

Iota energy of unicyclic and bicyclic signed digraphs

by

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**Dedicated
to my
Amman and Abba**

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Abstract

Spectral graph theory is the study of characteristics of a graph associated with the matrices and the eigenvalues of that graph. In this thesis, we focus on the properties of a graph in relation to its adjacency matrix. The energy of a sidigraph S of order n is defined by $E(S) = \sum_{j=1}^n |\operatorname{Re}(\lambda_j)|$, where $\operatorname{Re}(\lambda_j)$ is the real part of the eigenvalue λ_j , for $j = 1, \dots, n$.

In this dissertation, we extend notion of iota energy to sidigraphs such that the Coulson's integral formula remains valid. We compute iota energy formulas for the signed directed cycles and find extremal iota energies for unicyclic sidigraphs with fixed order. The set containing n -vertex sidigraphs with cycles each of length h is denoted by $S_{n,h}$. We discuss the increasing property of iota energy over some specific subclasses of the set $S_{n,h}$. We have also found those sidigraphs which give minimum and maximum values of iota energy among the class of bicyclic sidigraphs which are vertex disjoint.

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Chapter 1

Fundamentals of graph theory

This chapter includes some basic definitions and fundamental concepts that will be used in this dissertation. In order to clarify any ambiguities, supporting examples have also been discussed. The main idea is to discuss the properties of graphs, digraphs and signed digraphs.

1.1 History of graph theory

In our daily life we encounter many problems which can be represented by means of a graph. Whether the problem is to find the fastest route from one city to another or to minimize the travelling time of a postman to deliver letters, all such problems can be expressed by a set of points and the lines connecting certain pair of points. It was the study of these graphs that gave rise to the idea of graph theory.

The problem that initiated the study of graph theory was Königsberg's bridge problem. Königsberg was a city in Russia in which two islands were connected to the main land by seven bridges. Euler proposed a problem whether all the bridges can be traversed only once with the extra condition that the trip ends in the same place it began. Euler solved this problem in the form of a graph by a set of vertices depicting landmarks and the bridges connecting those landmarks by edges. He concluded that it was only possible

if every landmark has even number of bridges.

1.2 Introduction to graph

An ordered pair $G = (\mathcal{V}, \mathcal{E})$ is called a graph where \mathcal{V} is the set of vertices (or nodes) and is called the vertex set (or node set). The set \mathcal{E} contains edges and is called the edge set. If there is an edge between vertex w_1 and vertex w_2 , we represent it by w_1w_2 or w_2w_1 and the vertices w_1 and w_2 are called the endpoints of the edge w_1w_2 . If the vertex w_1 is the endpoint of the edge e then e is incident on v . If the vertices w_1 and w_2 are connected by an edge then they are said to be adjacent, otherwise non adjacent. Similarly, if two edges e and f share a common vertex then they are said to be adjacent. A loop is an edge whose starting and ending points are same. Multiple edges are those edges which have same pair of endpoints. A graph without loops and multiple edges is said to be a simple graph.

The degree of a vertex w_1 , represented by $d(w_1)$, is the number of edges incident on w_1 . A vertex for which $d(w_1) = 0$ is known as isolated vertex. The degree of a vertex increases by two if it has a loop. A graph $F = (\mathcal{P}', \mathcal{Q}')$ is called a subgraph of G if $\mathcal{P}' \subseteq \mathcal{V}$ and $\mathcal{Q}' \subseteq \mathcal{E}$.

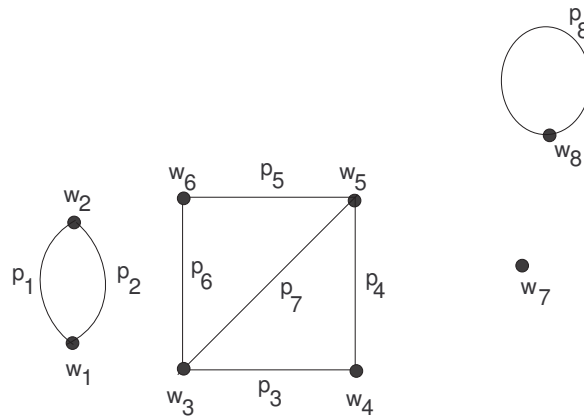


Figure 1.1: A graph $G = (\mathcal{V}, E)$

Example 1.1. The graph G in Fig. 1.1 has vertex set $\mathcal{V} = \{w_1, w_2, w_3, w_4, w_5, w_6, w_7, w_8\}$ and edge set $\mathcal{E} = \{p_1, p_2, p_3, p_4, p_5, p_6, p_7, p_8\}$. There exist multiple edges between vertices w_1 and w_2 . Vertex w_8 has a loop and vertex w_7 is an isolated vertex.

A walk is a finite alternating sequence $w_1e_1w_2e_2\dots e_nw_n$ of vertices and edges such that the edge e_j has endpoints w_j and w_{j+1} for $j = 1, 2, \dots, n - 1$. It is not necessary for a walk to have distinct vertices and edges. The total number of edges in a w_1, w_2 -walk, with endpoints w_1 and w_2 , is called the length of w_1, w_2 -walk. A walk with no repeated edge is called a trail. A w_1, w_2 -path on n -vertices with endpoints w_1 and w_2 is a trail with no repeated vertex. Number of edges in a path is the length of path. A trail in which the first and last vertices are equal is called a circuit. A cycle is a circuit without any repeated vertex except the first and last vertex. The number of edges in a cycle is called the length of a cycle.

A graph G is connected if there exists a w_1, w_2 -path for every pair of vertices $w_1, w_2 \in \mathcal{V}$. A simple graph on n -vertices in which vertices are pair-wise adjacent is known as a complete graph denoted by K_n . The component of a graph G is the largest connected subgraph of G . A graph which is either K_2 or C_n , $n \geq 3$ is called an elementary figure. A disconnected graph which has elementary figures as its components is called a basic figure.

1.3 Energy of graphs

Gutman [9] introduced the concept of graph energy. It has a vast number of applications in chemistry which can be studied in [8, 10, 20]. Graph energy is an invariant which is calculated from the eigenvalues of the graph.

An $n \times n$ symmetric matrix, denoted by $A(G) = [a_{ij}]$, is called the adjacency matrix of a simple graph $G = (\mathcal{V}, \mathcal{E})$ of order n , such that

$$a_{ij} = \begin{cases} 1 & \text{if there exists an edge between } v_i \text{ and } v_j \\ 0 & \text{otherwise.} \end{cases}$$

Let I be an $n \times n$ identity matrix then the polynomial $\phi_G(x) = \det(xI - A(G))$ is called the characteristic polynomial of the adjacency matrix. The zeros of this polynomial are considered as the eigenvalues of the graph G . The spectrum of G , denoted by $\text{Spec}(G)$, is the multiset of the eigenvalues of G .

The energy of a simple graph G is given by:

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

where z_1, \dots, z_n are the eigenvalues of G .

The coefficient theorem for graphs is as follows:

Theorem 1.2 (Cvetković et al. [4]). *Let \mathcal{L}_k be the set of all k -vertex basic figures L of an n -vertex graph G , $p(L)$ be the number of components of L and $c(L)$ the set of all cycles of L . Then the characteristic polynomial of G is as follows:*

$$\phi_G(x) = x^n + \sum_{k=1}^n a_k x^{n-k},$$

where

$$a_k = \sum_{L \in \mathcal{L}_k} (-1)^{p(L)2^{|c(L)|}}$$

for all $k = 1, 2, \dots, n$.

