \mathcal{E}(D_m^s[2, m-13]) > \dots > \mathcal{E}(D_m^s[4, 4]) \\
= \mathcal{E}(D_m^s[2, 4]) > \mathcal{E}(D_m^s[6, 2]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

Xang and Yang prove the following theorem about the extremal energy of those bicyclic sidigraphs in the class \mathcal{D}_m^s whose both cycles are of even length.

Theorem 4.14 (Xang and Yang [76]). *Suppose a sidigraph $\mathcal{S} \in \mathcal{D}_m^s$ has even directed cycles.*

- (i) *For $m \equiv 0 \pmod{4}$, the largest energy of \mathcal{S} is obtained if $\mathcal{S} \cong D_m^s[2, m-2]$.*
- (ii) *For $m \equiv 1 \pmod{4}$, the largest energy of \mathcal{S} is obtained if $\mathcal{S} \cong D_m^s[2, m-3]$.*
- (iii) *For $m \equiv 2 \pmod{4}$, the largest energy of \mathcal{S} is obtained if $\mathcal{S} \cong D_m^s[2, m-2]$.*
- (iv) *For $m \equiv 3 \pmod{4}$, the largest energy of \mathcal{S} is obtained if $\mathcal{S} \cong D_m^s[2, m-3]$.*
- (v) *The smallest energy of \mathcal{S} is obtained for $\mathcal{S} \cong D_m^s[2, 2]$.*

4.2.2 Both cycles are of odd length

In this subsection, we find energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s that contain cycles of odd length. Note that for $b \equiv 1 \pmod{2}$, $\mathcal{E}(C_b) = \mathcal{E}(C_b)$. Hence we only consider the case when both cycles are positive.

Lemma 4.15. *Suppose $m \equiv 0 \pmod{4}$ and $b \equiv 1 \pmod{2}$. Then $\mathcal{E}(D_m^s[b, m-b])$ attains largest value at $b = 3$. Therefore the following energy ordering holds:*

$$\mathcal{E}(D_m^s[3, m-3]) > \mathcal{E}(D_m^s[5, m-5]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right).$$

Proof. Using Equation (2.2), we get

$$\mathcal{E}(D_m^s[b, m-b]) = \csc \frac{\pi}{2b} + \csc \frac{\pi}{2(m-b)}.$$

By Part (1) of Lemma 4.8, we see that $\csc \frac{\pi}{2b} + \csc \frac{\pi}{2(m-b)}$ is decreasing on $[2, \frac{m}{2}]$ and increasing on $[\frac{m}{2}, m-2]$. Therefore the smallest odd number in $[2, \frac{m}{2}]$ where $\mathcal{E}(D_m^s[b, m-b])$ has maximum value is $b = 3$ and the largest odd number in $[\frac{m}{2}, m-2]$ where $\mathcal{E}(D_m^s[b, m-b])$ has maximum value is $b = m-3$. Thus we have

$$\mathcal{E}(D_m^s[3, m-3]) > \mathcal{E}(D_m^s[5, m-5]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m}{2}-1, \frac{m}{2}+1\right]\right).$$

The proof is completed. □

Similar to Lemma 4.15, the following result can be proved.

Lemma 4.16. *Suppose $m \equiv 2 \pmod{4}$ and $b \equiv 1 \pmod{2}$. Then $\mathcal{E}(D_m^s[b, m-b])$ attains largest value at $b = 3$. Therefore the following energy ordering holds:*

$$\mathcal{E}(D_m^s[3, m-3]) > \mathcal{E}(D_m^s[5, m-5]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right).$$

Lemma 4.17. *Suppose $m \equiv 1 \pmod{4}$ and $b \equiv 1 \pmod{2}$. Then $\mathcal{E}(D_m^s[b, m-b-1])$ has largest value at $b = 3$. Therefore the following energy ordering holds:*

$$\mathcal{E}(D_m^s[3, m-4]) > \mathcal{E}(D_m^s[5, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right).$$

Proof. Since $b \equiv 1 \pmod{2}$ and $m \equiv 1 \pmod{4}$, therefore $m - b - 1 \equiv \pmod{2}$. Using Equation (2.2), we have

$$\mathcal{E}(D_m^s[b, m - b - 1]) = \csc \frac{\pi}{2b} + \csc \frac{\pi}{2(m - b - 1)}.$$

Hence by changing m to $m - 1$ is Lemma 4.15, we get the desired result. \square

By changing m with Lemma 4.16 to $m - 1$, the following result is obtained.

Lemma 4.18. *Suppose $m \equiv 3 \pmod{4}$ and $b \equiv 1 \pmod{2}$. Then $\mathcal{E}(D_m^s[b, m - b - 1])$ has maximum value at $b = 3$. Therefore the following energy ordering holds:*

$$\mathcal{E}(D_m^s[3, m - 4]) > \mathcal{E}(D_m^s[5, m - 6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right).$$

Combining Lemmas 4.15 ~ 4.18, the following corollary is obtained.

Corollary 4.19. *Suppose $b \equiv 1 \pmod{2}$.*

(i) *For each $m \equiv 0 \pmod{2}$,*

$$\mathcal{E}(D_m^s[3, m - 3]) \geq \mathcal{E}(D_m^s[b, m - b]).$$

(ii) *For each $m \equiv 1 \pmod{2}$,*

$$\mathcal{E}(D_m^s[3, m - 4]) \geq \mathcal{E}(D_m^s[b, m - b - 1]).$$

Now we give the extremal energy of those bicyclic sidigraphs in the class \mathcal{D}_m^s whose both cycles are of odd length.

Theorem 4.20. *Suppose the sidigraph $\mathcal{S} \in \mathcal{D}_m^s$ has odd directed cycles.*

(i) *For $m \equiv 0 \pmod{2}$, the largest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[3, m - 3]$.*

(ii) *For $m \equiv 1 \pmod{2}$, the largest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[3, m - 4]$.*

(iii) *The smallest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[3, 3]$.*

Proof. The proof of Parts (i) and (ii) follows from Corollary 4.19.

(iii). As for odd integers b_1 and b_2 with $b_1 \geq b_2 \geq 3$, it holds that $\mathcal{E}(C_{b_1}) \geq \mathcal{E}(C_{b_2})$. Hence the smallest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[3, 3]$. \square

In next theorem, we give complete energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose both cycles are of odd length.

Theorem 4.21. *Suppose $m > 5$ and $b \in [2, m - 2]$.*

(i) *If $m \equiv 0 \pmod{4}$ then*

$$\begin{aligned} & \mathcal{E}(D_m^s[3, m-3]) > \mathcal{E}(D_m^s[5, m-5]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-2}{2}, \frac{m+2}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{m-6}{2}, \frac{m+2}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{m-10}{2}, \frac{m+2}{2}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[3, \frac{m+2}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[3, \frac{m-2}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[3, \frac{m-6}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[3, 3]). \end{aligned}$$

(ii) *If $m \equiv 1 \pmod{4}$ then*

$$\begin{aligned} & \mathcal{E}(D_m^s[3, m-4]) > \mathcal{E}(D_m^s[5, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-3}{2}, \frac{m+1}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{m-7}{2}, \frac{m+1}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{m-11}{2}, \frac{m+1}{2}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[3, \frac{m+1}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[3, \frac{m-3}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[3, \frac{m-7}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[3, 3]). \end{aligned}$$

(iii) *If $m \equiv 2 \pmod{4}$ then*

$$\begin{aligned} & \mathcal{E}(D_m^s[3, m-3]) > \mathcal{E}(D_m^s[5, m-5]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m}{2}, \frac{m}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{m-4}{2}, \frac{m}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{m-8}{2}, \frac{m}{2}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[3, \frac{m}{2}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[3, \frac{m-4}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[3, \frac{m-8}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[3, 3]). \end{aligned}$$

(iv) If $m \equiv 3 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[3, m-4]) > \mathcal{E}(D_m^s[5, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{m-1}{2}, \frac{m-1}{2}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{m-5}{2}, \frac{m-1}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{m-9}{2}, \frac{m-1}{2}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[3, \frac{m-1}{2}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[3, \frac{m-5}{2}\right]\right) > \mathcal{E}\left(D_m^s\left[3, \frac{m-9}{2}\right]\right) > \cdots > \mathcal{E}(D_m^s[3, 3]).
\end{aligned}$$

Proof. We know that $\csc z$ and $\cot z$ are decreasing for $z \in \left(0, \frac{\pi}{2}\right]$. Therefore we get the required energy ordering of bicyclic sidigraphs in \mathcal{D}_m^s when both cycles are of odd length. \square

4.2.3 One cycle is of odd length and one cycle is of even length

In this subsection, we find energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose one cycle is of even length and one is of odd length. For $m \equiv 0 \pmod{2}$, if $b \equiv 1 \pmod{2}$ then $m-b \equiv 1 \pmod{2}$ and if $b \equiv 0 \pmod{2}$ then $m-b \equiv 0 \pmod{2}$. So we only have to consider the case when $m \equiv 1 \pmod{2}$. Note that if $b \equiv 0 \pmod{2}$ and $m-b \equiv 1 \pmod{2}$ then $\mathcal{E}(D_m^s[b, m-b]) = \mathcal{E}(D_m^s[b, m-b])$. Hence we only have to give the energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose both cycles are positive or both cycles are negative.

Now we give the energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose both cycles are positive.

Lemma 4.22. *Suppose m is odd with $m \equiv 0 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:*

(i) Let $b \equiv 2 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right).$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right).$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right).$$

(ii) Let $b \equiv 0 \pmod{4}$.

(a) If $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

(b) If $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

Proof. (i). Suppose $b \equiv 2 \pmod{4}$ then $m-b \equiv 1 \pmod{2}$. Using Equation (2.2), we have

$$\mathcal{E}(D_m^s[b, m-b]) = 2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}.$$

By Part (2) of Lemma 4.8, we see that $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ is decreasing on $\left[2, \frac{2m}{3}\right]$. So the smallest even number where $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ attains maximum value is $b = 2$. Therefore we have

$$\mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right).$$

Also Part (2) of Lemma 4.8, we see that $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ is increasing on $\left[\frac{2m}{3}, m-2\right]$. So the largest even number where $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ attains maximum value is $b = m-3$ if $m-3 \equiv 2 \pmod{4}$ and $b = m-5$ if $m-3 \equiv 0 \pmod{4}$. Therefore we have

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right),$$

and

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right).$$

Analogously one can prove Part (ii). □

Next two lemmas have same proofs as of Lemma 4.22 and thus proofs are omitted.

Lemma 4.23. *Suppose m is odd with $m \equiv 1 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:*

(i) *Let $b \equiv 2 \pmod{4}$.*

(a) *If $b \in \left[2, \frac{2m}{3}\right]$ then*

$$\mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m-8}{3}, \frac{m+8}{3}\right]\right).$$

(b) *If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then*

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-4}{3}\right]\right).$$

(c) *If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then*

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-4}{3}\right]\right).$$

(ii) *Let $b \equiv 0 \pmod{4}$.*

(a) *If $m-3 \equiv 2 \pmod{4}$ then*

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

(b) *If $m-3 \equiv 0 \pmod{4}$ then*

$$\mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

Lemma 4.24. *Suppose m is odd with $m \equiv 2 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:*

(i) *Let $b \equiv 2 \pmod{4}$.*

(a) *If $b \in \left[2, \frac{2m}{3}\right]$ then*

$$\mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m-4}{3}, \frac{m+4}{3}\right]\right).$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-8}{3}\right]\right).$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-8}{3}\right]\right).$$

(ii) Let $b \equiv 0 \pmod{4}$.

(a) If $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

(b) If $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]).$$

Now we give the energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose both cycles are negative.

Lemma 4.25. *Suppose m is odd with $m \equiv 0 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:*

(i) Let $b \equiv 0 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m-6}{3}, \frac{m+6}{3}\right]\right).$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-6}{3}\right]\right).$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-6}{3}\right]\right).$$

(ii) Let $b \equiv 2 \pmod{4}$.

(a) If $m - 3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[\mathbf{m} - \mathbf{3}, \mathbf{3}]) > \mathcal{E}(D_m^s[\mathbf{m} - \mathbf{7}, \mathbf{7}]) > \cdots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m} - \mathbf{2}]).$$

(b) If $m - 3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[\mathbf{m} - \mathbf{5}, \mathbf{5}]) > \mathcal{E}(D_m^s[\mathbf{m} - \mathbf{9}, \mathbf{9}]) > \cdots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m} - \mathbf{2}]).$$

Proof. (i). Suppose $b \equiv 0 \pmod{4}$ then $m - b \equiv 1 \pmod{2}$. Using Equation (2.3), we get

$$\mathcal{E}(D_m^s[\mathbf{b}, \mathbf{m} - \mathbf{b}]) = 2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}.$$

Part (2) of Lemma 4.8 tells us that $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ is decreasing on $\left[2, \frac{2m}{3}\right]$. So the smallest even number where $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ has largest value is $b = 4$. Therefore we have

$$\mathcal{E}(D_m^s[\mathbf{4}, \mathbf{m} - \mathbf{4}]) > \mathcal{E}(D_m^s[\mathbf{8}, \mathbf{m} - \mathbf{8}]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{\mathbf{2m} - \mathbf{6}}{\mathbf{3}}, \frac{\mathbf{m} + \mathbf{6}}{\mathbf{3}}\right]\right).$$

Also Part (2) of Lemma 4.8, we see that $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ is increasing on $\left[\frac{2m}{3}, m - 2\right]$. So the largest even number where $2 \csc \frac{\pi}{b} + \csc \frac{\pi}{2(m-b)}$ attains largest value is $b = m - 3$ if $m - 3 \equiv 0 \pmod{4}$ and $b = m - 5$ if $m - 3 \equiv 2 \pmod{4}$. Therefore we have

$$\mathcal{E}(D_m^s[\mathbf{m} - \mathbf{3}, \mathbf{3}]) > \mathcal{E}(D_m^s[\mathbf{m} - \mathbf{7}, \mathbf{7}]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{\mathbf{2m} + \mathbf{6}}{\mathbf{3}}, \frac{\mathbf{m} - \mathbf{6}}{\mathbf{3}}\right]\right).$$

and

$$\mathcal{E}(D_m^s[\mathbf{m} - \mathbf{5}, \mathbf{5}]) > \mathcal{E}(D_m^s[\mathbf{m} - \mathbf{9}, \mathbf{9}]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{\mathbf{2m} + \mathbf{6}}{\mathbf{3}}, \frac{\mathbf{m} - \mathbf{6}}{\mathbf{3}}\right]\right).$$

Similarly, Part (ii) can be proved. □

Next two lemmas has same proof as of Lemma 4.25 and are thus neglected.

Lemma 4.26. *Suppose m is odd with $m \equiv 1 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:*

(i) Let $b \equiv 0 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m-2}{3}, \frac{m+2}{3}\right]\right).$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-10}{3}\right]\right).$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-10}{3}\right]\right).$$

(ii) Let $b \equiv 2 \pmod{4}$.

(a) If $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}(D_m^s[2, m-2]).$$

(b) If $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}(D_m^s[2, m-2]).$$

Lemma 4.27. Suppose m is odd with $m \equiv 2 \pmod{3}$ and $b \equiv 0 \pmod{2}$. Then the following energy ordering holds:

(i) Let $b \equiv 0 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m-10}{3}, \frac{m+10}{3}\right]\right).$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-2}{3}\right]\right).$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-2}{3}\right]\right).$$

(ii) Let $b \equiv 2 \pmod{4}$.

(a) If $m-3 \equiv 2 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}(D_m^s[2, m-2]).$$

(b) If $m-3 \equiv 0 \pmod{4}$ then

$$\mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[2, m-2]).$$

Now we give the extremal energy of those bicyclic sidigraphs in the class \mathcal{D}_m^s whose one cycle is of even length and one is of odd length.

Theorem 4.28. *Suppose a sidigraph $\mathcal{S} \in \mathcal{D}_m^s$ has one cycle of even length and one of odd length.*

(i) *For $m \equiv 1 \pmod{2}$, the largest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[2, m-2]$.*

(iii) *The smallest energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[2, 3]$.*

Proof. (i). For proof, see Theorem 7 [50].

(ii). Since for odd integers b_1 and b_2 with $b_1 \geq b_2 \geq 3$, it holds that $\mathcal{E}(C_{b_1}) \geq \mathcal{E}(C_{b_2})$ and $\mathcal{E}(C_2) = 0$. Hence the minimal energy of \mathcal{S} is attained if $\mathcal{S} \cong D_m^s[2, 3]$. \square

In next theorem, we give the complete energy ordering of those bicyclic sidigraphs in \mathcal{D}_m^s whose one cycle is of even length and one is of odd length.

Theorem 4.29. *Let $m > 5$ is odd and $b \in [2, m-2]$.*

(1) *Suppose $m \equiv 0 \pmod{3}$.*

(i) *Let $b \equiv 2 \pmod{4}$.*

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-12}{3}, \frac{m}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-24}{3}, \frac{m}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m-6}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-12}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m-6}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m-12}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, 3\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-12}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-24}{3}, 3\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m}{3}, \frac{m}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-12}{3}, \frac{m}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-24}{3}, \frac{m}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m-6}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-12}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(d) If $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}(D_m^s[2, m-2]) \\
& > \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[2, m-6]) > \dots > \mathcal{E}(D_m^s[2, 3]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(e) If $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}(D_m^s[2, m-2]) \\
& > \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[2, m-6]) > \dots > \mathcal{E}(D_m^s[2, 3]) > \mathcal{E}(D_m^s[2, 2]).
\end{aligned}$$

(ii) Let $b \equiv 0 \pmod{4}$.

(a) If $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(b) If $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(c) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m-6}{3}, \frac{m+6}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-18}{3}, \frac{m+6}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-30}{3}, \frac{m+6}{3}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[4, \frac{m+6}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-6}{3}\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(d) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-6}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-6}{3}, \frac{m-6}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-18}{3}, \frac{m-6}{3}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[4, \frac{m-6}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m-12}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-18}{3}\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(e) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-6}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-12}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, \frac{m-18}{3}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+6}{3}, 3\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-6}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-18}{3}, 3\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(2) Suppose $m \equiv 1 \pmod{3}$.

(i) Let $b \equiv 2 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m-8}{3}, \frac{m+8}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-20}{3}, \frac{m+8}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-32}{3}, \frac{m+8}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m+8}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m+2}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-4}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-4}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-8}{3}, \frac{m-4}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-20}{3}, \frac{m-4}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m-4}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m-10}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-16}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-4}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-10}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, \frac{m-16}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+4}{3}, 3\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-8}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-20}{3}, 3\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(d) If $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[\mathbf{m-3}, \mathbf{3}]) > \mathcal{E}(D_m^s[\mathbf{m-7}, \mathbf{7}]) > \dots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-2}]) \\
& > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-4}]) > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-6}]) > \dots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{3}]).
\end{aligned}$$

(e) If $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[\mathbf{m-5}, \mathbf{5}]) > \mathcal{E}(D_m^s[\mathbf{m-9}, \mathbf{9}]) > \dots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-2}]) \\
& > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-4}]) > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{m-6}]) > \dots > \mathcal{E}(D_m^s[\mathbf{2}, \mathbf{3}]).
\end{aligned}$$

(ii) Let $b \equiv 0 \pmod{4}$.

(a) If $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(b) If $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \cdots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(c) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m-2}{3}, \frac{m+2}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-14}{3}, \frac{m+2}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-26}{3}, \frac{m+2}{3}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[4, \frac{m+2}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m-4}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-10}{3}\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(d) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-10}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-2}{3}, \frac{m-10}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-14}{3}, \frac{m-10}{3}\right]\right) > \cdots > \mathcal{E}\left(D_m^s\left[4, \frac{m-10}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m-16}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-22}{3}\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(e) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \cdots > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-10}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-16}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, \frac{m-22}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+10}{3}, 3\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-2}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-14}{3}, 3\right]\right) > \cdots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(3) Suppose $m \equiv 2 \pmod{3}$.

(i) Let $b \equiv 2 \pmod{4}$.

(a) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[2, m-2]) > \mathcal{E}(D_m^s[6, m-6]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m-4}{3}, \frac{m+4}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-16}{3}, \frac{m+4}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-28}{3}, \frac{m+4}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m+4}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m-2}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-8}{3}\right]\right) > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(b) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-8}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-4}{3}, \frac{m-8}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-16}{3}, \frac{m-8}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[2, \frac{m-8}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[2, \frac{m-14}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[2, \frac{m-20}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(c) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-8}{3}\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-14}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, \frac{m-20}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+8}{3}, 3\right]\right) \\
& > \mathcal{E}\left(D_m^s\left[\frac{2m-4}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-16}{3}, 3\right]\right) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(d) If $m-3 \equiv 2 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}(D_m^s[2, m-2]) \\
& > \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[2, m-6]) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(e) If $m-3 \equiv 0 \pmod{4}$ then

$$\begin{aligned}
& \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}(D_m^s[2, m-2]) \\
& > \mathcal{E}(D_m^s[2, m-4]) > \mathcal{E}(D_m^s[2, m-6]) > \dots > \mathcal{E}(D_m^s[2, 3]).
\end{aligned}$$

(ii) Let $b \equiv 0 \pmod{4}$.

(a) If $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(b) If $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 5]) > \mathcal{E}(D_m^s[m-7, 9]) > \dots > \mathcal{E}(D_m^s[4, m-4]) \\ & > \mathcal{E}(D_m^s[4, m-6]) > \mathcal{E}(D_m^s[4, m-8]) > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(c) If $b \in \left[2, \frac{2m}{3}\right]$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[4, m-4]) > \mathcal{E}(D_m^s[8, m-8]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m-10}{3}, \frac{m+10}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-22}{3}, \frac{m+10}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-34}{3}, \frac{m+10}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[4, \frac{m+10}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m+4}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-2}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(d) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 2 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-5, 5]) > \mathcal{E}(D_m^s[m-9, 9]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-2}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-10}{3}, \frac{m-2}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-22}{3}, \frac{m-2}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-2}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[4, \frac{m-8}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[4, \frac{m-14}{3}\right]\right) > \dots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

(e) If $b \in \left[\frac{2m}{3}, m-2\right]$ and $m - 3 \equiv 0 \pmod{4}$ then

$$\begin{aligned} & \mathcal{E}(D_m^s[m-3, 3]) > \mathcal{E}(D_m^s[m-7, 7]) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-2}{3}\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-8}{3}\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, \frac{m-14}{3}\right]\right) > \dots > \mathcal{E}\left(D_m^s\left[\frac{2m+2}{3}, 3\right]\right) \\ & > \mathcal{E}\left(D_m^s\left[\frac{2m-10}{3}, 3\right]\right) > \mathcal{E}\left(D_m^s\left[\frac{2m-22}{3}, 3\right]\right) > \dots > \mathcal{E}(D_m^s[4, 3]) > \mathcal{E}(D_m^s[2, 3]). \end{aligned}$$

Proof. We know that $\csc z$ and $\cot z$ are decreasing for $z \in \left(0, \frac{\pi}{2}\right]$. Therefore we get the required energy ordering of bicyclic sidigraphs in \mathcal{D}_m^s when both cycles are of odd length. \square

4.3 Conclusion

Vertex-disjoint bicyclic sidigraphs are classified into three categories: the sidigraphs whose cycles are of even length, the sidigraphs whose cycles are of odd length and the sidigraphs whose one cycle is of even length and one is of odd length. In the current chapter, we separately investigated the energy ordering in each category. We also find largest and smallest energy in each category.

Chapter 5

Inverse sum indeg energy of graphs

In this chapter, we discuss about graph energy which is based on ISI matrix and study few properties of the ISI matrix. The ISI energy formula for some well-known graphs are determined. Some bounds for ISI energy of graphs are obtained. We also give integral representation of ISI energy of graphs. In the end, we give some noncospectral equienergetic graphs with respect to inverse sum indeg energy.

5.1 Inverse sum indeg energy

Let $\mathcal{G} = (\mathbb{V}_{\mathcal{G}}, \mathbb{E}_{\mathcal{G}})$ be a graph. Zangi et al. [77] defined the ISI matrix $\mathcal{A}_{\text{ISI}}(\mathcal{G}) = [a_{pq}]_{m \times m}$ of an m -vertex graph \mathcal{G} as:

$$a_{pq} = \begin{cases} \frac{d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}}{d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}} & \text{if } w_p w_q \in \mathbb{E}_{\mathcal{G}}, \\ 0 & \text{otherwise.} \end{cases}$$

The \mathcal{A}_{ISI} -characteristic polynomial of \mathcal{G} is given by:

$$\Psi_{\mathcal{G}}(\tilde{\theta}) = \det(\mathcal{A}_{\text{ISI}}(\mathcal{G}) - \tilde{\theta}I_m) \quad (5.1)$$

Let $\theta_1, \dots, \theta_m$ be the \mathcal{A}_{ISI} -eigenvalues of \mathcal{G} . Then Zangi et al. [77] define ISI energy of \mathcal{G} as

$$\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \sum_{q=1}^m |\theta_q|. \quad (5.2)$$

For convenience, we define some notations. Let

$$\mathcal{B} = 2 \sum_{1 \leq p < q \leq m} \left(\frac{d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}}{d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}} \right)^2, \quad \Upsilon = \det(\mathcal{A}_{\text{ISI}}(\mathcal{G})). \quad (5.3)$$

Theorem 5.1. *Suppose \mathcal{G}_m^r is a simple connected graph. Then*

$$\text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{G}_m^r)) \leq \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{K}_m)),$$

where the inequality becomes equality for $\mathcal{G}_m^r \cong \mathcal{K}_m$.

Proof. For convenience, write $\mathcal{H} = \mathcal{G}_m^r$. First, let $\mathcal{H} \not\cong \mathcal{K}_m$. Then $d_{\mathcal{H}}^{(w_p)} \leq m - 1$ for every vertex w_p of \mathcal{H} , $p = 1, \dots, m$. Therefore

$$\frac{d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}}{d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}} = \frac{1}{\frac{1}{d_{\mathcal{H}}^{(w_p)}} + \frac{1}{d_{\mathcal{H}}^{(w_q)}}} \leq \frac{1}{\frac{1}{m-1} + \frac{1}{m-1}} = \frac{m-1}{2}.$$

Now

$$\begin{aligned} \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{H})) &= 2 \sum_{1 \leq p < q \leq m} \left(\frac{d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}}{d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}} \right)^2 \\ &\leq \frac{2r(m-1)^2}{4} = \frac{r(m-1)^2}{2}. \end{aligned}$$

As $\mathcal{H} \not\cong \mathcal{K}_m$, it holds that $r < \frac{m(m-1)}{2}$. Consequently

$$\begin{aligned} \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{H})) &\leq \frac{r(m-1)^2}{2} < \frac{m(m-1)}{2} \times \frac{(m-1)^2}{2} \\ &= \frac{m}{4}(m-1)^3. \end{aligned}$$

Now let $\mathcal{H} \cong \mathcal{K}_m$. Lemma 2.16 implies

$$\begin{aligned} \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{K}_m)) &= 2 \left[\frac{m(m-1)}{2} \times \frac{(m-1)^2}{4} \right] \\ &= \frac{m}{4}(m-1)^3. \end{aligned}$$

Hence $\text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{H})) \leq \text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{K}_m))$. This proves the result. \square

A square diagonal matrix whose diagonal elements are square matrices and the non-diagonal elements are 0 is called a block diagonal matrix.

Next theorem determines the relationship among ISI energy of graph components and a graph.

Theorem 5.2. Suppose a graph \mathcal{G} has components $\mathcal{Q}_1, \mathcal{Q}_2, \dots, \mathcal{Q}_s$. Then $\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \sum_{q=1}^s \mathcal{E}_{\text{ISI}}(\mathcal{Q}_q)$.

Proof. Since $\mathcal{Q}_1, \mathcal{Q}_2, \dots, \mathcal{Q}_s$ are the components of \mathcal{G} , we can write $\mathcal{G} = \mathcal{Q}_1 \cup \mathcal{Q}_2 \cup \dots \cup \mathcal{Q}_s$. Then $\mathcal{A}_{\text{ISI}}(\mathcal{G})$ is a block diagonal matrix with diagonal elements $\mathcal{A}_{\text{ISI}}(\mathcal{Q}_1), \mathcal{A}_{\text{ISI}}(\mathcal{Q}_2), \dots, \mathcal{A}_{\text{ISI}}(\mathcal{Q}_s)$. Therefore

$$\text{spec}_{\text{ISI}}(\mathcal{G}) = \text{spec}_{\text{ISI}}(\mathcal{Q}_1) \cup \text{spec}_{\text{ISI}}(\mathcal{Q}_2) \cup \dots \cup \text{spec}_{\text{ISI}}(\mathcal{Q}_s).$$

Hence

$$\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \sum_{q=1}^s \mathcal{E}_{\text{ISI}}(\mathcal{Q}_q).$$

The proof is complete. □

Following result follows directly from ISI matrix of $\overline{\mathcal{K}}_m$.

Lemma 5.3. Suppose \mathcal{G} is a graph with $n_{\mathcal{G}} = m$. Then $\mathcal{E}_{\text{ISI}}(\mathcal{G}) = 0$ for $\mathcal{G} \cong \overline{\mathcal{K}}_m$.

Theorem 5.4. If a graph $\mathcal{G} \not\cong \overline{\mathcal{K}}_m$ and $\mathcal{E}_{\text{ISI}}(\mathcal{G})$ is an integer then $\mathcal{E}_{\text{ISI}}(\mathcal{G})$ be an even positive integer.

Proof. With no loss of generality, suppose that $\theta_1, \dots, \theta_s$ are positive and $\theta_{s+1}, \dots, \theta_m$ are non-negative. From Lemma 2.16, we have

$$\sum_{q=1}^s \theta_q + \sum_{q=s+1}^m \theta_q = \sum_{q=1}^m \theta_q = 0.$$

This gives

$$\sum_{q=1}^s \theta_q = - \sum_{q=s+1}^m \theta_q.$$

Now

$$\begin{aligned} \mathcal{E}_{\text{ISI}}(\mathcal{G}) &= \sum_{q=1}^m |\theta_q| \\ &= \sum_{q=1}^s \theta_q + \sum_{q=s+1}^m \theta_q \\ &= 2 \sum_{q=1}^s \theta_q. \end{aligned}$$

Therefore $\mathcal{E}_{\text{ISI}}(\mathcal{G})$ is an even integer. □

A matrix M is irreducible if the digraph associated with M is strongly connected. A matrix is non-negative if its all entries are non-negative.

Theorem 5.5 (Perron-Frobenius). *Let $A \neq 0$ be an irreducible matrix. Then A has a positive eigenvalue ν with corresponding eigenvector $y > 0$. If ω is another eigenvalue for A , then $\nu > |\omega|$.*

In the following two results, we determine some properties of the \mathcal{A}_{ISI} -eigenvalues of a graph \mathcal{G} . The idea of proof is taken from proof of Lemma 1.1 [17]

Lemma 5.6. *Suppose \mathcal{G} is a simple connected graph with $n_{\mathcal{G}} = m$, $m \geq 2$, and \mathcal{A}_{ISI} -eigenvalues $\theta_1 \geq \theta_2 \geq \dots \geq \theta_m$. If \mathcal{G} has diameter at least 3, then $\theta_1 > \theta_2 > 0$.*

Proof. Since the graph \mathcal{G} is connected therefore $\mathcal{A}_{\text{ISI}}(\mathcal{G})$ is an irreducible non-negative square matrix of order m . By Perron-Frobenius theorem, we have $\theta_1 > \theta_2$. Since the diameter of \mathcal{G} is at least 3, \mathcal{P}_4 is the subgraph of \mathcal{G} . So $\theta_2(\mathcal{G}) \geq \theta_2(\mathcal{P}_4) = \frac{4}{3} > 0$, where $\theta_2(\mathcal{G})$ is the second largest \mathcal{A}_{ISI} -eigenvalue of \mathcal{G} and $\theta_2(\mathcal{P}_4)$ is the second largest \mathcal{A}_{ISI} -eigenvalue of \mathcal{P}_4 . Hence $\theta_1 > \theta_2 > 0$. \square

Lemma 5.7 (Brouwer and Haemers [7]). *Suppose a connected graph \mathcal{G} has its largest \mathcal{A} -eigenvalue λ_1 . Then $-\lambda_1$ is an eigenvalue of \mathcal{G} if and only if it is bipartite.*

Theorem 5.8. *Suppose \mathcal{G} is a graph with $n_{\mathcal{G}} = m$, $m \geq 2$ and let its \mathcal{A} -spectrum and \mathcal{A}_{ISI} -spectrum are symmetric about the origin. Then $|\theta_1| = |\theta_2| = \dots = |\theta_q| > 0$ ($q \geq 2$) and rest of the \mathcal{A}_{ISI} -eigenvalues are zero (if exist) if and only if $\bigcup_{j=1}^t \mathcal{K}_{r,s} \cong \mathcal{G}$, where $t(r+s) = m$ and one of the r or s is greater than 1.*

Proof. First assume that

$$|\theta_1| = |\theta_2| = \dots = |\theta_q| > 0 \quad (q \geq 2), \quad (5.4)$$

and rest of the \mathcal{A}_{ISI} -eigenvalues are zero (if exist). Then each component of \mathcal{G} has atmost three distinct \mathcal{A}_{ISI} -eigenvalues. Let \mathcal{Q} be a component of \mathcal{G} . From Equation (5.4) and Lemma 5.7, we see that \mathcal{Q} is bipartite. The diameter of \mathcal{Q} is at least 3 if \mathcal{Q} is not a complete bipartite graph.

Therefore using Lemma 5.6 and Equation (5.4), we get a contradiction. Hence Q is a complete bipartite graph. As Q is arbitrary component of \mathcal{G} , therefore $\mathcal{G} \cong \bigcup_{j=1}^t \mathcal{K}_{r,s}$, where $t(r+s) = m$.

The converse statement is easy to prove. \square

5.2 ISI energy of some graphs

Now we prove ISI energy formula for some classes of graphs.

The \mathcal{A} -spectrum of \mathcal{K}_m and $\mathcal{K}_{m,n}$ is, respectively, given by

$$\begin{aligned} \text{spec}_{\mathcal{A}}(\mathcal{K}_m) &= \{(-1)^{m-1}, (m-1)\}, \\ \text{spec}_{\mathcal{A}}(\mathcal{K}_{m,n}) &= \{(0)^{m+n-2}, \pm \sqrt{mn}\}. \end{aligned}$$

Using Theorem 2.17, we get the following results.

Theorem 5.9. $\mathcal{E}_{\text{ISI}}(C_m) = \mathcal{E}(C_m)$.

Theorem 5.10. $\mathcal{E}_{\text{ISI}}(\mathcal{K}_m) = (m-1)^2$.

Remark 5.11. Let $m \equiv 2 \pmod{4}$. Then from energy formula of cycle C_m [4], one can see that $\mathcal{E}_{\text{ISI}}(C_m) = 2\mathcal{E}_{\text{ISI}}(C_{\frac{m}{2}})$.

Now we obtain the ISI energy formula for a complete bipartite graph.

Theorem 5.12. $\mathcal{E}_{\text{ISI}}(\mathcal{K}_{m,n}) = \frac{2(mn)^{\frac{3}{2}}}{m+n}$.

Proof. Let B be an $m \times n$ matrix and C be an $n \times m$ matrix, where each entry of B and C is equal to $\frac{mn}{m+n}$. Let O be a zero matrix of order $m \times m$ and O' be a zero matrix of order $n \times n$. Now

$$\mathcal{A}_{\text{ISI}}(\mathcal{K}_{m,n}) = \begin{bmatrix} O & B \\ C & O' \end{bmatrix}.$$

That is,

$$\mathcal{A}_{\text{ISI}}(\mathcal{K}_{m,n}) = \frac{mn}{m+n} \mathcal{A}(\mathcal{K}_{m,n}).$$

Hence

$$\text{spec}_{\text{ISI}}(\mathcal{K}_{m,n}) = \left\{ \frac{(mn)^{\frac{3}{2}}}{m+n}, 0^{(m+n-2)}, -\frac{(mn)^{\frac{3}{2}}}{m+n} \right\}.$$

Therefore

$$\begin{aligned} \mathcal{E}_{\text{ISI}}(\mathcal{K}_{m,n}) &= \sum_{q=1}^{m+n} |\theta_q^{\text{ISI}}| \\ &= \left| \frac{(mn)^{\frac{3}{2}}}{m+n} \right| + \left| -\frac{(mn)^{\frac{3}{2}}}{m+n} \right| \\ &= \frac{2(mn)^{\frac{3}{2}}}{m+n}. \end{aligned}$$

The proof is complete. \square

Next corollary is easily obtained from Theorem 5.12 .

Corollary 5.13. $\mathcal{E}_{\text{ISI}}(\mathcal{S}_m) = \frac{2(m-1)^{\frac{3}{2}}}{m}$.

Remark 5.14. By Theorem 5.2 and Theorem 5.10, it is easily seen that $\mathcal{E}_{\text{ISI}}(\overline{\mathcal{K}_{m,n}}) = m^2 + n^2 - 2(m-1+n)$.

Let $F = (f_{ij})$ be a $p \times p$ matrix with eigenvalues λ_k and B be a $q \times q$ matrix with eigenvalues β_l , $i, j, k = 1, \dots, p$, $l = 1, \dots, q$. The Kronecker product of F and B , represented by $F \otimes B$, gives the matrix which is formed by substituting each entry f_{ij} of F by $f_{ij} B$. The eigenvalues of $F \otimes B$ are $\lambda_k \beta_l$.