1.4 Signed graphs

An ordered pair $S = (G, \omega)$ is said to be a signed graph (shortly sigraph), where $G = (\mathcal{V}, \mathcal{E})$ is the underlying graph and $\omega : \mathcal{E} \rightarrow \{-1, 1\}$ is the signing function. That is, a $+1$ or a -1 sign is assigned to each edge of S . An edge which is assigned a $+1$ sign is called a positive edge. Similarly, a negative edge is the one which is assigned a -1 sign. In general, the edges of S are called signed edges. The sets \mathcal{E}^+ and \mathcal{E}^- represent the sets of positive and negative edges of S , respectively. Thus, $\mathcal{E} = \mathcal{E}^+ \cup \mathcal{E}^-$. The product of the sign of edges in S is called the sign of sigraph S . A sigraph S is positive (respectively,

negative) if the sign of S is positive (respectively, negative). If all cycles of a sigraph are positive then it is cycle balanced, otherwise non cycle balanced.

The adjacency matrix, denoted by $A(S) = [b_{mn}]$, of a sigraph S is a matrix of order n , where

$$b_{mn} = \begin{cases} \omega(v_m v_n) & \text{if there is an edge between } v_m \text{ and } v_n \\ 0 & \text{otherwise.} \end{cases}$$

The characteristic polynomial $\phi_S(x)$ of sigraph S is the $\det(xI - A(S))$. The roots of $\phi_S(x) = 0$ are called the eigenvalues of S . The multiset of the eigenvalues of S is the spectrum of S , denoted by $\text{Spec}(S)$.

The energy in sigraphs was introduced by Germina et. al. [7]. The energy of a sigraph S is

$$E(S) = \sum_{j=1}^n |\lambda_j|,$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of S . The coefficient theorem for sigraphs is as follows:

Theorem 1.3 (Acharya [1]). *Let S be an n -vertex sigraph and \mathcal{L}_k be the set of all k -vertex basic figures L . Further, suppose $p(L)$ is the number of components of L and $c(L)$ and $s(Z)$ denote the set of all cycles of L and the sign of cycle Z , respectively. Then the characteristic polynomial of S is as follows:*

$$\phi_S(x) = x^n + \sum_{k=1}^n c_k(S) x^{n-k},$$

where

$$c_k(S) = \sum_{L \in \mathcal{L}_k} (-1)^{p(L)2^{c(L)}} \prod_{z \in c(L)} s(Z)$$

for all $k = 1, 2, \dots, n$.

Applications of sigraphs in chemistry can be studied in [11, 14].

1.5 Digraphs and signed digraphs

A directed graph (or briefly digraph) is a pair $D = (\mathcal{V}, \mathcal{A})$, where \mathcal{V} represents the vertex set and \mathcal{A} represents set of arcs of D . An ordered pair $S = (D, \omega)$ is said to be a signed digraph (or briefly sidigraph), where $D = (\mathcal{V}, \mathcal{A})$ is said to be the underlying digraph and $\omega : \mathcal{A} \rightarrow \{-1, 1\}$ represents the signing function. A positive arc of S is an arc with a $+1$ sign. Similarly, a negative arc of S is an arc with a -1 sign. Generally, the arcs of S are called signed arcs. The sets of positive arcs (respectively, negative arcs) of S is represented by $\mathcal{A}^+(S)$ (respectively, $\mathcal{A}^-(S)$). Thus, $\mathcal{A}(S) = \mathcal{A}^+(S) \cup \mathcal{A}^-(S)$ is the set of signed arcs of S . Similarly, the number of positive arcs (respectively, negative arcs) of S are denoted by a^+ (respectively, a^-). Thus, $a = a^+ + a^-$ is the total number of arcs of S .

w_1w_2 denotes an arc of S from w_1 to w_2 . A sidigraph on n vertices w_1, \dots, w_n with signed arcs w_jw_{j+1} for $j = 1, \dots, n-1$ is called a signed directed path and is denoted by P_n . A sidigraph of order n having vertices w_1, \dots, w_n and signed arcs w_jw_{j+1} , $j = 1, \dots, n-1$ and w_nw_1 is called a signed directed cycle of length n . The product of sign of arcs of a sidigraph S is known as the sign of sidigraph S . A sidigraph having positive sign (respectively, negative sign) is said to be positive (respectively, negative). If each directed cycle of a sidigraph is positive then it is said to be cycle balanced; otherwise non cycle balanced. C_n^+ (respectively, C_n^-) denote a positive (respectively, negative) directed cycle of length n . Thus, a signed directed cycle which is either positive or negative is represented by C_n .

In a digraph D if for every pair of vertices w_1 and w_2 there exists a w_1, w_2 -path and a w_2, w_1 -path then D is called strongly connected digraph. The maximally connected subdigraphs of a digraph D are its strong components. Strongly connected sidigraphs and strong components of sidigraphs can be defined analogously. A digraph is unicyclic if it has a unique directed cycle and the number of vertices equals the number of arcs. A digraph is bicyclic if it has two directed cycles and the number of vertices is one less than the number of arcs. If D is unicyclic (respectively, bicyclic) then sidigraph $S = (D, \omega)$ is

unicyclic (respectively, bicyclic).

The total number of arcs entering a vertex w_1 is said to be the in-degree of vertex w_1 denoted by $d^+(w_1)$. Similarly, the total number of arcs leaving the vertex w_1 is the out-degree of vertex w_1 denoted by $d^-(w_1)$. A sidigraph is linear if $d^+(w_1) = d^-(w_1)$.

The adjacency matrix of a sidigraph $S = (D, \omega)$ with underlying digraph $D = (\mathcal{V}, \mathcal{A})$ whose vertices are w_1, w_2, \dots, w_n is a matrix $A(S) = [a_{mn}]$ of order n , where

$$a_{mn} = \begin{cases} \omega(w_m w_n) & \text{if there is an arc from } w_m \text{ to } w_n \\ 0 & \text{otherwise.} \end{cases} \quad (1.1)$$

The polynomial $\phi_S(x) = \det(xI - A(S))$ is known as the characteristic polynomial of S , where I is the identity matrix. The roots of $\phi_S(x) = 0$ are the eigenvalues of S . The multiset of these eigenvalues is known as the spectrum of S , denoted by $\text{Spec}(S)$. Two sidigraphs of same order having same spectrum are said to be cospectral; otherwise non-cospectral.

A sidigraph S is said to be symmetric if an arc $w_1 w_2 \in \mathcal{A}^+(S)$ (respectively, $w_1 w_2 \in \mathcal{A}^-(S)$) then $w_2 w_1 \in \mathcal{A}^+(S)$ (respectively, $w_2 w_1 \in \mathcal{A}^-(S)$), where $w_1, w_2 \in \mathcal{V}$.

Let $S_1 = (D_1, \omega_1)$ and $S_2 = (D_2, \omega_2)$ be two sidigraphs, where $D_1 = (\mathcal{V}_1, \mathcal{A}_1)$ and $D_2 = (\mathcal{V}_2, \mathcal{A}_2)$ are the underlying digraphs of S_1 and S_2 , respectively. The cartesian product $S_1 \times S_2$ of S_1 and S_2 is the sidigraph $S = (D, \omega)$, where $D = (\mathcal{V}, \mathcal{A})$, $\mathcal{V} = \mathcal{V}_1 \times \mathcal{V}_2$, the arc set \mathcal{A} is $\mathcal{A}(S_1 \times S_2) = \{(v_1, w_1)(v_2, w_2) \mid v_1 v_2 \in \mathcal{A}_1 \text{ and } w_1 = w_2 \text{ or } v_1 = v_2 \text{ and } w_1 w_2 \in \mathcal{A}_2\}$, and the signing function is defined by:

$$\omega((v_1, w_1)(v_2, w_2)) = \begin{cases} \omega_1(v_1 v_2) & \text{if } w_1 \text{ is equal to } w_2 \\ \omega_2(w_1 w_2) & \text{if } v_1 \text{ is equal to } v_2. \end{cases} \quad (1.2)$$

The concept of graph energy was further extended by Peña and Rada [17] to the energy of digraphs. It is obvious that eigenvalues of a digraph are not necessarily real. Khan et al. [12] studied the contribution of imaginary parts of the eigenvalues of a digraph towards its energy and introduced the notion of iota energy. Later, Pirzada and Bhat [18] defined the energy formula for sidigraphs.

1.6 Overview

The sequence of this dissertation is as follows:

In Chapter 2, we discuss some basic results related to energy of digraphs and sidigraphs.

In Chapter 3, we define the iota energy for sidigraphs and calculate the iota energy formulas for signed directed cycles. We also discuss the increasing property of iota energy over some specific subclasses of the set $S_{n,h}$, where $S_{n,h}$ contains sidigraphs of n vertices with cycles each of length h .

In Chapter 4, we find sidigraphs with extremal iota energy among the class of vertex disjoint bicyclic sidigraphs of fixed order.

Chapter 2

Energy of digraphs and sidigraphs

Peña and Rada [17] extended the idea of graph energy to the energy of digraphs. Germina et al. [7] introduced the concept of energy in sigraphs which was further extended to sidigraphs by Pirzada and Bhat [18]. In this chapter we discuss some known results related to the energy of digraphs and sidigraphs.

2.1 Energy of digraphs

The eigenvalues of a digraph maybe complex as its adjacency matrix is not symmetric. The energy of a digraph is defined as

$$E(D) = \sum_{j=1}^n |\operatorname{Re}(\lambda_j)|, \quad (2.1)$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of D . The coefficients for the characteristic polynomial of digraphs can be calculated using the following theorem.

Theorem 2.1 (Cvetkovic et al. [4]). *Let \mathcal{L}_k be the set of all k -vertex linear subdigraphs L of an n -vertex digraph D and $\operatorname{comp}(L)$ be the number of components of L . Then the characteristic polynomial of D is given by*

$$\phi_D(x) = x^n + \sum_{k=1}^n c_k x^{n-k},$$

where

$$c_k = \sum_{L \in \mathcal{L}_k} (-1)^{\text{comp}(L)}$$

for all $k = 1, 2, \dots, n$.

In the next theorem, Peña and Rada [17] gave the extremal energy of unicyclic digraphs on n vertices.

Theorem 2.2 (Peña and Rada [17]). *Let D be a unicyclic digraph on n vertices. Then smallest energy is attained by digraph D containing cycles of order 2, 3 or 4 and the cycle of order n has largest energy.*

Next theorem establishes a relationship between the energy of digraphs and its strong components.

Theorem 2.3 (Peña and Rada [17]). *Let D be an n -vertex digraph. Then*

$$E(D) = \sum_{j=1}^r E(D_j),$$

where D_1, \dots, D_r are the strong components of a digraph D .

Coulson's integral formula is useful in finding the energy of digraphs without calculating their eigenvalues. Throughout this dissertation, we represent the principal value of an integral $\int_{-\infty}^{\infty} F(x)dx$ by *p.v.* $\int_{-\infty}^{\infty} F(x)dx$. A polynomial in which leading coefficient is 1 is called a monic polynomial. In the following theorem, Mateljevic et al. [15] gave the formula to calculate the energy of a polynomial.

Theorem 2.4 (Mateljevic et al. [15]). *Let ϕ be a monic polynomial of degree n and let $\lambda_j, j = 1, \dots, n$, be its zeros. Then*

$$\sum_{j=1}^n |\text{Re}(\lambda_j)| = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \left(n - \frac{ix\phi'(ix)}{\phi(ix)} \right) dx,$$

where $\text{Re}(\lambda_j)$ represents the real part of λ_j .

Next theorem gives the energy of digraphs using Coulson's integral formula.

Theorem 2.5 (Peña and Rada [17]). *If D is an n -vertex digraph with characteristic polynomial $\phi_D(x)$ and $\operatorname{Re}(\lambda_k)$ denotes the real part of the eigenvalue λ_k , then*

$$E(D) = \sum_{k=1}^n |\operatorname{Re}(\lambda_k)| = \frac{1}{\pi} p.v \int_{-\infty}^{+\infty} \left(n - \frac{ix\phi'_D(ix)}{\phi_D(ix)} \right) dx.$$

An immediate consequence of Theorem 2.5 is as follows:

Corollary 2.6 (Peña and Rada [17]). *Define $\gamma(t) = t^n \phi(\frac{i}{t})$. If ϕ is an n -vertex monic polynomial with zeros $\lambda_1, \dots, \lambda_n$ and $\operatorname{Re}(\lambda_k)$ is the real part of λ_k , then*

$$\sum_{k=1}^n |\operatorname{Re}(\lambda_k)| = \frac{1}{\pi} p.v \int_{-\infty}^{+\infty} \log |\gamma(t)| \frac{dt}{t^2}.$$

In 2016, Khan et al. [12] studied the contribution of imaginary parts of the eigenvalues of a digraph towards its energy and defined the iota energy of a digraph D as

$$E_c(D) = \sum_{j=1}^n |\operatorname{Im}(z_j)|, \quad (2.2)$$

where z_1, \dots, z_n are the eigenvalues of D . The following theorem gives extremal iota energy of unicyclic sidigraphs with a positive directed cycle.

Theorem 2.7 (Khan et al. [12]). *The unicyclic n -vertex digraphs which contain a directed cycle C_2^+ have smallest iota energy among all n -vertex unicyclic digraphs. The directed cycle C_n^+ has the largest iota energy among all n -vertex unicyclic digraphs.*

2.2 Energy of sidigraphs

Let S be an n -vertex sidigraph. It is not necessary that the eigenvalues of sidigraphs are real. Thus, the energy of sidigraph S is given by

$$E(S) = \sum_{j=1}^n |\operatorname{Re}(\lambda_j)|, \quad (2.3)$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of S and $\operatorname{Re}(\lambda_j)$ is the real part of the eigenvalue λ_j [17].

The coefficients for the characteristic polynomial of sidigraphs can be calculated using the following theorem.

Theorem 2.8 (Acharya et al. [2]). *Let \mathcal{L}_k be the set of all k -vertex linear subdigraphs L of an n -vertex sidigraph S , $\text{comp}(L)$ be the number of components of L . Further suppose that $c(L)$ and $s(Z)$ denote the set of all cycles of L and the sign of cycle Z respectively. Then the characteristic polynomial of sidigraph S can be calculated by*

$$\phi_S(x) = x^n + \sum_{k=1}^n c_k x^{n-k},$$

where

$$c_k = \sum_{L \in \mathcal{L}_k} (-1)^{\text{comp}(L)} \prod_{Z \in c(L)} s(Z)$$

for all $k = 1, 2, \dots, n$.

Next theorem establishes a relationship between the energy of a sidigraph S and its strong components.

Theorem 2.9 (Pirzada and Bhat [18]). *Let S be a sidigraph on n vertices. Then*

$$E(S) = \sum_{j=1}^r E(S_j),$$

where S_1, \dots, S_r are the strong components of S .

Spectral criteria for cycle balanced sidigraphs is discussed in the following theorem.

Theorem 2.10 (Acharya [1]). *A sidigraph $S = (D, \omega)$ is said to be cycle balanced if and only if S and D are cospectral.*

In the following theorem, Khan et al. [12] compared the energy and iota energy of positive directed cycles.

Theorem 2.11 (Khan et al. [12]). *Energy and iota energy of the positive directed cycles C_k^+ satisfy the following relations, when $k \geq 2$.*

(1) $E(C_j^+) = E_c(C_j^+)$ if and only if $j \equiv 0 \pmod{4}$,

(2) $E(C_j^+) > E_c(C_j^+)$ if and only if $j \equiv 2 \pmod{4}$ or $j \equiv 1 \pmod{2}$.