Suppose $\mathcal{G}(\mathbb{V}_{\mathcal{G}}, \mathbb{E}_{\mathcal{G}})$ be a graph and \mathbb{V}' be the set such that $\mathbb{V}_{\mathcal{G}} \cap \mathbb{V}' = \phi$, $|\mathbb{V}_{\mathcal{G}}| = |\mathbb{V}'|$ and $\pi : \mathbb{V}_{\mathcal{G}} \rightarrow \mathbb{V}'$ is a bijection. For $w \in \mathbb{V}_{\mathcal{G}}$, we write $\pi(w) = w'$. The duplication of \mathcal{G} , represented by \mathcal{G}^* , is the graph with the property that $\mathbb{V}_{\mathcal{G}^*} = \mathbb{V}_{\mathcal{G}} \cup \mathbb{V}'$ and its edges are as follows: In \mathcal{G} , $wz \in \mathbb{E}_{\mathcal{G}}$ if and only if $wz' \in \mathbb{E}_{\mathcal{G}^*}$ and $zw' \in \mathbb{E}_{\mathcal{G}^*}$.

Let $\mathcal{H}_1, \dots, \mathcal{H}_d$ be the d copies of \mathcal{G} with vertex sets $\mathbb{V}_{\mathcal{H}_1}^1, \dots, \mathbb{V}_{\mathcal{H}_d}^d$ and let $\mathbb{V}_{\mathcal{H}_q}^q = \{w_{1q}, \dots, w_{mq}\}$, $q = 1, \dots, d$ and w_{jq} represents the j -th vertex of the q -th copy of \mathcal{G} , $j = 1, \dots, m$. The d -double graph \mathcal{G}^d of \mathcal{G} is the graph with the property that $\mathbb{V}_{\mathcal{G}^d} = \mathbb{V}_{\mathcal{H}_1}^1 \cup \dots \cup \mathbb{V}_{\mathcal{H}_d}^d$ and its edges are as follows: In \mathcal{G} , $w_1 w_2 \in \mathbb{E}_{\mathcal{G}}$ if and only if $w_{1i} w_{2k} \in \mathbb{E}_{\mathcal{G}^d}$ with $i \neq k$ and $k = 1, \dots, d$. See Figure 5.1.

Now we give the relation between $\mathcal{E}_{\text{ISI}}(\mathcal{G})$ and $\mathcal{E}_{\text{ISI}}(\mathcal{G}^*)$.

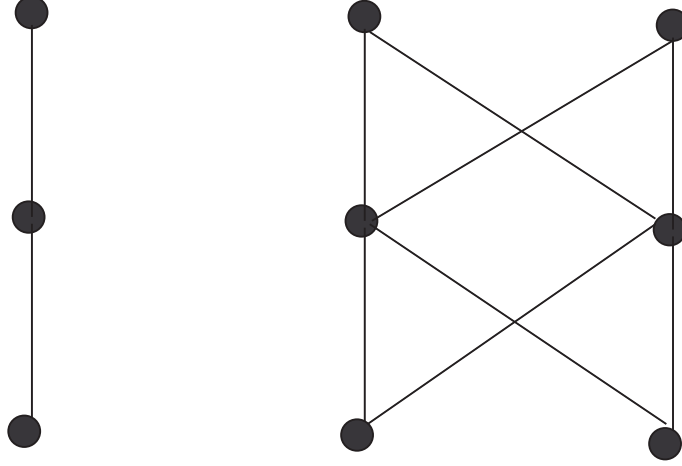


Figure 5.1: \mathcal{P}_3 and its 2-double graph \mathcal{P}_3^2 .

Theorem 5.15. $\mathcal{E}_{\text{ISI}}(\mathcal{G}^*) = 2 \mathcal{E}_{\text{ISI}}(\mathcal{G})$ for a graph \mathcal{G} with $n_{\mathcal{G}} = m$.

Proof. Let O be an $m \times m$ zero matrix. By proper labelling of the vertices in \mathcal{G}^* , we get

$$\mathcal{A}_{\text{ISI}}(\mathcal{G}^*) = \begin{bmatrix} O & \mathcal{A}_{\text{ISI}}(\mathcal{G}) \\ \mathcal{A}_{\text{ISI}}(\mathcal{G}) & O \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \mathcal{A}_{\text{ISI}}(\mathcal{G}).$$

Thus the spectrum of $\mathcal{A}_{\text{ISI}}(\mathcal{G}^*)$ is $\pm \theta_q^{\text{ISI}}$, $q = 1, \dots, m$. Hence $\mathcal{E}_{\text{ISI}}(\mathcal{G}^*) = 2 \mathcal{E}_{\text{ISI}}(\mathcal{G})$. \square

Theorem 5.16. $\mathcal{E}_{\text{ISI}}(\mathcal{G}^d) = d^2 \mathcal{E}_{\text{ISI}}(\mathcal{G})$ for a graph \mathcal{G} with $n_{\mathcal{G}} = m$.

Proof. Let J_d be a $d \times d$ matrix whose every entry is equal to 1. By proper labeling of the vertices in \mathcal{G}^d , we have

$$\mathcal{A}_{\text{ISI}}(\mathcal{G}^d) = \begin{bmatrix} d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & \dots & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) \\ d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & \dots & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) \\ \vdots & \vdots & \vdots & \vdots \\ d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) & \dots & d\mathcal{A}_{\text{ISI}}(\mathcal{G}) \end{bmatrix}_{dm \times dm}$$

Therefore $\mathcal{A}_{\text{ISI}}(\mathcal{G}^d) = d (\mathcal{A}_{\text{ISI}}(\mathcal{G}) \otimes J_d)$, where \mathcal{A} -spectrum of J_d is $d^{(1)}$ and $0^{(d-1)}$. By property of Kronecker product of matrices, the \mathcal{A}_{ISI} -spectrum of \mathcal{G}^d is 0 with multiplicity $d - 1$ and \mathcal{A}_{ISI} -spectrum of \mathcal{G} . Therefore we get $\mathcal{E}_{\text{ISI}}(\mathcal{G}^d) = d^2 \mathcal{E}_{\text{ISI}}(\mathcal{G})$. \square

5.3 Bounds and integral representation of ISI energy

In this section, few bounds on ISI energy of graphs are given. Das et al. [21] prove the following theorem for eigenvalues of degree-based energies of graphs.

Theorem 5.17 (Das et al. [21]). *For the eigenvalues $f_1 \geq f_2 \geq \dots \geq f_m$ of a matrix $\mathcal{A}_{TI}(\mathcal{G})$, the following inequalities hold.*

$$\begin{aligned} \sqrt{\frac{\text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{m(m-1)}} &\leq f_1 \leq \sqrt{\frac{(m-1) \text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{m}}, \\ -\sqrt{\frac{(m-1) \text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{m}} &\leq f_m \leq -\sqrt{\frac{\text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{m(m-1)}}, \\ -\sqrt{\frac{(k-1) \text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{m(m-k+1)}} &\leq f_k \leq \sqrt{\frac{(m-k) \text{tr}(\mathcal{A}_{TI}^2(\mathcal{G}))}{km}}, \end{aligned}$$

for each $k = 2, \dots, m-1$.

Next result is obtained by using Theorem 5.17.

Theorem 5.18. *For the eigenvalues $\theta_1 \geq \theta_2 \geq \dots \geq \theta_m$ of $\mathcal{A}_{\text{ISI}}(\mathcal{G})$, the following inequalities hold.*

$$\begin{aligned} \sqrt{\frac{\mathcal{B}}{m(m-1)}} &\leq \theta_1 \leq \sqrt{\frac{(m-1) \mathcal{B}}{m}}, \\ -\sqrt{\frac{(m-1) \mathcal{B}}{m}} &\leq \theta_m \leq -\sqrt{\frac{\mathcal{B}}{m(m-1)}}, \\ -\sqrt{\frac{(k-1) \mathcal{B}}{m(m-k+1)}} &\leq \theta_k \leq \sqrt{\frac{(m-k) \mathcal{B}}{km}}, \end{aligned}$$

for each $k = 2, \dots, m-1$ and \mathcal{B} is defined in Equation (5.3).

Next result is obtained using Theorem 5.1 and Theorem 5.18.

Theorem 5.19. *For \mathcal{A}_{ISI} -eigenvalues $\theta_1 \geq \theta_2 \geq \dots \geq \theta_m$ of a connected graph \mathcal{G} , the following*

inequalities hold.

$$\begin{aligned}\sqrt{\frac{\mathcal{B}}{m(m-1)}} &\leq \theta_1 \leq \mathcal{E}_{\text{ISI}}(\mathcal{K}_m), \\ -\mathcal{E}_{\text{ISI}}(\mathcal{K}_m) &\leq \theta_m \leq -\sqrt{\frac{\mathcal{B}}{m(m-1)}}, \\ -\sqrt{\frac{(k-1)(m-1)^3}{4(m-k+1)}} &\leq \theta_k \leq \sqrt{\frac{(m-k)(m-1)^3}{4k}},\end{aligned}$$

for each $k = 2, \dots, m-1$.

In next theorem, we find bounds for ISI energy using $\text{tr}(\mathcal{A}_{\text{ISI}}^2(\mathcal{G}))$ and $\det(\mathcal{A}_{\text{ISI}}(\mathcal{G}))$.

Theorem 5.20. *Suppose \mathcal{G} be a simple graph with $n_{\mathcal{G}} = m$, $m \geq 2$. Then*

$$m |\Upsilon|^{\frac{2}{m}} \leq \mathcal{E}_{\text{ISI}}(\mathcal{G}) \leq \sqrt{m \mathcal{B}},$$

where Υ and \mathcal{B} are defined in Equation (5.3).

Proof. We know that arithmetic mean is always less than quadratic mean. Therefore

$$\begin{aligned}\mathcal{E}_{\text{ISI}}(\mathcal{G}) &= \sum_{q=1}^m |\theta_q| \\ &\leq \sqrt{m \sum_{q=1}^m |\theta_q|^2} \\ &= \sqrt{m \sum_{q=1}^m \theta_q^2} = \sqrt{m \mathcal{B}}.\end{aligned}$$

Quadratic-Geometric mean inequality gives

$$\begin{aligned}[\mathcal{E}_{\text{ISI}}(\mathcal{G})]^2 &= \left[\sum_{q=1}^m |\theta_q| \right]^2 \\ &\geq \sum_{q=1}^m |\theta_q|^2 \\ &\geq m \left(\prod_{q=1}^m |\theta_q| \right)^{\frac{2}{m}} = m |\Upsilon|^{\frac{2}{m}}.\end{aligned}$$

This completes the proof. □

Now we have the following theorem. The proof is similar to the proof of Theorem 3 [21] and is thus excluded.

Theorem 5.21. *Suppose \mathcal{G} be a simple graph with $n_{\mathcal{G}} = m \geq 2$. Then*

$$\sqrt{\mathcal{B} + m |\Upsilon|_m^{\frac{2}{m}} (m-1)} \leq \mathcal{E}_{\text{ISI}}(\mathcal{G}) \leq \sqrt{(m-1) \mathcal{B} + m |\Upsilon|_m^{\frac{2}{m}}},$$

where Υ and \mathcal{B} are defined in Equation (5.3).

In Theorem 5.22, we obtain bounds for ISI energy using size, smallest and largest degrees of a simple graph.

Theorem 5.22. *Suppose $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a graph. Then*

$$\begin{aligned} \mathcal{E}_{\text{ISI}}(\mathcal{H}) &\geq \sqrt{\frac{r \delta_{\mathcal{H}}^2}{2} + m(m-1) |\Upsilon|_m^{\frac{2}{m}}} \\ \mathcal{E}_{\text{ISI}}(\mathcal{H}) &\leq \sqrt{r(m-1) \frac{\nabla_{\mathcal{H}}^2}{2} + m |\Upsilon|_m^{\frac{2}{m}}}. \end{aligned}$$

Proof. For each vertex w_p of \mathcal{H} , $\delta_{\mathcal{H}} \leq d_{\mathcal{H}}^{(w_p)} \leq \nabla_{\mathcal{H}}$, $p = 1, 2, \dots, m$. Using this fact, we get

$$\begin{aligned} \frac{1}{\frac{1}{d_{\mathcal{H}}^{(w_p)}} + \frac{1}{d_{\mathcal{H}}^{(w_q)}}} &\leq \frac{1}{\frac{1}{\nabla_{\mathcal{H}}} + \frac{1}{\nabla_{\mathcal{H}}}} = \frac{\nabla_{\mathcal{H}}}{2}, \\ \frac{1}{\frac{1}{d_{\mathcal{H}}^{(w_p)}} + \frac{1}{d_{\mathcal{H}}^{(w_q)}}} &\geq \frac{1}{\frac{1}{\delta_{\mathcal{H}}} + \frac{1}{\delta_{\mathcal{H}}}} = \frac{\delta_{\mathcal{H}}}{2}. \end{aligned}$$

Hence

$$\begin{aligned} \mathcal{B} &= 2 \sum_{1 \leq p < q \leq m} \left(\frac{d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}}{d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}} \right)^2 \leq 2r \frac{\nabla_{\mathcal{H}}^2}{4} = \frac{r \nabla_{\mathcal{H}}^2}{2}, \\ \mathcal{B} &= 2 \sum_{1 \leq p < q \leq m} \left(\frac{d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}}{d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}} \right)^2 \geq 2r \frac{\delta_{\mathcal{H}}^2}{4} = \frac{r \delta_{\mathcal{H}}^2}{2}. \end{aligned}$$

Now using Theorem 5.21, we obtain the desired result. \square

An analogue of Theorem 1.2 is Theorem 5.23.

Theorem 5.23. Suppose \mathcal{G} be a simple graph with $n_{\mathcal{G}} = m$ and \mathcal{A}_{ISI} -characteristic polynomial $\Psi(\theta)$. Then

$$\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(m - \frac{i\tilde{\theta} \Psi'_{\mathcal{G}}(i\tilde{\theta})}{\Psi_{\mathcal{G}}(i\tilde{\theta})} \right) d\tilde{\theta},$$

where $\Psi'_{\mathcal{G}}(\tilde{\theta}) = \frac{d}{d\tilde{\theta}} \Psi_{\mathcal{G}}(\tilde{\theta})$ and $i = \sqrt{-1}$.

Corollary 5.24. Suppose \mathcal{G} be a graph with $n_{\mathcal{G}} = m$. Then

$$\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{\tilde{\theta}^2} \ln \left(\tilde{\theta}^m \Psi_{\mathcal{G}}\left(\frac{i}{\tilde{\theta}}\right) \right) d\tilde{\theta}.$$

Next result is similar to graph energy.

Theorem 5.25. Let \mathcal{G} be a graph with $n_{\mathcal{G}} = m$ and \mathcal{A}_{ISI} -characteristic polynomial $\Psi_{\mathcal{G}}(\tilde{\theta}) = \tilde{\theta}^m + \sum_{q=1}^m b_q \tilde{\theta}^{m-q}$. Then

$$\begin{aligned} \mathcal{E}_{\text{ISI}}(\mathcal{G}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\tilde{\theta}^2} \log \left[\left(\sum_{q=0}^{\lfloor \frac{m}{2} \rfloor} (-1)^q b_{2q}(\mathcal{G}) \tilde{\theta}^{2q} \right)^2 \right. \\ \left. + \left(\sum_{q=0}^{\lfloor \frac{m}{2} \rfloor} (-1)^q b_{2q+1}(\mathcal{G}) \tilde{\theta}^{2q+1} \right)^2 \right] d\tilde{\theta}. \end{aligned}$$

5.4 \mathcal{A}_{ISI} -Equienergetic graphs

Two graphs with same \mathcal{A}_{ISI} -spectrum are said to be \mathcal{A}_{ISI} -cospectral, otherwise \mathcal{A}_{ISI} -noncospectral. Two \mathcal{A}_{ISI} -equienergetic graphs are the graphs with same ISI energy. Two isomorphic graphs are always \mathcal{A}_{ISI} -cospectral and thus are \mathcal{A}_{ISI} -equienergetic. In this section, we construct few classes of \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic graphs.

Suppose \mathcal{G} be a b -regular graph with $n_{\mathcal{G}} = m$. Let $\mathcal{L}^{(1)}(\mathcal{G}) = \mathcal{L}(\mathcal{G})$, $\mathcal{L}^{(q)}(\mathcal{G}) = \mathcal{L}(\mathcal{L}^{(q-1)}(\mathcal{G}))$, $q = 1, 2, \dots$, be the iterated line graphs of \mathcal{G} . Ramane et al. [65] prove the following energy formula for $\mathcal{L}^{(2)}(\mathcal{G})$.

$$\mathcal{E}(\mathcal{L}^{(2)}(\mathcal{G})) = 2mb(b-2). \quad (5.5)$$

Theorem 5.26. Suppose \mathcal{H}_1 and \mathcal{H}_2 are two b -regular m -vertex \mathcal{A} -noncospectral graphs. Then $\mathcal{L}^{(2)}(\mathcal{H}_1)$ and $\mathcal{L}^{(2)}(\mathcal{H}_2)$ are \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic graphs.

Proof. For an m -vertex b -regular \mathcal{G} , $\mathcal{L}^{(2)}(\mathcal{G})$ is $\frac{1}{2}mb(b-1)$ -vertex $(4b-6)$ -regular graph. By Theorem 2.17 and Equation (5.5), we get

$$\begin{aligned}\mathcal{E}_{\text{ISI}}(\mathcal{L}^{(2)}(\mathcal{G})) &= (2b-3) \mathcal{E}(\mathcal{L}^{(2)}(\mathcal{G})) \\ &= 2mb(2b-3)(b-2).\end{aligned}$$

Hence $\mathcal{E}_{\text{ISI}}(\mathcal{L}^{(2)}(\mathcal{H}_1)) = \mathcal{E}_{\text{ISI}}(\mathcal{L}^{(2)}(\mathcal{H}_2))$.

Since $\mathcal{A}_{\text{ISI}}(\mathcal{L}^{(2)}(\mathcal{G})) = (2b-3)\mathcal{A}(\mathcal{L}^{(2)}(\mathcal{G}))$ and $\mathcal{L}^{(2)}(\mathcal{H}_1)$ and $\mathcal{L}^{(2)}(\mathcal{H}_2)$ are \mathcal{A} -noncospectral graphs, therefore $\mathcal{L}^{(2)}(\mathcal{H}_1)$ and $\mathcal{L}^{(2)}(\mathcal{H}_2)$ are also \mathcal{A}_{ISI} -noncospectral graphs. \square

Corollary 5.27. *Suppose \mathcal{H}_1 and \mathcal{H}_2 are two b -regular m -vertex and \mathcal{A} -noncospectral graphs. Then for any $q \geq 2$, $\mathcal{L}^{(q)}(\mathcal{H}_1)$ and $\mathcal{L}^{(q)}(\mathcal{H}_2)$ are \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic.*

Theorem 5.28. *Suppose \mathcal{H}_1 and \mathcal{H}_2 are two m -vertex \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic. Then $\mathcal{H}_1 \cup \overline{\mathcal{K}}_r$ and $\mathcal{H}_2 \cup \overline{\mathcal{K}}_r$ are \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic.*

Proof. By Theorem 5.2, we have

$$\begin{aligned}\mathcal{E}_{\text{ISI}}(\mathcal{H}_1 \cup \overline{\mathcal{K}}_r) &= \mathcal{E}_{\text{ISI}}(\mathcal{H}_1) + \mathcal{E}_{\text{ISI}}(\overline{\mathcal{K}}_r) \\ &= \mathcal{E}_{\text{ISI}}(\mathcal{H}_2) + \mathcal{E}_{\text{ISI}}(\overline{\mathcal{K}}_r) \\ &= \mathcal{E}_{\text{ISI}}(\mathcal{H}_2 \cup \overline{\mathcal{K}}_r).\end{aligned}$$

Since \mathcal{H}_1 and \mathcal{H}_2 are \mathcal{A}_{ISI} -noncospectral, therefore $\mathcal{H}_1 \cup \overline{\mathcal{K}}_r$ and $\mathcal{H}_2 \cup \overline{\mathcal{K}}_r$ are also \mathcal{A}_{ISI} -noncospectral. \square

Corollary 5.29. *Suppose \mathcal{H}_1 and \mathcal{H}_2 are two b -regular m -vertex \mathcal{A} -noncospectral graphs. Then for any $q \geq 2$, $\mathcal{L}^{(q)}(\mathcal{H}_1) \cup \overline{\mathcal{K}}_r$ and $\mathcal{L}^{(q)}(\mathcal{H}_2) \cup \overline{\mathcal{K}}_r$ are \mathcal{A}_{ISI} -noncospectral \mathcal{A}_{ISI} -equienergetic.*

The following two theorems give some more classes of \mathcal{A}_{ISI} -equienergetic graphs.

Theorem 5.30. *Let \mathcal{G} be any m -vertex graph and $d \equiv 0 \pmod{2}$. Also let $\widetilde{\mathcal{G}}$ be the graph which is the union of $\frac{d^2}{2}$ copies of \mathcal{G}^* . Then $\mathcal{E}_{\text{ISI}}(\mathcal{G}^d) = \mathcal{E}_{\text{ISI}}(\widetilde{\mathcal{G}})$.*

Proof. By definition of $\tilde{\mathcal{G}}$ and proof of Theorem 5.2, note that $\mathcal{A}_{\text{ISI}}(\tilde{\mathcal{G}})$ is a block diagonal matrix with diagonal elements $\mathcal{A}_{\text{ISI}}(\mathcal{G}^*)$ and \mathcal{A}_{ISI} -spectrum of $\tilde{\mathcal{G}}$ is $\pm\tilde{\theta}_q$ each with multiplicity $\frac{d^2}{2}$, $q = 1, \dots, m$. Also in proof of Theorem 5.16, we see that the \mathcal{A}_{ISI} -spectrum of \mathcal{G}^d is 0 with multiplicity $d - 1$ and $d^2 \tilde{\theta}_q$, $q = 1, \dots, m$. Therefore $\tilde{\mathcal{G}}$ and \mathcal{G}^d are \mathcal{A}_{ISI} -noncospectral and \mathcal{A}_{ISI} -equienergetic graphs. \square

Theorem 5.31. *Let \mathcal{G} be an m -vertex graph whose at least one component is a cycle. Take another m -vertex graph \mathcal{H} with same components as of \mathcal{G} except for the component which is cycle. Corresponding to each cycle (say C_r) in \mathcal{G} , where $r \equiv 2 \pmod{4}$, the graph \mathcal{H} has two cycles of half the order of C_r (say $C_{\frac{r}{2}}, C_{\frac{r}{2}}$). Then \mathcal{G} and \mathcal{H} are \mathcal{A}_{ISI} -noncospectral and \mathcal{A}_{ISI} -equienergetic graphs.*

Proof. Using Theorem 5.2 and Remark 5.11, one can get the desired result.

5.5 Conclusion

The energy of a graph has wide range of applications in chemistry. Energy of many types of graphs can be found by using inverse sum indeg energy of those graphs. We present some properties of ISI energy and \mathcal{A}_{ISI} -spectra of graphs. We also find relation of ISI energy of some graphs with graph energy.

Chapter 6

On generalized inverse sum indeg index and energy of graphs

In this chapter, we introduce generalized inverse sum indeg index and generalized inverse sum indeg energy of graphs. Our strong motivation to define generalized ISI index and energy is the fact that the degree based topological indices and energies are derived from them by giving the specific values to the parameters involved. We study the generalized inverse sum indeg index and energy from an algebraic point of view. Extremal values of this index for some graph classes are determined. Some spectral properties of generalized inverse sum indeg matrix are studied. We also find Nordhaus-Gaddum-type results for generalized ISI index spectral radius and energy.

6.1 Basic results

Let $\mathcal{G} = (\mathbb{V}_{\mathcal{G}}, \mathbb{E}_{\mathcal{G}})$ be a graph. We define generalized inverse sum indeg index as

$$S_{\alpha, \beta}(\mathcal{G}) = \sum_{w_p w_q \in \mathbb{E}_{\mathcal{G}}} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{\beta}}, \quad (6.1)$$

where α and β are real numbers.

We define generalized ISI matrix $\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{G}) = [a_{pq}]_{m \times m}$ of an m -vertex graph \mathcal{G} as

$$a_{pq} = \begin{cases} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{\beta}} & \text{if } w_p w_q \in \mathbb{E}_{\mathcal{G}}, \\ 0 & \text{otherwise.} \end{cases}$$

The $\mathcal{A}_{S_{\alpha,\beta}}$ -characteristic polynomial of \mathcal{G} is given by:

$$\begin{aligned} \Psi_{\mathcal{G}}(\tilde{\theta}) &= \det(\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{G}) - \tilde{\theta}I_m) \\ &= \tilde{\theta}^m + \sum_{q=1}^m c_q \tilde{\theta}^{m-q}, \end{aligned} \quad (6.2)$$

where I_m is an $m \times m$ identity matrix. The $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues of \mathcal{G} are the roots of polynomial in Equation (6.2).

Let $\theta_1, \dots, \theta_m$ be the $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues of \mathcal{G} . Then we define the generalized ISI energy of graph \mathcal{G} as

$$\mathcal{E}_{\alpha,\beta}(\mathcal{G}) = \sum_{q=1}^m |\theta_q|. \quad (6.3)$$

We list here few degree-based topological indices and energies of a graph \mathcal{G} . These types of degree based indices and energies can be derived from generalized ISI index and energy by only giving specific values to α and β .

1. If $\alpha = 0$ and $\beta = -1$, then $S_{\alpha,\beta}(\mathcal{G}) = M_1(\mathcal{G})$ and matrix $\mathcal{A}_{0,-1}(\mathcal{G})$ is the first Zagreb matrix. The energy corresponding to $\mathcal{A}_{0,-1}(\mathcal{G})$ is the first Zagreb energy $\mathcal{E}_{M_1}(\mathcal{G})$. Note that $\mathcal{E}_{M_1}(\mathcal{G}) = \mathcal{E}_{0,-1}(\mathcal{G})$.
2. If $\alpha = 0$ and $\beta = 1/2$, then $S_{\alpha,\beta}(\mathcal{G}) = \chi(\mathcal{G})$ and matrix $\mathcal{A}_{0,1/2}(\mathcal{G})$ is the sum-connectivity matrix. The energy corresponding to $\mathcal{A}_{0,1/2}(\mathcal{G})$ is the sum-connectivity energy $\mathcal{E}_{\chi}(\mathcal{G})$. Now see that $\mathcal{E}_{\chi}(\mathcal{G}) = \mathcal{E}_{0,1/2}(\mathcal{G})$.
3. If $\alpha = 0$ and $\beta = -\alpha$ then $S_{\alpha,\beta}(\mathcal{G}) = \chi_{\alpha}(\mathcal{G})$ and matrix $\mathcal{A}_{0,-\alpha}(\mathcal{G})$ is the general sum-connectivity matrix. The energy corresponding to $\mathcal{A}_{0,-\alpha}(\mathcal{G})$ is the general sum-connectivity energy $\mathcal{E}_{\chi_{\alpha}}(\mathcal{G})$. Note that $\mathcal{E}_{\chi_{\alpha}}(\mathcal{G}) = \mathcal{E}_{0,-\alpha}(\mathcal{G})$.

4. If $\alpha = 1$ and $\beta = 0$ then $S_{\alpha,\beta}(\mathcal{G}) = M_2(\mathcal{G})$ and matrix $\mathcal{A}_{1,0}(\mathcal{G})$ is the second Zagreb matrix. The energy corresponding to $\mathcal{A}_{1,0}(\mathcal{G})$ is the second Zagreb energy $\mathcal{E}_{M_2}(\mathcal{G})$. Note that $\mathcal{E}_{M_2}(\mathcal{G}) = \mathcal{E}_{1,0}(\mathcal{G})$.
5. If $\alpha = -1/2$ and $\beta = 0$ then $S_{\alpha,\beta}(G) = R(G)$ and matrix $\mathcal{A}_{-1/2,0}(\mathcal{G})$ is the Randić matrix. The energy corresponding to $\mathcal{A}_{-1/2,0}(\mathcal{G})$ is the Randić energy $\mathcal{E}_R(\mathcal{G})$. Observe that $\mathcal{E}_R(\mathcal{G}) = \mathcal{E}_{-1/2,0}(\mathcal{G})$.
6. If $\beta = 0$ then $S_{\alpha,\beta}(G) = R_\alpha(G)$ and matrix $\mathcal{A}_{\alpha,0}(\mathcal{G})$ is the general Randić matrix. The energy corresponding to $\mathcal{A}_{\alpha,0}(\mathcal{G})$ is the general Randić energy $\mathcal{E}_{R_\alpha}(\mathcal{G})$. Note that $\mathcal{E}_{R_\alpha}(\mathcal{G}) = \mathcal{E}_{\alpha,0}(\mathcal{G})$.
7. If $\alpha = 1$ and $\beta = 1$ then $S_{\alpha,\beta}(\mathcal{G}) = \text{ISI}(\mathcal{G})$ and matrix $\mathcal{A}_{1,1}(\mathcal{G})$ is the inverse sum indeg matrix. The energy corresponding to $\mathcal{A}_{1,1}(\mathcal{G})$ is the inverse sum indeg energy $\mathcal{E}_{\text{ISI}}(\mathcal{G})$. Note that $\mathcal{E}_{\text{ISI}}(\mathcal{G}) = \mathcal{E}_{1,1}(\mathcal{G})$.

For study of more degree-based topological indices, see [28] and references therein.

Under certain conditions, we now determine the monotonicity of the generalized ISI index of a graph \mathcal{G} when new edges are added in \mathcal{G} .

Lemma 6.1. *Let w and z be two non-adjacent vertices of a graph \mathcal{G} . Also let $\mathcal{G} + \{wz\}$ is the graph formed from \mathcal{G} by joining w and z by an edge wz . If $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq 0$ and $\alpha \geq \beta$, then $S_{\alpha,\beta}(\mathcal{G} + \{wz\}) > S_{\alpha,\beta}(\mathcal{G})$.*

Proof. If $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq 0$ and $\alpha \geq \beta$, then for any real numbers $x, y \geq 1$, we have $\left(1 + \frac{1}{x}\right)^\alpha \geq \left(1 + \frac{1}{x+y}\right)^\beta$. This implies $\frac{(x+1)^\alpha}{(x+y+1)^\beta} \geq \frac{x^\alpha}{(x+y)^\beta}$. Hence $\frac{((x+1)y)^\alpha}{(x+y+1)^\beta} \geq \frac{(xy)^\alpha}{(x+y)^\beta}$.

Let $N_{\mathcal{G}}(w) = \{w_1, \dots, w_r\}$ and $N_{\mathcal{G}}(z) = \{z_1, \dots, z_t\}$. Then

$$\begin{aligned} S_{\alpha, \beta}(\mathcal{G} + \{wz\}) - S_{\alpha, \beta}(\mathcal{G}) &= \left[\frac{\left((d_{\mathcal{G}}^{(w)} + 1) (d_{\mathcal{G}}^{(z)} + 1) \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)} + 2 \right)^{\beta}} \right] \\ &+ \sum_{p=1}^r \left[\frac{\left((d_{\mathcal{G}}^{(w)} + 1) d_{\mathcal{G}}^{(w_p)} \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(w_p)} + 1 \right)^{\beta}} - \frac{\left(d_{\mathcal{G}}^{(w)} d_{\mathcal{G}}^{(w_p)} \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(w_p)} \right)^{\beta}} \right] \\ &+ \sum_{q=1}^t \left[\frac{\left((d_{\mathcal{G}}^{(z)} + 1) d_{\mathcal{G}}^{(z_q)} \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(z)} + d_{\mathcal{G}}^{(z_q)} + 1 \right)^{\beta}} - \frac{\left(d_{\mathcal{G}}^{(z)} d_{\mathcal{G}}^{(z_q)} \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(z)} + d_{\mathcal{G}}^{(z_q)} \right)^{\beta}} \right] \\ &> 0, \end{aligned}$$

where $\left[\frac{\left((d_{\mathcal{G}}^{(w)} + 1) (d_{\mathcal{G}}^{(z)} + 1) \right)^{\alpha}}{\left(d_{\mathcal{G}}^{(w)} + d_{\mathcal{G}}^{(z)} + 2 \right)^{\beta}} \right] > 0$. Therefore $S_{\alpha, \beta}(\mathcal{G} + \{wz\}) > S_{\alpha, \beta}(\mathcal{G})$. \square

Next corollary is obtained from Lemma 6.1.

Corollary 6.2. *Suppose $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq 0$ and $\alpha \geq \beta$. Also suppose \mathcal{T} is a spanning tree of a graph \mathcal{G} with $n_{\mathcal{G}} = m$ and $\mathcal{G} \not\cong \mathcal{T}$. Then $S_{\alpha, \beta}(\mathcal{G}) > S_{\alpha, \beta}(\mathcal{T})$.*

Next theorem relates $S_{\alpha, \beta}(\mathcal{G})$ with $\chi_{\beta}(\mathcal{G})$.

Theorem 6.3. *Suppose $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ is a graph.*

(1). *If $\alpha \geq 0$, then $S_{\alpha, \beta}(\mathcal{H}) \geq \frac{r^2 \delta_{\mathcal{H}}^{2\alpha}}{\chi_{\beta}(\mathcal{H})}$.*

(2). *If $\alpha \leq 0$, then $S_{\alpha, \beta}(\mathcal{H}) \geq \frac{r^2 \nabla_{\mathcal{H}}^{2\alpha}}{\chi_{\beta}(\mathcal{H})}$.*

In both cases, the inequality becomes equality if \mathcal{H} is a regular graph.

Proof. By arithmetic mean-harmonic mean inequality, we have

$$\frac{r}{S_{\alpha, \beta}(\mathcal{H})} = \frac{r}{\sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)} \right)^{\beta}}} \leq \frac{1}{r} \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)} \right)^{\beta}}{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{\alpha}}.$$

Now if $\alpha \geq 0$, then $\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^\alpha \geq \delta_{\mathcal{H}}^{2\alpha}$. Therefore

$$\frac{1}{r} \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^\beta}{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^\alpha} \leq \frac{1}{r} \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^\beta}{\delta_{\mathcal{H}}^{2\alpha}} = \frac{\chi_\beta(\mathcal{H})}{r\delta_{\mathcal{H}}^{2\alpha}}.$$

Hence $S_{\alpha,\beta}(\mathcal{H}) \geq \frac{r^2 \delta_{\mathcal{H}}^{2\alpha}}{\chi_\beta(\mathcal{H})}$. Now the above inequality becomes equality if and only if for every $w_p w_q \in \mathbb{E}_{\mathcal{H}}$, $\frac{(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)})^\alpha}{(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)})^\beta} = \frac{b^{2\alpha-\beta}}{2^\beta}$, where b is some positive constant. This is possible if and only if \mathcal{H} is a b -regular graph.

Analogously, one can prove (2). □

Now we give relationship between $S_{\alpha,\beta}(\mathcal{G})$ and $R_\alpha(\mathcal{G})$.

Theorem 6.4. *Suppose $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ is a graph. Then*

(1). *If $\beta \geq 0$, then $\frac{R_\alpha(\mathcal{H})}{2^\beta \Delta_{\mathcal{H}}^\beta} \leq S_{\alpha,\beta}(\mathcal{H}) \leq \frac{R_\alpha(\mathcal{H})}{2^\beta \delta_{\mathcal{H}}^\beta}$.*

(2). *If $\beta \leq 0$, then $\frac{R_\alpha(\mathcal{H})}{2^\beta \delta_{\mathcal{H}}^\beta} \leq S_{\alpha,\beta}(\mathcal{H}) \leq \frac{R_\alpha(\mathcal{H})}{2^\beta \nabla_{\mathcal{H}}^\beta}$.*

In both cases, the inequality becomes equality if \mathcal{H} is a regular graph.

Proof. (1). If $\beta \geq 0$, then $\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^\beta \leq (2\nabla_{\mathcal{H}})^\beta$ and $\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^\beta \geq (2\delta_{\mathcal{H}})^\beta$. Hence

$$\begin{aligned} \frac{R_\alpha(\mathcal{H})}{2^\beta \nabla_{\mathcal{H}}^\beta} &= \frac{\sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^\alpha}{2^\beta \nabla_{\mathcal{H}}^\beta} \leq \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^\alpha}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^\beta} \\ &= S_{\alpha,\beta}(\mathcal{H}) \leq \frac{\sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^\alpha}{2^\beta \delta_{\mathcal{H}}^\beta} = \frac{R_\alpha(\mathcal{H})}{2^\beta \delta_{\mathcal{H}}^\beta}. \end{aligned}$$

Clearly the inequality becomes equality if \mathcal{H} is a regular graph.

Part (2) can be proved analogously. □

By direct computation, the following results are obtained.

Theorem 6.5. *Suppose a graph \mathcal{G} has componenets Q_1, Q_2, \dots, Q_s . Then $\mathcal{E}_{\alpha,\beta}(\mathcal{G}) = \sum_{q=1}^s \mathcal{E}_{\alpha,\beta}(Q_q)$.*

Theorem 6.6. Suppose \mathcal{G} is an m -vertex and b -regular graph. Then $\mathcal{E}_{\alpha,\beta}(\mathcal{G}) = \frac{b^{2\alpha}}{2^\beta b^\beta} \mathcal{E}(\mathcal{G})$.

Theorem 6.7. $\mathcal{E}_{\alpha,\beta}(\mathcal{K}_{m,n}) = \frac{2(mn)^{\frac{1}{2}+\alpha}}{(m+n)^\beta}$.

Proof. Since $\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{K}_{m,n}) = \frac{(mn)^\alpha}{(m+n)^\beta} \mathcal{A}(\mathcal{K}_{m,n})$, therefore $\mathcal{E}_{\alpha,\beta}(\mathcal{K}_{m,n}) = \frac{(mn)^\alpha}{(m+n)^\beta} \mathcal{E}(\mathcal{K}_{m,n}) = \frac{2(mn)^{\frac{1}{2}+\alpha}}{(m+n)^\beta}$. \square

The following two results are obtained using Theorem 6.6.