Next theorem gives the Coulson's integral formula for the energy of sidigraphs

Theorem 2.12 (Pirzada and Bhat [18]). *If S is an n -vertex sidigraph with characteristic polynomial $\phi_D(x)$, then*

$$E(S) = \sum_{k=1}^n |\operatorname{Re}(\lambda_k)| = \frac{1}{\pi} p.v \int_{-\infty}^{+\infty} \left(n - \frac{ix\phi_D'(ix)}{\phi_D(ix)} \right) dx,$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of S and $\operatorname{Re}(\lambda_k)$ denotes the real part of the eigenvalue λ_k .

Next corollary can be easily deduced from Theorem 2.12.

Corollary 2.13 (Peña and Rada [17]). *Let ϕ be an n -th degree monic polynomial with zeros $\lambda_1, \lambda_2, \dots, \lambda_n$ and define $\gamma(t) = t^n \phi(\frac{i}{t})$. Then*

$$\sum_{k=1}^n |\operatorname{Re}(\lambda_k)| = \frac{1}{\pi} p.v \int_{-\infty}^{+\infty} \log |\gamma(t)| \frac{dt}{t^2},$$

where $\operatorname{Re}(\lambda_k)$ is the real part of λ_k .

Let $S_{n,h}$ be the set of sidigraphs with n vertices such that each sidigraph in $S_{n,h}$ has signed directed cycles of length h . In chapter 3, we study the increasing property of energy and iota energy of sidigraphs in $S_{n,h}$. The following results were useful to prove our main results.

Theorem 2.14 (Pirzada and Bhat [18]). *If $S \in S_{n,h}$ then $\phi_S(x) = x^n + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} (-1)^k c^*(S, kh) x^{n-kh}$, where $c^*(S, kh)$ is the number of positive linear subsidigraphs of order kh —number of negative linear subsidigraphs of order kh , for every $k = 1, \dots, \lfloor \frac{n}{h} \rfloor$.*

Pirzada and Bhat [18] defined a quasi-order relation \preceq over a subfamily $S_{n,h}^1$ of $S_{n,h}$ as follows:

Definition 2.15. [18] Let $S_{n,h}^1 = \{S \in S_{n,h} \mid c^*(S, kh) \geq 0, k = 1, \dots, \lfloor \frac{n}{h} \rfloor\}$. The quasi-order relation over $S_{n,h}^1$ is given by: Let S_1 and S_2 be two elements of $S_{n,h}^1$. Then $S_1 \preceq S_2$ if for all $k = 1, 2, \dots, \lfloor \frac{n}{h} \rfloor$, $c^*(S_1, kh) \leq c^*(S_2, kh)$. If $S_1 \preceq S_2$ and there exists k such that $c^*(S_1, kh) < c^*(S_2, kh)$ then $S_1 \prec S_2$. This relation \preceq is reflexive and transitive over $S_{n,h}^1$.

The following theorem gives increasing property of energy over the set $S_{n,h}^1$ when $h \equiv 2 \pmod{4}$.

Theorem 2.16 (Pirzada and Bhat [18]). *The energy of $S_{n,h}^1$ increases with respect to the quasi-order \preceq relation when $h \equiv 2 \pmod{4}$. That is, if $S_1 \preceq S_2$ then $E(S_1) \leq E(S_2)$.*

Let c_m^+ denote the number of m -length positive directed closed walks and c_m^- denote the number of m -length negative directed closed walks. The following corollary and lemma will be useful in obtaining the main result of upper bound for the iota energy of sidigraphs.

Corollary 2.17 (Pirzada and Bhat [18]). *If z_1, \dots, z_n are the eigenvalues of a sidigraph S , then*

$$\sum_{j=1}^n z_j^m = c_m^+ - c_m^-. \quad (2.4)$$

Lemma 2.18 (Pirzada and Bhat [18]). *Let S be a sidigraph having n -vertices, a arcs and n eigenvalues namely z_1, \dots, z_n . Then*

$$(1) \sum_{j=1}^n (\operatorname{Re}(z_j))^2 - \sum_{j=1}^n (\operatorname{Im}(z_j))^2 = c_2^+ - c_2^-.$$

$$(2) \sum_{j=1}^n (\operatorname{Re}(z_j))^2 + \sum_{j=1}^n (\operatorname{Im}(z_j))^2 \leq a.$$

Recall that a^+ and a^- represent the number of positive and negative arcs respectively.

Theorem 2.19 (Pirzada and Bhat [18]). *Let S be a sidigraph with n vertices and $a = a^+ + a^-$ arcs. Further suppose z_1, \dots, z_n be its eigenvalues. Then*

$$E(S) \leq \sqrt{\frac{1}{2}n(a + c_2^+ - c_2^-)}.$$

The equality holds if $S = \frac{n}{2}C_2^+$, n is even or S is a skew symmetric sidigraph.

Recall that K_2 is a complete graph on two vertices.

Theorem 2.20 (Rada [19]). *Let D be a digraph with a arcs and \overleftrightarrow{K}_2 be a symmetric digraph on two vertices. Then $E(D) \leq a$. Moreover, $E(D) = a$ if and only if D is $\frac{a}{2}\overleftrightarrow{K}_2$ plus some isolated vertices.*

In the following theorem, Pirzada and Bhat [18] found a sidigraph whose energy is equal to its number of vertices.

Theorem 2.21 (Pirzada and Bhat [18]). *Let S be a sidigraph of order n having eigenvalues z_1, \dots, z_n such that $|\operatorname{Re}(z_k)| \leq 1$ for every $k = 1, 2, \dots, n$. Then*

$$E(S \times C_2^+) = 2n.$$

Chapter 3

Iota energy of unicyclic signed digraphs

Recently, the concept of iota energy of digraphs is introduced. In this chapter, we extend notion of iota energy to signed digraphs. We compute iota energy formulas for the signed directed cycles. We find the unicyclic signed digraphs with extremal iota energies among the class of unicyclic signed digraphs with fixed order such that the Coulson's integral formula remains valid for signed digraphs. We also discuss the increasing property of iota energy over some specific subclasses of the set $S_{n,h}$, where the set $S_{n,h}$ contains n -vertex signed digraphs with cycles each of length h .

3.1 Iota energy of signed digraphs

Let S be an n -vertex sidigraph with eigenvalues z_1, \dots, z_n . We define the iota energy of S as follow:

$$E_c(S) = \sum_{k=1}^n |\operatorname{Im}(z_k)|, \quad (3.1)$$

where $\operatorname{Im}(z_k)$ is the imaginary part of the eigenvalue z_k .

Example 3.1. Let S be a sidigraph shown in Fig. 3.1. Dotted lines represent the negative

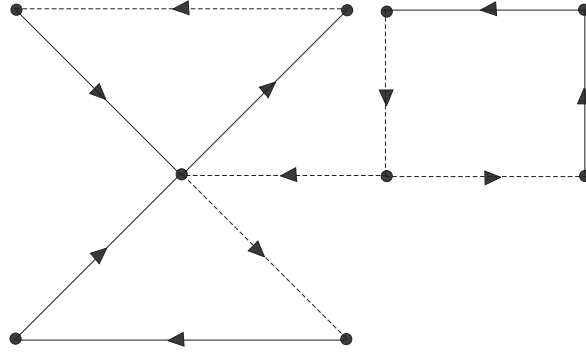


Figure 3.1: A sidigraph with both positive and negative directed cycles

arcs and solid lines represent positive arcs. According to Theorem 2.8, the characteristic polynomial of S is $\phi_S(x) = x^9 + 2x^6 - x^5 - 2x^2$ and the corresponding eigenvalues are $0, 0, \pm 1, \pm i, -2^{\frac{1}{3}}, \frac{2^{\frac{1}{3}} \pm i 2^{\frac{1}{3}} \sqrt{3}}{2}$. Thus, $E_c(S) = 2 + 2^{\frac{1}{3}} \sqrt{3}$.

Example 3.2. Let S be an n -vertex acyclic sidigraph. Then by Theorem 2.8, the characteristic polynomial of S is $\phi_S(x) = x^n$. All eigenvalues of S are zero thus $E_c(S) = 0$.