Theorem 6.8. $\mathcal{E}_{\alpha,\beta}(\mathcal{C}_m) = 4^{\alpha-\beta} \mathcal{E}(\mathcal{C}_m)$.

Theorem 6.9. $\mathcal{E}_{\alpha,\beta}(\mathcal{K}_m) = 2^{1-\beta} (m-1)^{2\alpha-\beta+1}$.

6.2 Extremal values of generalized ISI index

In the current section, we find extremal values of graphs with respect to generalized ISI index in some graph classes.

Theorem 6.10. Suppose \mathcal{T} is a tree with $n_{\mathcal{T}} = m$. If $\alpha = \beta$ and $0 \leq \alpha \leq 1$, then

$$S_{\alpha,\beta}(\mathcal{T}) \geq \frac{(m-1)(m-1)^\alpha}{m^\alpha},$$

where the inequality becomes equality if $\mathcal{T} \cong \mathcal{S}_m$.

Proof. The result is proved by induction on m .

For $m \in \{1, 2, 3\}$, the only tree is the star graph \mathcal{S}_m . So the statement follows trivially for $m \leq 3$. Now assume that the statement holds true for $m \geq 4$.

Suppose \mathcal{T} is a tree with $n_{\mathcal{T}} = m$. Let wz be a pendent edge of \mathcal{T} with $d_{\mathcal{T}}^{(z)} = 1$ and $d_{\mathcal{T}}^{(w)} = t$. As $m \geq 4$, we have $2 \leq t \leq m$. Further, since \mathcal{T} is not isomorphic to a star, we have that there exists at least one neighbor u of w in \mathcal{T} with $d_{\mathcal{T}}(u) \geq 2$. Let $N_{\mathcal{T}}(w) \setminus \{z, u\} = \{w_1, \dots, w_{t-2}\}$.

Let $\tilde{\mathcal{T}} = \mathcal{T} \setminus \{z\}$. Then $n_{\tilde{\mathcal{T}}} = m - 1$. By induction hypothesis

$$S_{\alpha,\beta}(\tilde{\mathcal{T}}) \geq \frac{(m-2)(m-2)^\alpha}{(m-1)^\alpha}.$$

Hence

$$S_{\alpha,\beta}(\mathcal{T}) - S_{\alpha,\beta}(\tilde{\mathcal{T}}) = \left(\frac{t}{t+1}\right)^\alpha + \left[\left(\frac{d_{\mathcal{T}}^{(u)} t}{d_{\mathcal{T}}^{(u)} + t}\right)^\alpha - \left(\frac{d_{\mathcal{T}}^{(u)}(t-1)}{d_{\mathcal{T}}^{(u)} + t - 1}\right)^\alpha\right] + \sum_{q=1}^{t-2} \left[\left(\frac{d_{\mathcal{T}}^{(w_q)} t}{d_{\mathcal{T}}^{(w_q)} + t}\right)^\alpha - \left(\frac{d_{\mathcal{T}}^{(w_q)}(t-1)}{d_{\mathcal{T}}^{(w_q)} + t - 1}\right)^\alpha\right].$$

Let $\xi > 0$ and define

$$g(\xi) = \left(\frac{\xi t}{\xi + t}\right)^\alpha - \left(\frac{\xi(t-1)}{\xi + t - 1}\right)^\alpha.$$

Then

$$\begin{aligned} g'(\xi) &= \alpha \xi^{\alpha-1} \left[\left(\frac{t}{\xi + t}\right)^{\alpha+1} - \left(\frac{t-1}{\xi + t - 1}\right)^{\alpha+1} \right] \\ &= \alpha \xi^{\alpha-1} \left[\frac{(\xi t + t^2 - t)^{\alpha+1} - (\xi t + t^2 - t - \xi)^{\alpha+1}}{(\xi + t)^{\alpha+1} (\xi + t - 1)^{\alpha+1}} \right]. \end{aligned}$$

As $t \geq 2$, $0 \leq \alpha \leq 1$ and $\xi > 0$, we have $(\xi + t)^{\alpha+1} > 0$ and $(\xi + t - 1)^{\alpha+1} > 0$. Also $(\xi t + t^2 - t) > (\xi t + t^2 - t - \xi)$. Therefore $(\xi t + t^2 - t)^{\alpha+1} > (\xi t + t^2 - t - \xi)^{\alpha+1}$. Hence $g'(\xi) > 0$ and thus $g(\xi)$ is strictly increasing for $\xi > 0$. Also $2^\alpha > 1$ for $0 \leq \alpha \leq 1$, $d_{\mathcal{T}}^{(w_q)} \geq 1$ and $d_{\mathcal{T}}^{(u)} \geq 2$, we have

$$\begin{aligned} S_{\alpha,\beta}(\mathcal{T}) - S_{\alpha,\beta}(\widetilde{\mathcal{T}}) &\geq \left(\frac{t}{t+1}\right)^\alpha + \left[\left(\frac{2t}{2+t}\right)^\alpha - \left(\frac{2(t-1)}{t+1}\right)^\alpha\right] + \sum_{q=1}^{t-2} \left[\left(\frac{t}{t+1}\right)^\alpha - \left(\frac{t-1}{t}\right)^\alpha\right] \\ &\geq \left(\frac{t}{t+1}\right)^\alpha + \left[\left(\frac{2t}{2+t}\right)^\alpha - \left(\frac{2(t-1)}{t+1}\right)^\alpha\right] > \left(\frac{t}{t+1}\right)^\alpha + 2^\alpha \left(\frac{t}{2+t}\right)^\alpha \\ &> \left(\frac{t}{t+2}\right)^\alpha + 2^\alpha \left(\frac{t}{t+2}\right)^\alpha = \left(\frac{t}{t+2}\right)^\alpha (1 + 2^\alpha) > 2 \left(\frac{t}{t+2}\right)^\alpha. \end{aligned}$$

Since $t \geq 2$, we have

$$\begin{aligned} S_{\alpha,\beta}(\mathcal{T}) - S_{\alpha,\beta}(\widetilde{\mathcal{T}}) &> 2 \left(\frac{t}{t+2}\right)^\alpha > 1 \\ &\geq \frac{(m-1)(m-1)^\alpha}{m^\alpha} - \frac{(m-2)(m-2)^\alpha}{(m-1)^\alpha} = S_{\alpha,\beta}(\mathcal{S}_m) - S_{\alpha,\beta}(\mathcal{S}_{m-1}) \end{aligned}$$

Therefore by induction hypothesis $S_{\alpha,\beta}(\mathcal{T}) - S_{\alpha,\beta}(\mathcal{S}_m) > S_{\alpha,\beta}(\widetilde{\mathcal{T}}) - S_{\alpha,\beta}(\mathcal{S}_{m-1}) \geq 0$. This concludes the proof by induction and clearly equality holds if $\mathcal{T} \cong \mathcal{S}_m$. \square

Next theorem gives the minimal graph with respect to generalized ISI index in the set of all connected graphs with smallest degree 2.

Theorem 6.11. *Among all connected graphs $\mathcal{H} = \mathcal{G}_m^r$ with smallest degree 2, we have*

- (1). *If $\alpha \geq 0$ and $\beta \leq 0$, then $S_{\alpha,\beta}(\mathcal{H}) \geq r 4^{\alpha-\beta}$.*
- (2). *If $\alpha = \beta \geq 0$, then $S_{\alpha,\beta}(\mathcal{H}) \geq r$.*

In both cases, the inequality becomes equality for $\mathcal{H} \cong C_m$.

Proof. (1). If $\alpha \geq 0$ and $\beta \leq 0$, then for any $w_p, w_q \in \mathbb{V}_{\mathcal{H}}$, we have $\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha} \geq 4^{\alpha}$ and $\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta} \leq 4^{\beta}$. Therefore

$$S_{\alpha, \beta}(\mathcal{H}) = \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta}} \geq r 4^{\alpha - \beta}.$$

Now $S_{\alpha, \beta}(\mathcal{H}) = r 4^{\alpha - \beta}$ if and only if $d_{\mathcal{H}}^{(w_p)} = d_{\mathcal{H}}^{(w_q)} = 2$ for every edge $w_p w_q \in \mathbb{E}_{\mathcal{H}}$. Therefore the inequality becomes equality for $\mathcal{H} \cong C_m$.

(2). Since $\delta_{\mathcal{H}} = 2$, therefore $\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right) \geq \left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)$. Hence

$$S_{\alpha, \beta}(\mathcal{H}) = \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta}} \geq r.$$

Similar to the proof of Part (1), the inequality becomes equality for $\mathcal{H} \cong C_m$. □

Next theorem has same proof as of Theorem 3.2 [2] and thus neglected.

Theorem 6.12. *Suppose $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq 0$ and $\alpha \geq \beta$. Also let $m \geq 4$ and \mathcal{G} be a connected graph with $n_{\mathcal{G}} = m$ and independence number σ . Then*

$$S_{\alpha, \beta}(\mathcal{G}) \leq \frac{(m - \sigma)(m - 1)^{2\alpha - \beta}(m - \sigma - 1)}{2^{\beta + 1}} + \sigma(m - \sigma) \left[\frac{(m - \sigma)^{\alpha}(m - 1)^{\alpha}}{(2m - \sigma - 1)^{\beta}} \right],$$

where the inequality becomes equality when $\mathcal{G} \cong \overline{\mathcal{K}}_{\sigma} \wedge \mathcal{K}_{m - \sigma}$.

6.3 On spectral radius and spread of the generalized ISI matrix

In this section, we give bounds on spectral radius and spread of graphs with respect to generalized ISI matrix. For any complex $m \times m$ matrix M with eigenvalues μ_1, \dots, μ_m , the spread $s(M)$ of M is introduced in [57] and is defined as $s(M) = \max_{p, q} |\mu_p - \mu_q|$.

Let $\omega_1 \geq \cdots \geq \omega_m$ be the $\mathcal{A}_{\mathcal{S}_{\alpha,\beta}}$ -eigenvalues of a simple graph \mathcal{G} . Then spread of $\mathcal{A}_{\mathcal{S}_{\alpha,\beta}}(\mathcal{G})$ is defined as $s(\mathcal{A}_{\mathcal{S}_{\alpha,\beta}}(\mathcal{G})) = \omega_1 - \omega_m$, since the eigenvalues $\omega \geq \cdots \geq \omega_m$ are all real.

For convenience, we define some notations. Let

$$\mathcal{J} = \sum_{1 \leq p < q \leq m} \frac{(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)})^{2\alpha}}{(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)})^{2\beta}}, \quad \Omega = \det(\mathcal{A}_{\mathcal{S}_{\alpha,\beta}}(\mathcal{G})). \quad (6.4)$$

We first give some lemmas that are used for proving our main results.

Lemma 6.13. *Let \mathcal{G} be an m -vertex graph and $\omega_1, \dots, \omega_m$ be its $\mathcal{A}_{\mathcal{S}_{\alpha,\beta}}$ -eigenvalues. Then*

- (1). $\sum_{q=1}^m \omega_q = 0$,
- (2). $\sum_{q=1}^m \omega_q^2 = 2 \mathcal{J}$.

Proof. The proof is straight forward. □

Lemma 6.14 (Zhang [81]). *Suppose $y \in \mathbb{R}^m$ with $y \neq 0$. For any $m \times m$ symmetric matrix C with eigenvalues $\eta_1 \geq \cdots \geq \eta_m$, it holds that,*

$$y^T C y \leq \eta_1 y^T y,$$

where y^T is the transpose of y . The inequality becomes equality if and only if y is an eigenvector of C corresponding to η_1 .

Lemma 6.15 (Horn and Johnson [44]). *Let $A_1 = [a_{pq}]_{m \times m}$ and $A_2 = [b_{pq}]_{m \times m}$ be $m \times m$ symmetric and non-negative matrices. If $A_1 \geq A_2$, that is, $a_{pq} \geq b_{pq}$ for each $p, q = 1, \dots, m$, then $\eta_1(A_1) \geq \eta_1(A_2)$, where $\eta_1(A_k)$, $k = 1, 2$ is the greatest eigenvalue of the respective matrix.*

Theorem 6.16 (Hong [43]). *Suppose \mathcal{G}_m^r is a connected graph having \mathcal{A} -eigenvalues $\lambda_1 \geq \cdots \geq \lambda_m$. Then*

$$\lambda_1 \leq \sqrt{2r - m + 1}.$$

The inequality becomes equality if and only if $\mathcal{G}_m^r \cong \mathcal{S}_m$ or $\mathcal{G}_m^r \cong \mathcal{K}_m$.

Theorem 6.17 (Cao [11]). Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a graph with \mathcal{A} -eigenvalues $\lambda_1 \geq \dots \geq \lambda_m$ and $\delta_{\mathcal{H}} \geq 1$. Then

$$\lambda_1 \leq \sqrt{2r - \delta_{\mathcal{H}}(m-1) + (\delta_{\mathcal{H}} - 1)\nabla_{\mathcal{H}}}.$$

Now we give bounds on largest $\mathcal{A}_{\mathcal{S}_{\alpha, \beta}}$ -eigenvalue of a graph.

Theorem 6.18. Let $m \geq 2$. Also let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph with $\mathcal{A}_{\mathcal{S}_{\alpha, \beta}}$ -eigenvalues $\omega_1 \geq \dots \geq \omega_m$ and $\alpha, \beta \in \mathbb{R}$.

(1). If $\alpha, \beta \geq 0$ then

$$\frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}} \leq \omega_1 \leq \frac{(m-1)^{2\alpha} \sqrt{2r - m + 1}}{2^{\beta}}.$$

(2). If $\alpha, \beta \leq 0$ then

$$\frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}} \leq \omega_1 \leq \frac{\sqrt{2r - m + 1}}{2^{\beta} (m-1)^{\beta}}.$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

$$\frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}} \leq \omega_1 \leq \frac{(m-1)^{2\alpha-\beta} \sqrt{2r - m + 1}}{2^{\beta}}.$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

$$\frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}} \leq \omega_1 \leq \frac{\sqrt{2r - m + 1}}{2^{\beta}}.$$

Proof. (1). Let $y \in \mathbb{R}^m$ such that $y = (y_1, y_2, \dots, y_m)^T$. Then

$$\begin{aligned} y^T \mathcal{A}_{\mathcal{S}_{\alpha, \beta}}(\mathcal{H}) y &= \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)} \right)^{\beta}} y_p y_q \\ &\geq \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{\alpha}}{2^{\beta} \nabla_{\mathcal{H}}^{\beta}} y_p y_q. \end{aligned}$$

Taking $y = \left(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \dots, \frac{1}{\sqrt{m}} \right)^T$, we get $\frac{1}{2^{\beta} \nabla_{\mathcal{H}}^{\beta}} \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{\alpha} y_p y_q = \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}}$. Therefore by

Lemma 6.14, $\omega_1 \geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}}$.

Now for any vertex $w_p \in \mathbb{V}_{\mathcal{G}}$, $p = 1, \dots, m$, we have $1 \leq \delta_{\mathcal{H}} \leq d_{\mathcal{H}}^{(w_p)} \leq \nabla_{\mathcal{H}} \leq (m-1)$.

Therefore

$$\frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta}} \leq \frac{\nabla_{\mathcal{H}}^{2\alpha}}{2^{\beta} \delta_{\mathcal{H}}^{\beta}} \leq \frac{(m-1)^{2\alpha}}{2^{\beta}}.$$

If η_1 is the spectral radius of a matrix $\frac{(m-1)^{2\alpha}}{2^{\beta}} \mathcal{A}(\mathcal{H})$, then by Lemma 6.15 and Theorem 6.16, we obtain

$$\omega_1 \leq \eta_1 = \frac{(m-1)^{2\alpha} \lambda_1}{2^{\beta}} \leq \frac{(m-1)^{2\alpha} \sqrt{2r-m+1}}{2^{\beta}},$$

where λ_1 is the spectral radius of $\mathcal{A}(\mathcal{H})$.

(2). Let $y \in \mathbb{R}^m$ such that $y = (y_1, y_2, \dots, y_m)^T$. Then

$$\begin{aligned} y^T \mathcal{A}_{\mathcal{S}_{\alpha, \beta}}(\mathcal{H}) y &= \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta}} y_p y_q \\ &\geq \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{2^{\beta} \delta_{\mathcal{H}}^{\beta}} y_p y_q. \end{aligned}$$

Taking $y = \left(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \dots, \frac{1}{\sqrt{m}}\right)^T$, we get $\frac{1}{2^{\beta} \delta_{\mathcal{H}}^{\beta}} \sum_{w_p w_q \in \mathbb{E}_{\mathcal{H}}} \left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha} y_p y_q = \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}}$. Therefore by Lemma 6.14, $\omega_1 \geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}}$.

Now for any vertex $w_p \in \mathbb{V}_{\mathcal{G}}$, $p = 1, \dots, m$, we have $1 \leq \delta_{\mathcal{H}} \leq d_{\mathcal{H}}^{(w_p)} \leq \nabla_{\mathcal{H}} \leq (m-1)$. Since $\alpha, \beta \leq 0$, therefore $\delta_{\mathcal{H}}^{2\alpha} \leq 1$ and $\nabla_{\mathcal{H}}^{\beta} \geq (m-1)^{\beta}$. Now

$$\frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)}\right)^{\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)}\right)^{\beta}} \leq \frac{\delta_{\mathcal{H}}^{2\alpha}}{2^{\beta} \nabla_{\mathcal{H}}^{\beta}} \leq \frac{1}{2^{\beta} (m-1)^{\beta}}.$$

If η_1 is the spectral radius of a matrix $\frac{1}{2^{\beta} (m-1)^{\beta}} \mathcal{A}(\mathcal{H})$, then by Lemma 6.15 and Theorem 6.16, we obtain

$$\omega_1 \leq \eta_1 = \frac{\lambda_1}{2^{\beta} (m-1)^{\beta}} \leq \frac{\sqrt{2r-m+1}}{2^{\beta} (m-1)^{\beta}},$$

where λ_1 is the spectral radius of $\mathcal{A}(\mathcal{H})$.

Parts (3) and (4) can be proved analogously. \square

Next theorem gives bounds on the smallest $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalue of a graph.

Theorem 6.19. *Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a graph with $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues $\omega_1 \geq \dots \geq \omega_m$.*

Then

$$\sqrt{\frac{2\mathcal{J} + (m-1)(m-2)\Omega^{2/m-1}}{2}} \leq \omega_m \leq \sqrt{\frac{2(m-1)\mathcal{J}}{m}},$$

where $\alpha, \beta \in \mathbb{R}$ and \mathcal{J} is defined in Equation (6.4).