Example 3.3. Let S be an n -vertex symmetric sidigraph, $n \geq 2$. Then all eigenvalues of the sidigraph S are real as S has symmetric adjacency matrix. Thus, $E_c(S) = 0$.

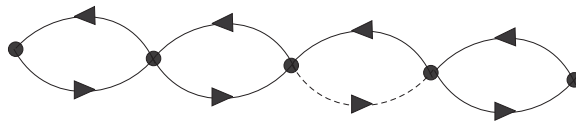


Figure 3.2: A sidigraph with four signed directed cycles

Example 3.4. Let S be a sidigraph shown in Fig. 3.2. Dotted lines represent the negative arcs and solid lines represent positive arcs. By Theorem 2.8, we have $\phi_S(x) = x^5 - 2x^3 + x$ and the corresponding eigenvalues are $0, -1, -1, 1$ and 1 . Thus, $E_c(S) = 0$.

The following theorem is analogue of the Theorem 2.9.

Theorem 3.5. *Let S be a sidigraph on n vertices and S_1, \dots, S_r be its strong components.*

Then

$$E_c(S) = \sum_{k=1}^r E_c(S_k).$$

By Theorem 2.10, we conclude that a directed cycle and a positive directed cycle are considered cospectral. Hence, we can consider directed cycles to be positive directed cycles. Using Theorem 2.8, the characteristic polynomial of a positive directed cycle C_n^+ is given by:

$$\phi_{C_n^+}(x) = x^n - 1.$$

Thus, the eigenvalues of C_n^+ are given by $\exp\left(\frac{2k\pi i}{n}\right)$, where $k = 0, 1, \dots, n-1$. Therefore, by (2.3) and (3.1), the energy and iota energy of C_n^+ are given by:

$$E(C_n^+) = \sum_{k=0}^{n-1} \left| \cos \frac{2k\pi}{n} \right|, \quad (3.2)$$

$$E_c(C_n^+) = \sum_{k=0}^{n-1} \left| \sin \frac{2k\pi}{n} \right|. \quad (3.3)$$

Using (3.2), Pirzada and Bhat [18] calculated the following energy formulas for a positive directed cycle C_n^+ , $n \geq 2$.

$$E(C_n^+) = \begin{cases} 2 \cot \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}4) \\ 2 \csc \frac{\pi}{n} & \text{if } n \equiv 2(\text{mod}4) \\ \csc \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (3.4)$$

Khan et al. [12] calculated the iota energy formulas for a positive directed cycle C_n^+ , $n \geq 2$.

$$E_c(C_n^+) = \begin{cases} 2 \cot \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}2) \\ \cot \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (3.5)$$

Again, using Theorem 2.8, the characteristic polynomial of a negative directed cycle C_n^- is given by:

$$\phi_{C_n^-}(x) = x^n + 1.$$

The eigenvalues of C_n^- are given by $\exp\left(\frac{(2k+1)\pi i}{n}\right)$, where $k = 0, 1, \dots, n-1$. Thus, the energy and iota energy of C_n^- are computed by:

$$E(C_n^-) = \sum_{k=0}^{n-1} \left| \cos \frac{(2k+1)\pi}{n} \right|, \quad (3.6)$$

$$E_c(C_n^-) = \sum_{k=0}^{n-1} \left| \sin \frac{(2k+1)\pi}{n} \right|. \quad (3.7)$$

Using (3.6), Pirzada and Bhat [18] calculated the energy of a negative directed cycle C_n^- , $n \geq 2$ as follow:

$$E(C_n^-) = \begin{cases} 2 \csc \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}4) \\ 2 \cot \frac{\pi}{n} & \text{if } n \equiv 2(\text{mod}4) \\ \csc \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (3.8)$$

Next, we calculate the iota energy formulas for a negative directed cycle C_n^- .

Case:1 When $n \equiv 0(\text{mod} 2)$. Then (3.7) yields

$$\begin{aligned} E_c(C_n^-) &= \sum_{k=0}^{n-1} \left| \sin \frac{(2k+1)\pi}{n} \right| \\ &= 2 \sum_{k=0}^{\frac{n}{2}-1} \left| \sin \frac{(2k+1)\pi}{n} \right| \\ &= 2 \frac{(\sin(\frac{n}{2} - 1 + 1) \frac{\pi}{n})^2}{\sin \frac{\pi}{n}} \\ &= 2 \frac{(\sin \frac{\pi}{2})^2}{\sin \frac{\pi}{n}} = 2 \csc \frac{\pi}{n}. \end{aligned}$$

Case 2: When $n \equiv 1(\text{mod} 2)$. Then from (3.7), we get

$$\begin{aligned} E_c(C_n^-) &= \sum_{k=0}^{n-1} \left| \sin \frac{(2k+1)\pi}{n} \right| \\ &= \sum_{k=1}^{\frac{n}{2}-1} \left| \sin \frac{k\pi}{n} \right| = \frac{\sin \frac{n\pi}{2n} \sin(n-1) \frac{\pi}{2n}}{\sin \frac{\pi}{2n}} \\ &= \frac{\sin(\frac{\pi}{2} - \frac{\pi}{2n})}{\sin \frac{\pi}{2n}} = \cot \frac{\pi}{2n}. \end{aligned}$$

In brief, we can write:

$$E_c(C_n^-) = \begin{cases} 2 \csc \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}2) \\ \cot \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (3.9)$$

If S is a unicyclic sidigraph on n vertices having a unique directed cycle C_m of length m ($2 \leq m \leq n$) then Theorem 2.8 gives

$$\begin{aligned} \phi_S(x) &= x^n + (-1)^s x^{n-m} \\ &= x^{n-m}(x^m + (-1)^s) \\ &= x^{n-m} \phi_{C_m}(x). \end{aligned}$$

Thus the iota energy of S is given by

$$E_c(S) = E_c(C_m). \quad (3.10)$$

The following theorem gives relationship between energy of positive directed cycle and negative directed cycles.

Theorem 3.6. *Iota energy of positive and negative directed cycles satisfy the following:*

- (1) $E_c(C_n^+) = E_c(C_n^-)$ if and only if $n \equiv 1(\text{mod} 2)$,
- (2) $E_c(C_n^+) < E_c(C_n^-)$ if and only if $n \equiv 0(\text{mod} 2)$.

Proof. Proof follows from (3.5) and (3.9). □

Next theorem compares the energy and iota energy of negative directed cycles.

Theorem 3.7. *Let $n \geq 2$, then energy and iota energy of a negative directed cycle C_n^- satisfy the following:*

- (1) $E(C_n^-) = E_c(C_n^-)$ if and only if $n \equiv 0(\text{mod} 4)$,
- (2) $E(C_n^-) < E_c(C_n^-)$ if and only if $n \equiv 2(\text{mod} 4)$,
- (3) $E(C_n^-) > E_c(C_n^-)$ if and only if $n \equiv 1(\text{mod} 2)$.

Proof. Proof follows from (3.8) and (3.9). □

Combining (3.10) and Theorem 3.7, we get the following corollary.

Corollary 3.8. *For a unicyclic sidigraph S on n vertices containing a unique negative directed cycle C_r^- , where $2 \leq r \leq n$, the following hold:*

- (1) $E(S) = E_c(S)$ if and only if $r \equiv 0 \pmod{4}$,
- (2) $E(S) < E_c(S)$ if and only if $r \equiv 2 \pmod{4}$,
- (3) $E(S) > E_c(S)$ if and only if $r \equiv 1 \pmod{2}$.

In the following lemma, we show that the iota energy of C_n^- is twice the energy of $C_{\frac{n}{2}}^-$ when $n \equiv 2 \pmod{4}$.