Proof. By Part (1) of Lemma 6.13, we get

$$\omega_m^2 = \left(- \sum_{q=1}^{m-1} \omega_q \right)^2 = \sum_{q=1}^{m-1} \omega_q^2 + 2 \sum_{1 \leq p < q \leq m-1} \omega_p \omega_q.$$

Now by arithmetic-geometric mean inequality, we get

$$\begin{aligned} \frac{2}{(m-1)(m-2)} \sum_{1 \leq p < q \leq m-1} \omega_p \omega_q &\geq \left(\omega_1^{m-2} \omega_2^{m-2} \dots \omega_m^{m-2} \right)^{2/(m-1)(m-2)} \\ &= \left(\det(\mathcal{A}_{\alpha,\beta}(\mathcal{H})) \right)^{2/m-1} = \Omega^{2/m-1}. \end{aligned}$$

Hence $\omega_m^2 \geq 2\mathcal{J} - \omega_m^2 + (m-1)(m-2)\Omega^{2/m-1}$ and $\omega_m \geq \sqrt{\frac{2\mathcal{J} + (m-1)(m-2)\Omega^{2/m-1}}{2}}$.

Again using Part (1) of Lemma 6.13 and Cauchy-Schwartz inequality, we have

$$\omega_m^2 \leq (m-1) \sum_{q=1}^{m-1} \omega_q^2 = (m-1)(2\mathcal{J} - \omega_m^2).$$

Hence $\omega_m \leq \sqrt{\frac{2(m-1)\mathcal{J}}{m}}$. □

In the following theorem, we give bounds on spread of the generalized ISI matrix of a graph.

Theorem 6.20. *Suppose $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a graph having $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues $\omega_1 \geq \dots \geq \omega_m$.*

(1). *If $\alpha, \beta \geq 0$ then*

$$\begin{aligned} s(\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{H})) &\geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}} - \frac{(m-1)^{2\alpha}}{2^{\beta}} \sqrt{\frac{2r(m-1)}{m}}, \\ s(\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{H})) &\leq \frac{(m-1)^{2\alpha} \sqrt{2r-m+1}}{2^{\beta}} - \frac{\sqrt{2r+2^{2\beta}(m-1)^{2\beta+1}(m-2)\Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta}(m-1)^{\beta}}. \end{aligned}$$

(2). If $\alpha, \beta \leq 0$ then

$$\begin{aligned} s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}} - \frac{1}{2^{\beta} (m-1)^{\beta}} \sqrt{\frac{2r(m-1)}{m}}, \\ s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\leq \frac{\sqrt{2r-m+1}}{2^{\beta} (m-1)^{\beta}} - \frac{\sqrt{2r(m-1)^{4\alpha} + 2^{2\beta} (m-1)(m-2) \Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta}}. \end{aligned}$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

$$\begin{aligned} s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \delta_{\mathcal{H}}^{\beta}} - \frac{(m-1)^{2\alpha-\beta}}{2^{\beta}} \sqrt{\frac{2r(m-1)}{m}}, \\ s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\leq \frac{(m-1)^{2\alpha-\beta} \sqrt{2r-m+1}}{2^{\beta}} - \frac{\sqrt{2r + 2^{2\beta} (m-1)(m-2) \Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta}}. \end{aligned}$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

$$\begin{aligned} s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\geq \frac{R_{\alpha}(\mathcal{H})}{m 2^{\beta} \nabla_{\mathcal{H}}^{\beta}} - \frac{1}{2^{\beta}} \sqrt{\frac{2r(m-1)}{m}}, \\ s(\mathcal{A}_{S_{\alpha, \beta}}(\mathcal{H})) &\leq \frac{\sqrt{2r-m+1}}{2^{\beta}} - \frac{\sqrt{2r(m-1)^{4\alpha} + 2^{2\beta} (m-1)^{1+2\beta} (m-2) \Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta} (m-1)^{\beta}}. \end{aligned}$$

Proof. (1). We have $1 \leq \delta_{\mathcal{H}} \leq d_{\mathcal{H}}^{(w_p)} \leq \nabla_{\mathcal{H}} \leq (m-1)$ for any vertex $w_p \in \mathbb{V}_{\mathcal{H}}$, $p = 1, \dots, m$.

Using Equation (6.4), we get

$$\begin{aligned} 2\mathcal{J} &= 2 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{2\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{2\beta}} \\ &\geq 2 \sum_{1 \leq p < q \leq m} \frac{\delta_{\mathcal{H}}^{4\alpha}}{2^{2\beta} \nabla_{\mathcal{H}}^{2\beta}} \geq \frac{r 2^{1-2\beta}}{(m-1)^{2\beta}}. \end{aligned} \tag{6.5}$$

Also

$$\begin{aligned} 2\mathcal{J} &= 2 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{2\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{2\beta}} \\ &\leq 2 \sum_{1 \leq p < q \leq m} \frac{\nabla_{\mathcal{H}}^{4\alpha}}{2^{2\beta} \delta_{\mathcal{H}}^{2\beta}} \leq r 2^{1-2\beta} (m-1)^{4\alpha}. \end{aligned} \tag{6.6}$$

Hence using Theorem 6.18, Theorem 6.19 and Equations (6.5) and (6.6), we get

$$\begin{aligned}
s(\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{H})) &= \omega_1 - \omega_m \\
&\leq \frac{(m-1)^{2\alpha} \sqrt{2r-m+1}}{2^\beta} - \sqrt{\frac{2\mathcal{J} + (m-1)(m-2)\Omega^{2/m-1}}{2}} \\
&\leq \frac{(m-1)^{2\alpha} \sqrt{2r-m+1}}{2^\beta} - \frac{1}{2} \sqrt{\frac{2r}{(2(m-1))^{2\beta}} + (m-1)(m-2)\Omega^{2/m-1}} \\
&= \frac{(m-1)^{2\alpha} \sqrt{2r-m+1}}{2^\beta} - \frac{\sqrt{2r+2^{2\beta}(m-1)^{2\beta+1}(m-2)\Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta}(m-1)^\beta}.
\end{aligned}$$

Also

$$\begin{aligned}
s(\mathcal{A}_{\alpha,\beta}(\mathcal{H})) &= \omega_1 - \omega_m \\
&\geq \frac{R_\alpha(\mathcal{H})}{m 2^\beta \nabla_{\mathcal{H}}^\beta} - \sqrt{\frac{2(m-1)\mathcal{J}}{m}} \\
&\geq \frac{R_\alpha(\mathcal{H})}{m 2^\beta \nabla_{\mathcal{H}}^\beta} - \frac{(m-1)^{2\alpha}}{2^\beta} \sqrt{\frac{2r(m-1)}{m}}.
\end{aligned}$$

(2). We have $1 \leq \delta_{\mathcal{H}} \leq d_{\mathcal{H}}^{(w_p)} \leq \nabla_{\mathcal{H}} \leq (m-1)$ for any vertex $w_p \in \mathbb{V}_{\mathcal{H}}$, $p = 1, \dots, m$. Since $\alpha, \beta \leq 0$, therefore $\nabla_{\mathcal{H}}^\alpha \geq (m-1)^\alpha$ and $\delta_{\mathcal{H}}^\beta \leq 1$. Using Equation (6.4), we obtain

$$\begin{aligned}
2\mathcal{J} &= 2 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{2\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{2\beta}} \\
&\geq 2 \sum_{1 \leq p < q \leq m} \frac{\nabla_{\mathcal{H}}^{4\alpha}}{2^{2\beta} \delta_{\mathcal{H}}^{2\beta}} \geq r 2^{1-2\beta} (m-1)^{4\alpha}.
\end{aligned} \tag{6.7}$$

Also

$$\begin{aligned}
2\mathcal{J} &= 2 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\mathcal{G}}^{(w_p)} d_{\mathcal{G}}^{(w_q)}\right)^{2\alpha}}{\left(d_{\mathcal{G}}^{(w_p)} + d_{\mathcal{G}}^{(w_q)}\right)^{2\beta}} \\
&\leq 2 \sum_{1 \leq p < q \leq m} \frac{\delta_{\mathcal{H}}^{4\alpha}}{2^{2\beta} \nabla_{\mathcal{H}}^{2\beta}} = \frac{r 2^{1-2\beta}}{(m-1)^{2\beta}}.
\end{aligned} \tag{6.8}$$

Hence using Theorem 6.18, Theorem 6.19 and Equations (6.7) and (6.8), we get

$$\begin{aligned}
s(\mathcal{A}_{S_{\alpha,\beta}}(\mathcal{H})) &= \omega_1 - \omega_m \\
&\leq \frac{\sqrt{2r - m + 1}}{2^\beta (m - 1)^\beta} - \sqrt{\frac{2\mathcal{J} + (m - 1)(m - 2)\Omega^{2/m-1}}{2}} \\
&\leq \frac{\sqrt{2r - m + 1}}{2^\beta (m - 1)^\beta} - \frac{1}{2} \sqrt{\frac{2r(m - 1)^{4\alpha}}{2^{2\beta}} + (m - 1)(m - 2)\Omega^{2/m-1}} \\
&= \frac{\sqrt{2r - m + 1}}{2^\beta (m - 1)^\beta} - \frac{\sqrt{2r(m - 1)^{4\alpha} + 2^{2\beta}(m - 1)(m - 2)\Omega^{2/m-1}}}{2^{\frac{1}{2}+\beta}}.
\end{aligned}$$

Also

$$\begin{aligned}
s(\mathcal{A}_{\alpha,\beta}(\mathcal{H})) &= \omega_1 - \omega_m \\
&\geq \frac{R_\alpha(\mathcal{H})}{m 2^\beta \delta_{\mathcal{H}}^\beta} - \sqrt{\frac{2(m - 1)\mathcal{J}}{m}} \\
&\geq \frac{R_\alpha(\mathcal{H})}{m 2^\beta \delta_{\mathcal{H}}^\beta} - \frac{1}{2^\beta (m - 1)^\beta} \sqrt{\frac{2r(m - 1)}{m}}.
\end{aligned}$$

Similarly, one can prove Parts (3) and (4).

The proof is complete. \square

6.4 Bounds on generalized ISI energy

In the current section, some bounds for the generalized ISI energy of graphs are given. We would like to mention that the idea of proof of next theorem is taken from Theorem 13 [20].

Theorem 6.21. *Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph having $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues $\omega_1 \geq \dots \geq \omega_m$ and $\alpha, \beta \in \mathbb{R}$.*

(1). *If $\alpha, \beta \geq 0$ then*

$$\frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m(m - 1)^\beta} \leq \mathcal{E}_{\alpha,\beta}(\mathcal{H}) \leq \frac{(m - 1)^{2\alpha}}{2^\beta} \sqrt{2mr}.$$

(2). *If $\alpha, \beta \leq 0$ then*

$$\frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m} \leq \mathcal{E}_{\alpha,\beta}(\mathcal{H}) \leq \frac{1}{2^\beta (m - 1)^\beta} \sqrt{2mr}.$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

$$\frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m} \leq \mathcal{E}_{\alpha,\beta}(\mathcal{H}) \leq \frac{(m-1)^{2\alpha-\beta}}{2^\beta} \sqrt{2mr}.$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

$$\frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m(m-1)^\beta} \leq \mathcal{E}_{\alpha,\beta}(\mathcal{H}) \leq \frac{1}{2^\beta} \sqrt{2mr}.$$

Proof. (1). With no loss of generality, suppose that $\omega_1, \dots, \omega_t$ are positive and $\omega_{t+1}, \dots, \omega_m$ are negative. Using Theorem 6.18, we get

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &= \sum_{q=1}^m |\omega_q| = 2 \sum_{q=1}^t \omega_q \\ &\geq 2 \omega_1 \geq \frac{2 R_\alpha(\mathcal{H})}{m 2^\beta \nabla_{\mathcal{H}}^\beta} \geq \frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m(m-1)^\beta}. \end{aligned}$$

Now applying Cauchy-Schwartz inequality, Part (2) of Lemma 6.13 and Equation (6.6), we have

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &= \sum_{q=1}^m |\omega_q| \leq \sqrt{m \sum_{q=1}^m \omega_q^2} = \sqrt{2m \mathcal{J}} \\ &\leq \sqrt{\frac{2mr(m-1)^{4\alpha}}{2^{2\beta}}} = \frac{(m-1)^{2\alpha}}{2^\beta} \sqrt{2mr}. \end{aligned}$$

(2). With no loss of generality, suppose that $\omega_1, \dots, \omega_t$ are positive and $\omega_{t+1}, \dots, \omega_m$ are negative. Since $\alpha, \beta \leq 0$ therefore $\delta_{\mathcal{H}}^\beta \leq 1$. Now using Theorem 6.18 (2), we get

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &= \sum_{q=1}^m |\omega_q| = 2 \sum_{q=1}^t \omega_q \\ &\geq 2 \omega_1 \geq \frac{2 R_\alpha(\mathcal{H})}{m 2^\beta \delta_{\mathcal{H}}^\beta} \geq \frac{2^{1-\beta} R_\alpha(\mathcal{H})}{m}. \end{aligned}$$

Now applying Cauchy-Schwartz inequality, Part (2) of Lemma 6.13 and Equation (6.8), we have

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &= \sum_{q=1}^m |\omega_q| \leq \sqrt{m \sum_{q=1}^m \omega_q^2} = \sqrt{2m \mathcal{J}} \\ &\leq \sqrt{\frac{2mr}{(m-1)^{2\beta} 2^{2\beta}}} = \frac{1}{2^\beta (m-1)^\beta} \sqrt{2mr}. \end{aligned}$$

One can prove Parts (3) and (4) in a similar manner.

The result is proved. \square

Theorem 6.22. Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph with $\mathcal{A}_{S_{\alpha, \beta}}$ -eigenvalues $\omega_1 \geq \dots \geq \omega_m$.

(1). If $\alpha, \beta \geq 0$ then

$$\frac{2^{1-\beta} \sqrt{r}}{(m-1)^\beta} \leq \mathcal{E}_{\alpha, \beta}(\mathcal{H}) \leq \frac{(m-1)^{2\alpha}}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r(m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)^{1-2\beta-4\alpha}}{m^2}} \right].$$

(2). If $\alpha, \beta \leq 0$ then

$$2^{1-\beta}(m-1)^{2\alpha} \sqrt{r} \leq \mathcal{E}_{\alpha, \beta}(\mathcal{H}) \leq \frac{1}{2^\beta (m-1)^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r(m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)^{1+2\beta}}{m^2 \delta_{\mathcal{H}}^{2\beta}}} \right].$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

$$2^{1-\beta} \sqrt{r} \leq \mathcal{E}_{\alpha, \beta}(\mathcal{H}) \leq \frac{(m-1)^{2\alpha-\beta}}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r(m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)^{1+2\beta-4\alpha}}{m^2 \delta_{\mathcal{H}}^{2\beta}}} \right].$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

$$2^{1-\beta} (m-1)^{2\alpha-\beta} \sqrt{r} \leq \mathcal{E}_{\alpha, \beta}(\mathcal{H}) \leq \frac{1}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r(m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)}{m^2 \nabla_{\mathcal{H}}^{2\beta}}} \right].$$

Proof. (1). By Part (1) of Lemma 6.13, we have $\sum_{q=1}^m \omega_q^2 = -2 \sum_{1 \leq p < q \leq m} \omega_p \omega_q$. Using Part (2) of Lemma 6.13, we obtain

$$\begin{aligned} (\mathcal{E}_{\alpha, \beta}(\mathcal{H}))^2 &= \left(\sum_{q=1}^m |\omega_q| \right)^2 \\ &= \sum_{q=1}^m \omega_q^2 + 2 \sum_{1 \leq p < q \leq m} |\omega_p \omega_q| \\ &\geq 2\mathcal{J} + 2 \left| \sum_{1 \leq p < q \leq m} \omega_p \omega_q \right| = 4\mathcal{J}. \end{aligned}$$

Now

$$4\mathcal{J} = 4 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^{2\alpha}}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)} \right)^{2\beta}} \geq \sum_{1 \leq p < q \leq m} \frac{4\delta_{\mathcal{H}}^{4\alpha}}{2^{2\beta} \nabla_{\mathcal{H}}^{2\beta}} \geq \frac{r 2^{2-2\beta}}{(m-1)^{2\beta}}.$$

Hence $\mathcal{E}_{\alpha,\beta}(\mathcal{H}) \geq \frac{2^{1-\beta} \sqrt{r}}{(m-1)^\beta}$.

To prove inequality on the right side, we apply Cauchy-Schwartz inequality to obtain $(\sum_{q=2}^m |\omega_q|)^2 \leq (m-1) \sum_{q=2}^m \omega_q^2$. Therefore using Part (2) of Lemma 6.13, $(\mathcal{E}_{\alpha,\beta}(\mathcal{H}) - \omega_1)^2 \leq (m-1) (2\mathcal{J} - \omega_1^2)$.

Hence by Theorem 6.18 (1), we get

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &\leq \omega_1 + \sqrt{(m-1) (2\mathcal{J} - \omega_1^2)} \\ &\leq \frac{(m-1)^{2\alpha} \sqrt{2r - m + 1}}{2^\beta} + \sqrt{(m-1) \left[r 2^{1-2\beta} (m-1)^{4\alpha} - \frac{R_\alpha^2(\mathcal{H})}{m^2 2^{2\beta} (m-1)^{2\beta}} \right]} \\ &= \frac{(m-1)^{2\alpha}}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r (m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)^{1-2\beta-4\alpha}}{m^2}} \right]. \end{aligned}$$

(2). Using Equation (6.7), we get

$$4\mathcal{J} = 2(2\mathcal{J}) \geq 2^{2-2\beta} r (m-1)^{4\alpha}.$$

Hence $\mathcal{E}_{\alpha,\beta}(\mathcal{H}) \geq 2^{1-\beta} (m-1)^{2\alpha} \sqrt{r}$.

Now using Theorem 6.18 (2) and Equation (6.8), we get

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\mathcal{H}) &\leq \omega_1 + \sqrt{(m-1) (2\mathcal{J} - \omega_1^2)} \\ &\leq \frac{\sqrt{2r - m + 1}}{2^\beta (m-1)^\beta} + \sqrt{(m-1) \left[\frac{r 2^{1-2\beta}}{(m-1)^{2\beta}} - \frac{R_\alpha^2(\mathcal{H})}{m^2 2^{2\beta} \delta_{\mathcal{H}}^{2\beta}} \right]} \\ &= \frac{1}{2^\beta (m-1)^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r (m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)^{1+2\beta}}{m^2 \delta_{\mathcal{H}}^{2\beta}}} \right]. \end{aligned}$$

This gives the required result.

Analogously, one can prove Parts (3) and (4). □

6.5 Nordhaus-Gaddum-type results for generalized ISI spectral radius and energy

Suppose the $\mathcal{A}_{S_{\alpha,\beta}}$ -eigenvalues of $\overline{\mathcal{G}}$ are v_q , $q = 1, 2, \dots, m$.

We first present bounds on $\omega_1 + v_1$.

Theorem 6.23. Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph and $\alpha, \beta \in \mathbb{R}$.

(1). If $\beta \geq 0$ then

$$\omega_1 + \nu_1 \geq \frac{1}{m 2^\beta} \left[\frac{\mathbf{R}_\alpha(\mathcal{H})}{(m-1)^\beta} + \frac{\mathbf{R}_\alpha(\overline{\mathcal{H}})}{(m-1-\delta_{\mathcal{H}})^\beta} \right].$$

(2). If $\beta \leq 0$ then

$$\omega_1 + \nu_1 \geq \frac{1}{m 2^\beta} \left[\frac{\mathbf{R}_\alpha(\mathcal{H})}{\delta_{\mathcal{H}}^\beta} + \frac{\mathbf{R}_\alpha(\overline{\mathcal{H}})}{(m-1-\nabla_{\mathcal{H}})^\beta} \right].$$

Proof. (1). Let $y \in \mathbb{R}^m$ such that $y = (y_1, y_2, \dots, y_m)^T$. Then

$$\begin{aligned} y^T \left[\mathcal{A}_{\mathcal{S}_{\alpha, \beta}}(\mathcal{H}) + \mathcal{A}_{\mathcal{S}_{\alpha, \beta}}(\overline{\mathcal{H}}) \right] y &= \sum_{w_p, w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^\alpha}{\left(d_{\mathcal{H}}^{(w_p)} + d_{\mathcal{H}}^{(w_q)} \right)^\beta} y_p y_q + \sum_{w_p, w_q \in \mathbb{E}_{\overline{\mathcal{H}}}} \frac{\left(d_{\overline{\mathcal{H}}}^{(w_p)} d_{\overline{\mathcal{H}}}^{(w_q)} \right)^\alpha}{\left(d_{\overline{\mathcal{H}}}^{(w_p)} + d_{\overline{\mathcal{H}}}^{(w_q)} \right)^\beta} y_p y_q \\ &\geq \sum_{w_p, w_q \in \mathbb{E}_{\mathcal{H}}} \frac{\left(d_{\mathcal{H}}^{(w_p)} d_{\mathcal{H}}^{(w_q)} \right)^\alpha}{2^\beta \nabla_{\mathcal{H}}^\beta} y_p y_q + \sum_{w_p, w_q \in \mathbb{E}_{\overline{\mathcal{H}}}} \frac{\left(d_{\overline{\mathcal{H}}}^{(w_p)} d_{\overline{\mathcal{H}}}^{(w_q)} \right)^\alpha}{2^\beta \nabla_{\overline{\mathcal{H}}}^\beta} y_p y_q. \end{aligned}$$

Since $\nabla_{\overline{\mathcal{H}}} = m-1-\delta_{\mathcal{H}}$ and $\nabla_{\mathcal{H}} \leq m-1$ therefore taking $y = (\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \dots, \frac{1}{\sqrt{m}})^T$ and using Lemma 6.14, we obtain

$$\omega_1 + \nu_1 \geq \frac{1}{m 2^\beta} \left[\frac{\mathbf{R}_\alpha(\mathcal{H})}{(m-1)^\beta} + \frac{\mathbf{R}_\alpha(\overline{\mathcal{H}})}{(m-1-\delta_{\mathcal{H}})^\beta} \right].$$

Similarly Part (2) can be proved. □

Theorem 6.24. Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph and \mathcal{H}_1 is a connected component of $\overline{\mathcal{H}}$ with $\nu_1 = \omega_1(\mathcal{H}_1)$.

(1). Let $\alpha, \beta \geq 0$.

(a). If $\nabla_{\mathcal{H}} = m-1$ or $\nabla_{\overline{\mathcal{H}}} = m-1$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta} \left[(m-1)^{2\alpha} \sqrt{2r-m+1} + (n_{\mathcal{H}_1}-1)^{2\alpha} \sqrt{2e_{\mathcal{H}_1}-n_{\mathcal{H}_1}+1} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m-2$ and $\nabla_{\overline{\mathcal{H}}} \leq m-2$, then

$$\omega_1 + \nu_1 \leq \frac{(m-2)^{2\alpha}}{2^\beta} \left[\sqrt{2r-m+1} + \sqrt{(m^2-2m-2r+1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)} \right].$$

(2) Let $\alpha, \beta \leq 0$.

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{G}}} = m - 1$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta} \left[\frac{\sqrt{2r - m + 1}}{(m - 1)^\beta} + \frac{\sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1}}{(n_{\mathcal{H}_1} - 1)^\beta} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta (m - 2)^\beta} \left[\sqrt{2r - m + 1} + \sqrt{(m^2 - 2m - 2r + 1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)} \right].$$

(3). Let $\alpha \geq 0$ and $\beta \leq 0$.

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{G}}} = m - 1$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta} \left[(m - 1)^{2\alpha - \beta} \sqrt{2r - m + 1} + (n_{\mathcal{H}_1} - 1)^{2\alpha - \beta} \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\omega_1 + \nu_1 \leq \frac{(m - 2)^{2\alpha - \beta}}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{(m^2 - 2m - 2r + 1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)} \right].$$

(4) Let $\alpha \leq 0$ and $\beta \geq 0$.

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{G}}} = m - 1$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\omega_1 + \nu_1 \leq \frac{1}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{(m^2 - 2m - 2r + 1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)} \right].$$

Proof. (1).

(a). Assume that $\nabla_{\mathcal{H}} = m - 1$. From Theorem 6.18, we have

$$\omega_1 \leq \frac{(m - 1)^{2\alpha} \sqrt{2r - m + 1}}{2^\beta}. \quad (6.9)$$

Let $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_t$ be connected components of $\overline{\mathcal{H}}$. With no loss of generality, assume that $\omega_1(\mathcal{H}_1) \geq \omega_1(\mathcal{H}_2) \geq \dots \geq \omega_1(\mathcal{H}_t)$. Also note that $v_1 = \omega_1(\mathcal{H}_1)$. Therefore using Theorem 6.18, we get

$$v_1 \leq \frac{(n_{\mathcal{H}_1} - 1)^{2\alpha} \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1}}{2^\beta}. \quad (6.10)$$

The desired result is obtained by adding equations (6.9) and (6.10).

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then $\delta_{\overline{\mathcal{H}}} \geq 1$. From Theorem 6.18, we have

$$\omega_1 \leq \frac{(m - 2)^{2\alpha} \sqrt{2r - m + 1}}{2^\beta}. \quad (6.11)$$

Now using inequalities $\delta_{\overline{\mathcal{H}}} = m - 1 - \nabla_{\mathcal{H}}$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, Theorem 6.17 and proof of Theorem 6.18, we get

$$\begin{aligned} v_1 &\leq \frac{(m - 2)^{2\alpha} \sqrt{2\binom{m}{2} - 2r - \delta_{\overline{\mathcal{H}}}(m - 1) + (\delta_{\overline{\mathcal{H}}} - 1) \nabla_{\overline{\mathcal{H}}}}}{2^\beta \delta_{\overline{\mathcal{H}}}^\beta} \\ &= \frac{(m - 2)^{2\alpha}}{2^\beta \delta_{\overline{\mathcal{H}}}^\beta} \sqrt{(m^2 - 2m - 2r + 1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)} \\ &\leq \frac{(m - 2)^{2\alpha}}{2^\beta} \sqrt{(m^2 - 2m - 2r + 1) + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)}. \end{aligned} \quad (6.12)$$

By adding Equations (6.11) and (6.12), we get the result.

Now similarly using Theorem 6.17 and Theorem 6.18, one can prove Parts (2) ~ (4). \square

We now give bounds on $\mathcal{E}_{\alpha, \beta}(\mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})) + \mathcal{E}_{\alpha, \beta}(\overline{\mathcal{G}}(m, r, \nabla_{\overline{\mathcal{G}}}, \delta_{\overline{\mathcal{G}}}))$.

Theorem 6.25. *Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph and \mathcal{H}_1 is a connected component of $\overline{\mathcal{H}}$ with $v_1 = \omega_1(\mathcal{H}_1)$.*

(1). *If $\alpha, \beta \geq 0$ then*

(a). *If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{H}}} = m - 1$, then*

$$\mathcal{E}_{\alpha, \beta}(\mathcal{H}) + \mathcal{E}_{\alpha, \beta}(\overline{\mathcal{H}}) \leq \frac{(m - 1)^{2\alpha}}{2^\beta} U + \frac{1}{2^\beta} \left[(n_{\mathcal{H}_1} - 1)^{2\alpha} \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} + W_1 \right],$$

(b). *If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then*

$$\mathcal{E}_{\alpha, \beta}(\mathcal{H}) + \mathcal{E}_{\alpha, \beta}(\overline{\mathcal{H}}) \leq \frac{(m - 2)^{2\alpha}}{2^\beta} U' + \frac{(m - 1 - \delta_{\mathcal{H}})^{2\alpha} \sqrt{m^2 - m - 2r}}{2^\beta (m - 1 - \nabla_{\mathcal{H}})^\beta} W_2,$$

(2). If $\alpha, \beta \leq 0$ then

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{H}}} = m - 1$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{1}{2^\beta (m-1)^\beta} U_1 + \frac{1}{2^\beta} \left[\frac{\sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1}}{(n_{\mathcal{H}_1} - 1)^\beta} + \frac{W_3 \sqrt{m^2 - m - 2r}}{(m-1 - \delta_{\mathcal{H}})^\beta (m-1 - \nabla_{\mathcal{H}})^\beta} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{1}{2^\beta (m-2)^\beta} U'_1 + \frac{(m-1 - \nabla_{\mathcal{H}})^{2\alpha} \sqrt{m^2 - m - 2r}}{2^\beta (m-1 - \delta_{\mathcal{H}})^\beta} W_4.$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{H}}} = m - 1$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{(m-1)^{2\alpha-\beta}}{2^\beta} U_2 + \frac{1}{2^\beta} \left[\sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} (n_{\mathcal{H}_1} - 1)^{2\alpha-\beta} + W_5 \frac{\sqrt{m^2 - m - 2r}}{2^\beta} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{(m-2)^{2\alpha-\beta}}{2^\beta} U'_2 + \frac{(m-1 - \delta_{\mathcal{H}})^{2\alpha-\beta} \sqrt{m^2 - m - 2r}}{2^\beta} W_6.$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

(a). If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{H}}} = m - 1$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{1}{2^\beta} U_3 + \frac{1}{2^\beta} \left[\sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} + W_7 \sqrt{m^2 - m - 2r} \right],$$

(b). If $\nabla_{\mathcal{H}} \leq m - 2$ and $\nabla_{\overline{\mathcal{H}}} \leq m - 2$, then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \leq \frac{1}{2^\beta} U_3 + \frac{(m-1 - \nabla_{\mathcal{H}})^{2\alpha-\beta} \sqrt{m^2 - m - 2r}}{2^\beta} W_8.$$

where

$$\begin{aligned}
U &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)^{1-4\alpha-2\beta}}{m^2}}, \\
U' &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)}{m^2(m - 2)^{4\alpha+2\beta}}}, \\
U_1 &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)^{1+2\beta}}{m^2 \delta_{\mathcal{H}}^{2\beta}}}, \\
U'_1 &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)(m - 2)^{2\beta}}{m^2 \delta_{\mathcal{H}}^{2\beta}}}, \\
U_2 &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)^{1-4\alpha+2\beta}}{m^2 \delta_{\mathcal{H}}^{2\beta}}}, \\
U'_2 &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)}{m^2(m - 2)^{4\alpha-2\beta} \delta_{\mathcal{H}}^{2\beta}}}, \\
U_3 &= \sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{R_\alpha^2(\mathcal{H})(m - 1)}{m^2 \nabla_{\mathcal{H}}^{2\beta}}}, \\
W_1 &= \sqrt{(m - 1) \left[\frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha} (m^2 - m - 2r)}{(m - 1 - \nabla_{\mathcal{H}})^{2\beta}} - \frac{(m - 1 - \nabla_{\mathcal{H}})^{4\alpha} (m^2 - m - 2r)^2}{4m^2 (m - 1 - \delta_{\mathcal{H}})^{2\beta}} \right]}, \\
W_2 &= \sqrt{1 + \frac{1 - m + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)}{m^2 - m - 2r}} + \sqrt{(m - 1) - \frac{(m - 1)(m - 1 - \nabla_{\mathcal{H}})^{4\alpha+2\beta} (m^2 - m - 2r)}{4m^2 (m - 1 - \delta_{\mathcal{H}})^{2\beta+4\alpha}}}, \\
W_3 &= \sqrt{(m - 1) \left[(m - 1 - \nabla_{\mathcal{H}})^{4\alpha+2\beta} - \frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha+2\beta} (m^2 - m - 2r)}{4m^2} \right]}, \\
W_4 &= \sqrt{1 + \frac{1 - m + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)}{m^2 - m - 2r}} + \sqrt{(m - 1) - \frac{(m - 1)(m - 1 - \delta_{\mathcal{H}})^{4\alpha+2\beta} (m^2 - m - 2r)}{4m^2 (m - 1 - \nabla_{\mathcal{H}})^{2\beta+4\alpha}}}, \\
W_5 &= \sqrt{(m - 1) \left[(m - 1 - \delta_{\mathcal{H}})^{4\alpha-2\beta} - \frac{(m - 1 - \nabla_{\mathcal{H}})^{4\alpha-2\beta} (m^2 - m - 2r)}{4m^2} \right]}, \\
W_6 &= \sqrt{1 + \frac{1 - m + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)}{m^2 - m - 2r}} + \sqrt{(m - 1) - \frac{(m - 1)(m - 1 - \nabla_{\mathcal{H}})^{4\alpha-2\beta} (m^2 - m - 2r)}{4m^2 (m - 1 - \delta_{\mathcal{H}})^{4\alpha-2\beta}}}, \\
W_7 &= \sqrt{(m - 1) \left[(m - 1 - \nabla_{\mathcal{H}})^{4\alpha-2\beta} - \frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha-2\beta} (m^2 - m - 2r)}{4m^2} \right]}, \\
W_8 &= \sqrt{1 + \frac{1 - m + \delta_{\mathcal{H}}(2 + \nabla_{\mathcal{H}} - m)}{m^2 - m - 2r}} + \sqrt{(m - 1) - \frac{(m - 1)(m - 1 - \delta_{\mathcal{H}})^{4\alpha-2\beta} (m^2 - m - 2r)}{4m^2 (m - 1 - \nabla_{\mathcal{H}})^{4\alpha-2\beta}}}.
\end{aligned}$$

Proof. (1). Note that $\nabla_{\overline{\mathcal{H}}} = m - 1 - \delta_{\mathcal{H}}$ and $\delta_{\overline{\mathcal{H}}} = m - 1 - \nabla_{\mathcal{H}}$. Using Part (2) of Lemma 6.13 on \mathcal{H} , we see that

$$\begin{aligned}
2\mathcal{J} &= 2 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\overline{\mathcal{H}}}^{(w_p)} d_{\overline{\mathcal{H}}}^{(w_q)}\right)^{2\alpha}}{\left(d_{\overline{\mathcal{H}}}^{(w_p)} + d_{\overline{\mathcal{H}}}^{(w_q)}\right)^{2\beta}} \\
&\leq 2 \sum_{w_p w_q \in \mathbb{E}_{\overline{\mathcal{H}}}} \frac{(\nabla_{\overline{\mathcal{H}}})^{4\alpha}}{2^{2\beta} (\delta_{\overline{\mathcal{H}}})^{2\beta}} \\
&= 2 \left[\binom{m}{2} - r \right] \frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha}}{2^{2\beta} (m - 1 - \nabla_{\mathcal{H}})^{2\beta}} \\
&= \frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha} (m^2 - m - 2r)}{2^{2\beta} (m - 1 - \nabla_{\mathcal{H}})^{2\beta}}.
\end{aligned}$$

Similar to the proof of Theorem 6.18, we get

$$v_1 \geq \frac{(\delta_{\overline{\mathcal{H}}})^{2\alpha} (m^2 - m - 2r)}{m^{2\beta+1} (\nabla_{\overline{\mathcal{H}}})^\beta} = \frac{(m - 1 - \nabla_{\mathcal{H}})^{2\alpha} (m^2 - m - 2r)}{m^{2\beta+1} (m - 1 - \delta_{\mathcal{H}})^\beta}. \quad (6.13)$$

Applying Cauchy-Schwartz inequality we obtain $(\sum_{q=2}^m |v_q|)^2 \leq (m - 1) \sum_{q=2}^m v_q^2$. Therefore using Part (2) of Lemma 6.13, $(\mathcal{E}_{\alpha, \beta}(\overline{\mathcal{H}}) - v_1)^2 \leq (m - 1) (2\mathcal{J} - v_1^2)$.

(a). From Theorem 6.22, we see that

$$\mathcal{E}_{\alpha, \beta}(\mathcal{H}) \leq \frac{(m - 1)^{2\alpha}}{2^\beta} \left[\sqrt{2r - m + 1} + \sqrt{2r(m - 1) - \frac{\mathbf{R}_\alpha^2(\mathcal{H})(m - 1)^{1-2\beta-4\alpha}}{m^2}} \right]. \quad (6.14)$$

If $\nabla_{\mathcal{H}} = m - 1$ or $\nabla_{\overline{\mathcal{H}}} = m - 1$, then by using inequality (6.10), we obtain

$$\begin{aligned}
\mathcal{E}_{\alpha, \beta}(\overline{\mathcal{H}}) &\leq v_1 + \sqrt{(m - 1) (2\mathcal{J} - v_1^2)} \\
&\leq \frac{(n_{\mathcal{H}_1} - 1)^{2\alpha} \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1}}{2^\beta} \\
&\quad + \sqrt{(m - 1) \left[\frac{(m - 1 - \delta_{\mathcal{H}})^{4\alpha} (m^2 - m - 2r)}{2^{2\beta} (m - 1 - \nabla_{\mathcal{H}})^{2\beta}} - \frac{(m - 1 - \nabla_{\mathcal{H}})^{4\alpha} (m^2 - m - 2r)^2}{m^2 2^{2\beta+2} (m - 1 - \delta_{\mathcal{H}})^{2\beta}} \right]} \\
&= \frac{1}{2^\beta} \left[(n_{\mathcal{H}_1} - 1)^{2\alpha} \sqrt{2e_{\mathcal{H}_1} - n_{\mathcal{H}_1} + 1} + W_1 \right].
\end{aligned} \quad (6.15)$$

By adding Equations (6.14) and (6.15), we get the desired result.

(b). From proof of Theorem 6.22 (1), we see that

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) \leq \frac{(m-2)^{2\alpha}}{2^\beta} \left[\sqrt{2r-m+1} + \sqrt{2r(m-1) - \frac{R_\alpha^2(\mathcal{H})(m-1)}{m^2(m-2)^{2\beta+4\alpha}}} \right]. \quad (6.16)$$

If $\nabla_{\mathcal{H}} \leq m-2$ and $\nabla_{\overline{\mathcal{H}}} \leq m-2$, then using Lemma 6.17 and proof of Theorem 6.18, we get

$$\begin{aligned} \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) &\leq \nu_1 + \sqrt{(m-1)(2\mathcal{J} - \nu_1^2)} \\ &\leq \frac{(m-1-\delta_{\mathcal{H}})^{2\alpha}}{2^\beta(m-1-\nabla_{\mathcal{H}})^\beta} \sqrt{(m^2-2m-2r+1) + \delta_{\mathcal{H}}(2+\nabla_{\mathcal{H}}-m)} \\ &\quad + \sqrt{(m-1) \left[\frac{(m-1-\delta_{\mathcal{H}})^{4\alpha}(m^2-m-2r)}{2^{2\beta}(m-1-\nabla_{\mathcal{H}})^{2\beta}} - \frac{(m-1-\nabla_{\mathcal{H}})^{4\alpha}(m^2-m-2r)^2}{m^2 2^{2\beta+2}(m-1-\delta_{\mathcal{H}})^{2\beta}} \right]} \\ &= \frac{(m-1-\delta_{\mathcal{H}})^{2\alpha} \sqrt{m^2-m-2r}}{2^\beta(m-1-\nabla_{\mathcal{H}})^\beta} W_2 \end{aligned} \quad (6.17)$$

The desired result is obtained by adding Equations (6.16) and (6.17).