Lemma 3.9. *Let n be an even integer. Then $E_c(C_n^-) = 2E(C_{\frac{n}{2}}^-)$ if and only if $n \equiv 2 \pmod{4}$.*

Proof. Suppose that $E_c(C_n^-) = 2E(C_{\frac{n}{2}}^-)$. On contrary, assume that $n \not\equiv 2 \pmod{4}$, that is, $n \equiv 0 \pmod{4}$. Then there are two cases: either $\frac{n}{2} \equiv 0 \pmod{4}$ or $\frac{n}{2} \equiv 2 \pmod{4}$.

Case 1: If $\frac{n}{2} \equiv 0 \pmod{4}$ then from (3.8) and (3.9) we get

$$\begin{aligned} E_c(C_n^-) &= 2 \csc \frac{\pi}{n}, \\ E(C_{\frac{n}{2}}^-) &= 2 \csc \frac{2\pi}{n}. \end{aligned}$$

From the above two equations together with the equation $E_c(C_n^-) = 2E(C_{\frac{n}{2}}^-)$, we obtain

$$2 \csc \frac{\pi}{n} = 4 \csc \frac{2\pi}{n}. \tag{3.11}$$

Simplifying the above equation, we get

$$\sin \frac{\pi}{n} \left(\cos \frac{\pi}{n} - 1 \right) = 0.$$

If $\sin \frac{\pi}{n} = 0$ then $\frac{\pi}{n} = m\pi$, where m is an integer. This implies that $mn = 1$, which is a contradiction. If $\cos \frac{\pi}{n} = 1$ then $\frac{\pi}{n} = 2m\pi$, where m is an integer. This gives $2mn = 1$,

which is again not possible.

Case 2: If $\frac{n}{2} \equiv 2 \pmod{4}$ then from (3.8) and (3.9) we get

$$\begin{aligned} E_c(C_n^-) &= 2 \csc \frac{\pi}{n}, \\ E(C_{\frac{n}{2}}^-) &= 2 \cot \frac{2\pi}{n}. \end{aligned}$$

The above two equations together with the equation $E_c(C_n^-) = 2E(C_{\frac{n}{2}}^-)$ imply

$$2 \csc \frac{\pi}{n} = 4 \cot \frac{2\pi}{n},$$

that is,

$$\cos \frac{\pi}{n} = \cos \frac{2\pi}{n}.$$

This is not possible. Thus Case 1 and Case 2 imply that $n \equiv 2 \pmod{4}$.

Conversely, suppose that $n \equiv 2 \pmod{4}$. Then $\frac{n}{2} \equiv 1 \pmod{2}$. By (3.8) and (3.9), we have

$$\begin{aligned} E_c(C_n^-) &= 2 \csc \frac{\pi}{n}, \\ E(C_{\frac{n}{2}}^-) &= \csc \frac{\pi}{n}. \end{aligned}$$

From the above two equations, we obtain

$$E_c(C_n^-) = 2E(C_{\frac{n}{2}}^-).$$

This completes the proof. □

Theorem 3.10. *Let S_1 be an n -vertex sidigraph with k vertex disjoint negative directed cycles $C_{r_1}^-, \dots, C_{r_k}^-$ of lengths r_1, \dots, r_k , respectively, where $r_j \equiv 2 \pmod{4}$, $j = 1, 2, \dots, k$*

Take another n -vertex sidigraph S_2 with $2k$ vertex disjoint negative directed cycles $C_{\frac{r_1}{2}}^-, C_{\frac{r_1}{2}}^-, \dots, C_{\frac{r_k}{2}}^-, C_{\frac{r_k}{2}}^-$ of lengths $\frac{r_1}{2}, \frac{r_1}{2}, \frac{r_2}{2}, \frac{r_2}{2}, \dots, \frac{r_k}{2}, \frac{r_k}{2}$. Then S_1 and S_2 satisfy the following:

$$E_c(S_1) = E(S_2).$$

Proof. By Theorem 3.5, we have

$$E_c(S_1) = \sum_{i=1}^k E_c(C_{r_i}^-)$$

Applying Lemma 3.9, we get

$$\begin{aligned} \sum_{i=1}^k E_c(C_{r_i}^-) &= 2 \sum_{i=1}^k E(C_{\frac{r_i}{2}}) \\ &= E(S_2) \end{aligned}$$

Thus, we have

$$E_c(S_1) = E(S_2)$$

This completes the proof. □

The next two lemmas will be helpful to prove a few results.

Lemma 3.11 (Farooq et al. [5]). *For $z \in (0, \frac{\pi}{2}]$, the following inequality holds:*

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

Lemma 3.12 (Khan et al. [13]). *Let z, p be real numbers such that $z \geq p > 0$ and $q > 0$.*

Then

$$\frac{2z\pi}{bz^2 - \pi^2} \leq \frac{2p\pi}{qp^2 - \pi^2}.$$

For any real number z with $z \in (0, \frac{\pi}{2})$, we have the following inequality:

$$z - \frac{z^3}{3!} \leq \sin z \leq z. \tag{3.12}$$

Next theorem gives smallest and largest iota energies of unicyclic sidigraphs with negative directed cycle.

Theorem 3.13. *Among n -vertex unicyclic sidigraphs with negative directed cycle, the sidigraph containing C_3^- has smallest iota energy. Moreover, among all non cycle balanced sidigraphs on n vertices, C_n^- has the largest iota energy.*

Proof. We first show that the iota energy of negative directed cycles increases monotonically with respect to their length, where the length is greater than 2. Let $r \geq 3$ be an integer then we have following two cases:

Case 1: Let $r \equiv 0 \pmod{2}$. Then by using (3.9) and (3.12), we get

$$\begin{aligned} E_c(C_r^-) &= 2 \csc \frac{\pi}{r} \leq \frac{2}{\frac{\pi}{r} \left(1 - \frac{\pi^2}{6r^2}\right)} \\ &= \frac{2r}{\pi} + \frac{2r\pi}{6r^2 - \pi^2}. \end{aligned}$$

Applying Lemma 3.12, we get

$$E_c(C_r^-) \leq \frac{2r}{\pi} + 0.2918. \quad (3.13)$$

On the other hand, by using (3.9) and Lemma 3.11, we obtain

$$\begin{aligned} E_c(C_{r+1}^-) &= \cot \frac{\pi}{2(r+1)} \\ &\geq \frac{2(r+1)}{\pi} - 0.429 \frac{\pi}{2(r+1)}. \end{aligned}$$

As $r \geq 3$, we get

$$E_c(C_{r+1}^-) > \frac{2r}{\pi} + 0.412. \quad (3.14)$$

Inequalities (3.13) and (3.14) give $E_c(C_r^-) < E_c(C_{r+1}^-)$.

Case 2: Let $r \equiv 1 \pmod{2}$. Then by using (3.9) and Lemma 3.11, we get

$$E_c(C_r^-) = \cot \frac{\pi}{2r} \leq \frac{2r}{\pi} - \frac{\pi}{6r} < \frac{2r}{\pi}. \quad (3.15)$$

On the other hand, by using (3.12), we obtain

$$E_c(C_{r+1}^-) = 2 \csc \frac{\pi}{r+1} \geq \frac{2r}{\pi} + \frac{2}{\pi} > \frac{2r}{\pi}. \quad (3.16)$$

Inequalities (3.15) and (3.16) imply that $E_c(C_r^-) < E_c(C_{r+1}^-)$.

Thus, we observed a monotonic increase in the iota energy of negative directed cycles with respect to their length when length is greater than 2. Therefore, C_n^- has the largest iota energy.

From (3.9), it is clear that $E_c(C_2^-) = 2$ and $E_c(C_3^-) = \sqrt{3}$. Let S be an n -vertex unicyclic sidigraph which contains a negative directed cycle C_3^- . Then by (3.10), $E_c(S) = E_c(C_3^-) = \sqrt{3}$, which is the smallest iota energy among unicyclic sidigraphs of order $n \geq 2$ which contain a negative directed cycle. \square

Next theorem gives extremal iota energy of unicyclic sidigraphs.