Similarly, one can prove Parts (2) ~ (4). □

Theorem 6.26. Let $\mathcal{H} = \mathcal{G}(m, r, \nabla_{\mathcal{G}}, \delta_{\mathcal{G}})$ be a connected graph and α, β are real numbers.

(1). If $\alpha, \beta \geq 0$ then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \geq \frac{2^{1-\beta} \sqrt{r}}{(m-1)^\beta} + \frac{\sqrt{2(m^2-m-2r)}(m-1-\nabla_{\mathcal{H}})^{2\alpha}}{2^\beta(m-1-\delta_{\mathcal{H}})^\beta}.$$

(2). If $\alpha, \beta \leq 0$ then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \geq 2^{1-\beta} (m-1)^{2\alpha} \sqrt{r} + \frac{\sqrt{2(m^2-m-2r)}(m-1-\delta_{\mathcal{H}})^{2\alpha}}{2^\beta(m-1-\nabla_{\mathcal{H}})^\beta}.$$

(3). If $\alpha \geq 0$ and $\beta \leq 0$ then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \geq 2^{1-\beta} \sqrt{r} + \frac{\sqrt{2(m^2-m-2r)}(m-1-\nabla_{\mathcal{H}})^{2\alpha-\beta}}{2^\beta}.$$

(4). If $\alpha \leq 0$ and $\beta \geq 0$ then

$$\mathcal{E}_{\alpha,\beta}(\mathcal{H}) + \mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \geq 2^{1-\beta} (m-1)^{2\alpha-\beta} \sqrt{r} + \frac{\sqrt{2(m^2-m-2r)}(m-1-\delta_{\mathcal{H}})^{2\alpha-\beta}}{2^\beta}.$$

Proof. (1). From Theorem 6.22 (1), we see that

$$E_{\alpha,\beta}(\mathcal{H}) \geq \frac{2^{1-\beta} \sqrt{r}}{(m-1)^\beta}. \quad (6.18)$$

By Part (1) of Lemma 6.13, we have $\sum_{q=1}^m v_q^2 = -2 \sum_{1 \leq p < q \leq m} v_p v_q$. Using Part (2) of Lemma 6.13, we obtain

$$\begin{aligned} (\mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}))^2 &= \left(\sum_{q=1}^m |v_q| \right)^2 \\ &= \sum_{q=1}^m v_q^2 + 2 \sum_{1 \leq p < q \leq m} |v_p v_q| \\ &\geq 2\mathcal{J} + 2 \left| \sum_{1 \leq p < q \leq m} v_p v_q \right| = 4\mathcal{J}. \end{aligned}$$

We know that $\nabla_{\overline{\mathcal{H}}} = m - 1 - \delta_{\mathcal{H}}$ and $\delta_{\overline{\mathcal{H}}} = m - 1 - \nabla_{\mathcal{H}}$. Now

$$4\mathcal{J} = 4 \sum_{1 \leq p < q \leq m} \frac{\left(d_{\overline{\mathcal{H}}}^{(w_p)} d_{\overline{\mathcal{H}}}^{(w_q)} \right)^{2\alpha}}{\left(d_{\overline{\mathcal{H}}}^{(w_p)} + d_{\overline{\mathcal{H}}}^{(w_q)} \right)^{2\beta}} \geq \sum_{1 \leq p < q \leq m} \frac{4(\delta_{\overline{\mathcal{H}}})^{4\alpha}}{2^{2\beta} (\nabla_{\overline{\mathcal{H}}})^{2\beta}} = \frac{2^{1-2\beta} (m^2 - m - 2r) (m - 1 - \nabla_{\mathcal{H}})^{4\alpha}}{(m - 1 - \delta_{\mathcal{H}})^{2\beta}}.$$

Hence

$$\mathcal{E}_{\alpha,\beta}(\overline{\mathcal{H}}) \geq \frac{(m - 1 - \nabla_{\mathcal{H}})^{2\alpha} \sqrt{2(m^2 - m - 2r)}}{2^\beta (m - 1 - \delta_{\mathcal{H}})^\beta}. \quad (6.19)$$

The result is obtained by adding equations (6.18) and (6.19).

Now using Theorem 6.22, one can prove Parts (2) ~ (4) in a similar manner. \square

6.6 Conclusion

We introduce generalized inverse sum indeg index and energy of graphs. Under certain conditions, we discuss the monotonicity of generalized ISI index by adding edges to a graph. We find extremal graphs with respect to generalized ISI index in class of trees, a class of connected graphs with smallest degree 2 and a class of graphs with given independence number. Bounds on spectral radius and spread of generalized ISI matrix are determined. We also find bounds on generalized ISI energy and Nordhaus-Gaddum-type results for generalized inverse sum indeg index spectral radius and energy.

Chapter 7

Some open problems

In the current chapter, we discuss about some open problems related to energy of graphs and digraphs. We also give few conjectures that are based on our numerical computation and proof of which are so far not available.

7.1 Energy of digraphs

The iota energy of a digraph \mathcal{D} (sidigraph \mathcal{S}) is defined as the sum of absolute values of imaginary parts of its eigenvalues, represented by $\mathcal{E}_c(\mathcal{D})$ ($\mathcal{E}_c(\mathcal{S})$). Recall that \mathcal{B}_m represents the set of all m -vertex bicyclic digraphs and $D_m^s[q, s] = C_q \cup C_s$. Also recall that $\vartheta[g, r, t]$ represents a ϑ -sidigraph with parameters g, r and t whose both cycles are positive and $\Theta[q, s]$ represents a Θ -sidigraph in which both cycles are positive. Khan et al. [23] determine the extremal iota energy in the class of vertex-disjoint bicyclic digraphs. Since $\mathcal{E}_c(D_m^s[2, 2]) = 2 \cot \frac{\pi}{2} = 0$, therefore, the digraph having minimal iota energy in \mathcal{B}_m is $D_m^s[2, 2]$. We mention here a related iota energy problem.

Problem 1: Find the bicyclic digraphs with maximal iota energy in the class of all bicyclic digraphs.

Based on our numerical computation we give following conjectures about Problem 1. The results are obtained using MATLAB. The validity of these conjectures up to $m = 20$ was ver-

ified by computing the values of iota energy for these bicyclic digraphs. Assuming that the results also hold for $m > 20$, we arrived at these given conjectures. We give here some of the computational results which prove the validity of the given conjectures. See Table 7.1 and Table 7.2.

Conjecture 7.1. If $q \geq s \geq 2$ then $\mathcal{E}_c(\Theta[q, s]) \leq \mathcal{E}_c(D_m^s[q, s])$.

Conjecture 7.2. Let $g \geq r$, $(g, r) \neq (1, 1)$ and $g+r+t-1 \leq m$. Then $\mathcal{E}_c(\vartheta[g, r, t]) \leq \mathcal{E}_c(\vartheta[3, 1, m-3])$.

Conjecture 7.3. Let $m \geq 8$. Then $\mathcal{E}_c(\vartheta[3, 1, m-3])$ is greater than the maximal value of iota energy of the vertex-disjoint bicyclic digraph for each m .

For study of maximal iota energy in class of vertex-disjoint bicyclic digraphs see [23].

By proving the Conjectures 7.1 ~ 7.3, one can obtain the the following result.

Conjecture 7.4. Let $m \geq 8$ and $\mathcal{D} \in \mathcal{B}_m$. Then $\mathcal{E}_c(\mathcal{D}) \leq \mathcal{E}_c(\vartheta[3, 1, m-3])$.

Table 7.1: Values of Iota energy of bicyclic digraphs.

q	s	$\mathcal{E}_c(D_m^s[q, s])$	$\mathcal{E}_c(\Theta[q, s])$	q	s	$\mathcal{E}_c(D_m^s[q, s])$	$\mathcal{E}_c(\Theta[q, s])$
2	6	3.4641	2.9104	2	8	4.8284	4.2118
3	5	4.8097	3.2254	3	7	6.1133	4.4503
4	4	4	2.3784	4	6	5.4641	3.4999
2	7	4.3813	3.6979	5	5	6.1554	3.5353
3	6	5.1962	3.5088	2	9	5.6713	4.9650
4	5	5.0777	2.8729	3	8	6.5605	4.8490
				4	7	6.3813	4.1906
				5	6	6.5418	3.4762

Now we give some more problems related to iota energy of digraphs (sidigraphs).

Problem 2: Find the bicyclic sidigraphs with extremal iota energy in class of all bicyclic sidigraphs.

Table 7.2: Values of Iota energy of bicyclic digraphs.

m	g	r	t	$\mathcal{E}_c(\vartheta[g, r, t])$	m	g	r	t	$\mathcal{E}_c(\vartheta[g, r, t])$
8	2	1	6	4.8056	9	2	1	7	5.5378
	2	2	5	4.8373		2	2	6	5.2654
	3	1	5	4.9414		3	1	6	5.8449
	3	2	4	4.2326		3	2	5	4.8056
	3	3	3	3.8883		3	3	4	4.8373
	4	1	4	4.8646		4	1	5	5.5608
	4	2	3	4.5503		4	2	4	4.9414
	4	3	2	3.4762		4	3	3	4.2326
	4	4	1	3.5353		4	4	2	3.8883
	5	1	3	4.7635		5	1	4	5.7662
	5	2	2	4.1906		5	2	3	4.8646
	5	3	1	3.4999		5	3	2	4.5503
	6	1	2	4.8490		5	4	1	3.4762
	6	2	1	4.4503		6	1	3	5.4695
7	1	1	4.2118	6	2	2	4.7635		
					7	1	2	5.7035	
					7	2	1	4.8490	
					8	1	1	4.9650	

Problem 3: Give the lower bounds for iota energy energy of sidigraphs and find extremal sidigraphs satisfying these lower bounds.

Problem 4: Determine the extremal iota energy in the class of those digraphs which contain no even cycles.

Khan et al. [47] find the digraphs having equal iota energy and these digraphs contains cycles as their strong components. Therefore we suggest the following problem.

Problem 5: Find the equienergetic digraphs with respect to iota energy that are not regular.

In Chapter 4, we determine the energy ordering of vertex-disjoint bicyclic sidigraphs and Yang and Wang [75] determine the energy and iota energy ordering of vertex-disjoint bicyclic digraphs. The following two problems are not solved yet.

Problem 6: Determine the energy ordering of all digraphs in \mathcal{B}_m and all sidigraphs in \mathcal{B}_m^s .

Problem 7: Determine the iota energy ordering of all digraphs in \mathcal{B}_m and all sidigraphs in \mathcal{B}_m^s .

Hafeez and Mehtab [39] find the extremal energy of those vertex-disjoint bicyclic weighted digraphs whose weights of both cycles are between -1 and 1 . One may consider the following problem.

Problem 8: Compute the extremal energy of all those bicyclic weighted digraphs whose weights of both cycles are between -1 and 1 .

7.2 Degree-based topological index and energy of graphs

In this section, we give some open problems related to inverse sum indeg energy and generalized inverse sum indeg index and energy of graphs.

We mention here a problem related to the ISI energy of trees.

Problem 9: In class of trees, find the graphs having minimal and maximal ISI energy.

Now we give the following conjecture about Problem 9 which is based on our numerical testing. To prove the conjecture using the Coulson-type integral expressions was (so far) not successful.

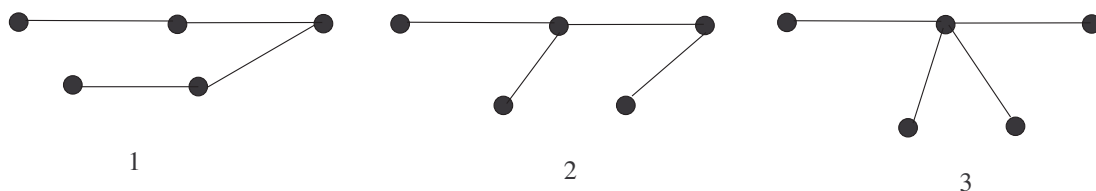


Figure 7.1: All trees of order 5.

Conjecture 7.5. In the class of m -vertex trees, \mathcal{S}_m has the smallest ISI energy and \mathcal{P}_m has the largest ISI energy.

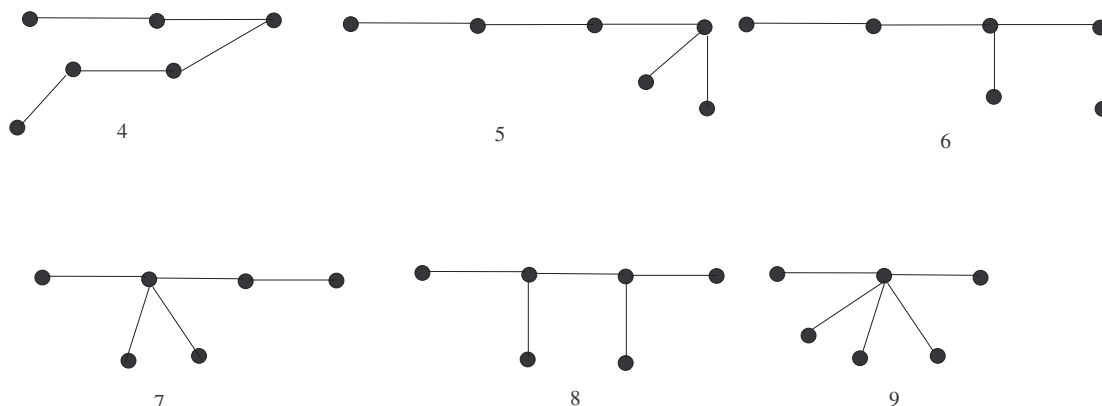


Figure 7.2: All trees of order 6.

The validity of Conjecture 7.5 up to $m = 10$ was verified by computing the \mathcal{E}_{ISI} values of all trees with 10 vertices. Assuming that the conjecture holds also for $m > 10$, we arrived at a most likely guess about the structure of the extremal trees with respect to ISI energy. We give here some of the computational results about ISI energy which shows the validity of Conjecture 7.5 for all trees with $m = 5$ and $m = 6$. See Figure 7.1, 7.2 and Table 7.3.

Table 7.3: ISI energy values.

Tree \mathcal{T}	$\mathcal{E}_{\text{ISI}}(\mathcal{T})$	Tree \mathcal{T}	$\mathcal{E}_{\text{ISI}}(\mathcal{T})$
1	4.4602	6	5.7546
2	3.4118	7	4.8948
3	3.2	8	5.1962
4	5.8703	9	3.7268
5	5.0698		

One may also consider the following problems.

Problem 10: In class of chemical trees, unicyclic graphs and bicyclic graphs, find the graphs having minimal and maximal ISI energy.

Problem 11: Find the extremal ISI energy in the class of graphs with fixed minimum or maximum degree or with fixed pendant vertices and fixed diameter.

In Chapter 5, we determine some classes of graphs having same ISI energy. The following problem can also be considered.

Problem 12: Find some more classes of graphs having same ISI energy.

We now give some problems related to generalized ISI index.

Problem 13: In the class of trees, compute the extremal value of generalized ISI index and finds the corresponding graphs.

The following result about minimal value of generalized ISI index in class of trees as stated in Problem 11 is based on our numerical testing. To prove the conjecture using the technique as in Theorem 6.10 was not so far successful.

Conjecture 7.6. Suppose \mathcal{T} is a tree with $n_{\mathcal{T}} = m$. If $\alpha = \beta$ and $\alpha > 1$, then

$$S_{\alpha, \beta}(\mathcal{T}) \geq \frac{(m-1)(m-1)^\alpha}{m^\alpha},$$

where the inequality becomes equality if $\mathcal{T} \cong \mathcal{S}_m$.

The validity of Conjecture 7.6 in the class of trees up to $m = 10$ and $1 < \alpha \leq 10$ was verified by computing the values of generalized ISI index. Assuming that the conjecture holds also for $m > 10$, we arrived at a most likely guess about the structure of the minimal tree with respect to generalized ISI index. We give here some of the computational results about generalized ISI index for all trees with $m = 5$ and $m = 6$ which shows the validity of Conjecture 7.6. We take $\alpha \in [1, 4]$ with a difference of 0.5. See Figure 7.1, 7.2 and Table 7.4.

The following problems can also be considered.

Problem 14: Find the extremal value of generalized ISI index in class of chemical trees, unicyclic graphs, bicyclic graphs or in the class of graphs with fixed pendant vertices, fixed diameter and fixed independence number etc.

The total transformation graph denoted by $T(\mathcal{G})$ is a graph with vertex set $\mathbb{V}_{\mathcal{G}} \cup \mathbb{E}_{\mathcal{G}}$, such that two vertices are adjacent in $T(\mathcal{G})$ if and only if they are either adjacent or incident in \mathcal{G} .

Problem 15: Compute the extremal value of generalized ISI index of total transformation graphs.

Table 7.4: Values of generalized ISI index of trees.

Tree \mathcal{T}	$S_{\alpha,\beta}(\mathcal{T})$						
	$\alpha = 1$	$\alpha = 1.5$	$\alpha = 2$	$\alpha = 2.5$	$\alpha = 3$	$\alpha = 3.5$	$\alpha = 4$
1	3.3333	3.0887	2.8889	2.7258	2.5926	2.4838	2.3951
2	3.3667	3.1579	3.0094	2.9146	2.8680	2.8656	2.9039
3	3.2000	2.8622	2.5600	2.2897	2.0480	1.8318	1.6384
4	4.3333	4.0887	3.8889	3.7258	3.5926	3.4838	3.3951
5	4.2833	4.0527	3.8914	3.7904	3.7425	3.7421	3.7851
6	4.4833	4.3672	4.3314	4.3678	4.4705	4.6351	4.8587
7	4.4000	4.2306	4.1422	4.1330	4.2027	4.3528	4.5868
8	4.5000	4.4352	4.5000	4.7042	5.0625	5.5949	6.3281
9	4.1667	3.8036	3.4722	3.1697	2.8935	2.6414	2.4113

We now give some problems related to generalized ISI energy.

Problem 16: Compute the graphs that are equienergetic with respect to generalized ISI energy.

Problem 17: Find the extremal value of generalized ISI energy in class of trees, chemical trees, unicyclic graphs, bicyclic graphs or in the class of graphs with fixed pendant vertices, fixed diameter and fixed independence number etc.

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