Theorem 3.14. *Among the class of n -vertex unicyclic sidigraphs, C_2^+ has the smallest iota energy while C_n^- has the largest iota energy.*

Proof. We see that $E_c(C_2^+) = 0$ and $E_c(C_3^-) = \sqrt{3}$. Also, Theorem 3.6 implies that C_n^- has the largest iota energy among the class of n -vertex unicyclic sidigraphs. Thus, the assertion follows from Theorem 2.7 and Theorem 3.13. \square

3.2 Iota energy of sidigraphs with complex adjacency matrix

Khan et al. [12] introduced the notion of complex adjacency matrix $A_c(D) = [a_{jk}]$ for a digraph $D = (\mathcal{V}, \mathcal{A})$ as follows:

$$a_{jk} = \begin{cases} -i & \text{if } v_j v_k \in \mathcal{A} \\ 0 & \text{otherwise.} \end{cases}$$

In this section, we define the complex adjacency matrix for sidigraphs. Let $S = (D, \omega)$ be a sidigraph, where $D = (\mathcal{V}, \mathcal{A})$ is known as the underlying digraph and $\omega : \mathcal{A} \rightarrow \{-1, 1\}$ is called the signing function. We define the complex adjacency matrix $A_c(S) = [s_{jk}]$ of S by:

$$s_{jk} = \begin{cases} i\omega(v_j v_k) & \text{if } v_j v_k \in \mathcal{A} \\ 0 & \text{otherwise.} \end{cases} \quad (3.17)$$

We will use the notation A_c for the complex adjacency matrix throughout this paper. A_c -eigenvalues are the eigenvalues calculated from the complex adjacency matrix A_c of

S . The A_c -spectrum of S , denoted by $\text{Spec}_c(S)$, is the set containing A_c -eigenvalues of S together with their multiplicities. According to (1.1), the adjacency matrix of S is represented by A . Since $A_c = iA$, it follows that $\text{Spec}_c(S) = i\text{Spec}(S)$. It can be observed that for every eigenvalue $z = x + iy$ of S , there exists an A_c -eigenvalue $iz = -y + ix$ of S . That is, $|\text{Im}(z)| = |\text{Re}(iz)|$. Let A_c -eigenvalues of the sidigraph S be z_1, \dots, z_n . Then, the iota energy of the sidigraph S can also be defined as:

$$E_c(S) = \sum_{k=1}^n |\text{Re}(z_k)|,$$

where $\text{Re}(z_k)$ is the real part of the A_c -eigenvalue z_k .

The coefficient theorem for sidigraphs in case of complex adjacency is given in the following theorem.

Theorem 3.15. *Let \mathcal{L}_k be the set of all k -vertex linear subdigraphs of an n -vertex sidigraph S . The number of components of a subdigraph L of S is denoted by $\text{comp}(L)$. Moreover, $c(L)$ and $s(Z)$ represent the set of all cycles of L and the sign of cycle Z , respectively. Then the characteristic polynomial of S according to complex adjacency matrix $A_c(S)$ is given by*

$$\phi_S^c(x) = x^n + \sum_{k=1}^n c_k(i)^k x^{n-k},$$

where

$$c_k = \sum_{L \in \mathcal{L}_k} (-1)^{\text{comp}(L)} \prod_{Z \in c(L)} s(Z)$$

for all $k = 1, 2, \dots, n$.

In [12, 18] the authors gave a scheme to find the energy and iota energy of the corresponding adjacency matrices without finding their eigenvalues. Therefore, it is natural to study it for iota energy of the sidigraphs. We restate Theorem 2.4 in terms of sidigraphs as follows.

Theorem 3.16. Let S be an n -vertex sidigraph having characteristic polynomial $\phi_S^c(x)$ of its complex adjacency matrix $A_c(S)$. Let z_1, \dots, z_n be the A_c -eigenvalues of S . Then

$$E_c(S) = \sum_{k=1}^n |\operatorname{Re}(z_k)| = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \left(n - \frac{ix\phi_S^c(ix)}{\phi_S^c(ix)} \right) dx,$$

where $\operatorname{Re}(z_k)$ is the real part of z_k .

An immediate outcome of Theorem 3.16 is given in following corollary.

Corollary 3.17. Let ϕ be a monic polynomial of degree n . Let $z_k, k = 1, 2, \dots, n$, be its roots, and let $\gamma(t) = t^n \phi(\frac{i}{t})$. Then

$$\sum_{k=1}^n |\operatorname{Re}(z_k)| = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \log |\gamma(t)| \frac{dt}{t^2},$$

where $\operatorname{Re}(z_k)$ is the real part of z_k .

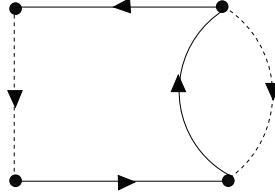


Figure 3.3: A sidigraph

Example 3.18. Consider the sidigraph S in Fig. 3.3. Then the characteristic polynomial,

$\phi_S^c(x) = x^4 - x^2 + 1$. Note that

$$\begin{aligned} \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \left(4 - \frac{ix\phi_S^c(ix)}{\phi_S^c(ix)} \right) dx &= \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \left(4 - \frac{ix(4(ix)^3 - 2(ix))}{(ix)^4 - (ix)^2 + 1} \right) \\ &= \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \left(\frac{2x^2 + 4}{x^4 + x^2 + 1} \right) dx \\ &= \frac{1}{\pi} \text{p.v.} \left(\int_{-\infty}^{\infty} \left(\frac{x+2}{x^2+x+1} \right) dx + \int_{-\infty}^{\infty} \left(\frac{-x+2}{x^2-x+1} \right) dx \right) \\ &= \frac{1}{\pi} \lim_{a \rightarrow \infty} \left(\frac{1}{2} \ln \frac{x^2+x+1}{x^2-x+1} + \sqrt{3} \left(\tan^{-1} \frac{2x+1}{\sqrt{3}} - \tan^{-1} \frac{2x-1}{\sqrt{3}} \right) \right). \end{aligned}$$

Thus, by Theorem 3.16, we obtain

$$E_c(S) = 2\sqrt{3}.$$

3.3 Increasing property of energy and iota energy of sidigraphs

Recall that $S_{n,h}$ is the set of sidigraphs of order n such that each sidigraph in $S_{n,h}$ has signed directed cycles of length h . In this section, we study the increasing property of energy and iota energy of sidigraphs in $S_{n,h}$. The following example shows that the increasing property of energy (respectively, iota energy) over the set $S_{n,h}^1$ may not hold when $h \equiv 0 \pmod{4}$.

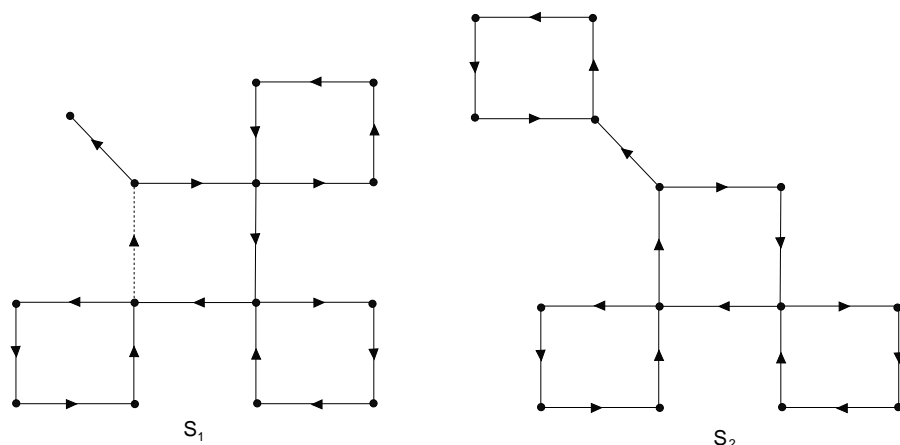


Figure 3.4: $S_1, S_2 \in S_{14,4}^1$

Example 3.19. Consider the sidigraphs $S_1, S_2 \in S_{14,4}^1$ in Fig. 3.4. Negative arcs are represented by dotted lines and positive arcs are represented by solid lines. Using Theorem

2.14, the characteristic polynomials of S_1 and S_2 are:

$$\phi_{S_1}(x) = x^{14} - 4x^{10} + 3x^6 - x^2,$$

$$\phi_{S_2}(x) = x^{14} - 4x^{10} + 4x^6 - x^2.$$

One can easily see that $c^*(S_1, kh) \leq c^*(S_2, kh)$, $k = 1, 2, 3$. Also, $E(S_1) = E_c(S_1) = 7.05$ and $E(S_2) = E_c(S_2) = 6.1163$. This proves that the energy (respectively, iota energy) may not increase with respect to the quasi-order relation defined over the set $S_{n,h}^1$ when $h \equiv 0(\text{mod } 4)$.

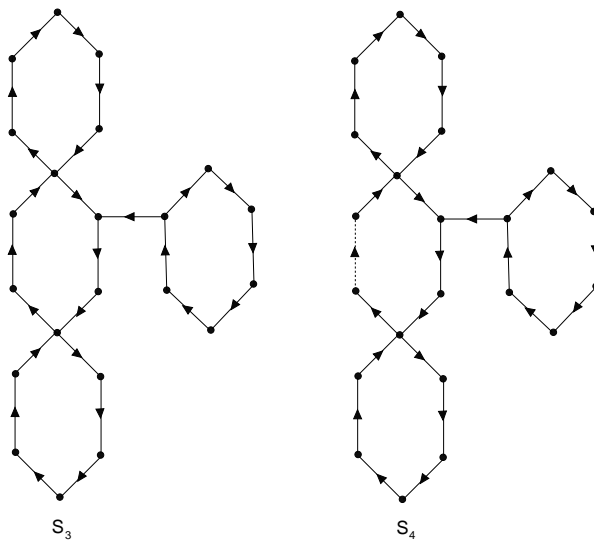


Figure 3.5: $S_3, S_4 \in S_{22,6}^1$

Example 3.20. Consider the sidigraphs S_3 and S_4 in Fig. 3.5, where $h \equiv 2(\text{mod } 4)$. The characteristic polynomials of S_3 and S_4 according to Theorem 2.14 are

$$\phi_{S_3}(x) = x^{22} - 4x^{16} + 4x^{10} - x^4,$$

$$\phi_{S_4}(x) = x^{22} - 2x^{16} + 2x^{10} - x^4.$$

Here $c^*(S_3, kh) \geq c^*(S_4, kh)$, $k = 1, 2, 3$. However, $E_c(S_3) = 10.4816$ and $E_c(S_4) = 11.8785$. Clearly $E_c(S_3) \leq E_c(S_4)$. Thus the iota energy may not increase with respect to the quasi-order relation over the set $S_{n,h}^1$ when $h \equiv 2(\text{mod } 4)$.

The following example shows that iota energy does not increase when $h \equiv 1 \pmod{2}$.

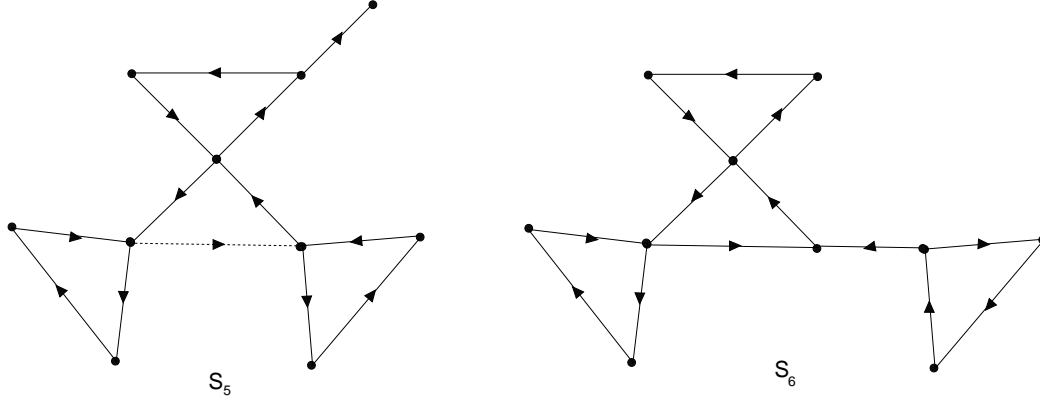


Figure 3.6: $S_5, S_6 \in S_{10,3}^1$

Example 3.21. Consider sidigraphs S_5 and S_6 shown in Fig. 3.6. According to Theorem 2.14, following are the characteristic polynomials of S_5 and S_6 .

$$\phi_{S_5}(x) = x^{10} - 2x^7 + 3x^4 - x,$$

$$\phi_{S_6}(x) = x^{10} - 4x^7 + 4x^4 - x.$$

Observe that $c^*(S_5, kh) \leq c^*(S_6, kh)$ but $E_c(S_5) = 5.8367$ and $E_c(S_6) = 5.3759$, that is, $E_c(S_5) > E_c(S_6)$.

Next, we define a new family $S_{n,h}^2$ of sidigraphs such that each sidigraph in $S_{n,h}^2$ has negative cycle of length h . Clearly, $S_{n,h}^2 \subset S_{n,h}$. The following theorem gives the characteristic polynomial for the sidigraphs in $S_{n,h}^2$.

Theorem 3.22. *Let $S \in S_{n,h}^2$. Then the characteristic polynomial of S according to the adjacency matrix $A(S)$ is given by*

$$\phi_S(x) = x^n + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} c(S, kh)x^{n-kh}, \quad (3.18)$$

where $c(S, kh) \geq 0$ for every $k = 1, \dots, \lfloor \frac{n}{h} \rfloor$.

Proof. Let S be a sidigraph of order n . Then using Theorem 2.8, $\phi_S(x) = x^n + \sum_{k=1}^n c_k x^{n-kh}$, where $c_k = \sum_{L \in \mathcal{L}_k} (-1)^{\text{comp}(L)} \prod_{Z \in c(L)} s(Z)$. Since the length of each cycle of S is h , it follows that $L \in \mathcal{L}_k$ if and only if k is a multiple of h . As each cycle of $S_{n,h}^2$ is negative so $c_{kh} = c(S, kh)$, where $c(S, kh)$ denotes the number of linear subsidigraphs of S containing k cycles of length h . This completes the proof. \square

A quasi-order relation over $S_{n,h}^2$ is defined as: Let S_1 and S_2 be two elements of $S_{n,h}^2$. Then $S_1 \preceq S_2$ if for all $k = 0, 1, \dots, \lfloor \frac{n}{h} \rfloor$, $c(S_1, kh) \leq c(S_2, kh)$. If $S_1 \preceq S_2$ and there exists k such that $c(S_1, kh) < c(S_2, kh)$ then $S_1 \prec S_2$. This relation \preceq is reflexive and transitive over $S_{n,h}^2$. The analogue of Theorem 3.22 is as follows:

Theorem 3.23. *Let $S \in S_{n,h}^2$. Then the characteristic polynomial of S according to the complex adjacency matrix $A_c(S)$ is defined by*

$$\phi_S^c(x) = x^n + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} i^{kh} c(S, kh) x^{n-kh}, \quad (3.19)$$

where $c(S, kh)$ is the number of linear subsidigraphs of order kh .

In the following theorem, we discuss the increasing property of the iota energy of sidigraphs with respect to the quasi-order relation \preceq defined over $S_{n,h}^2$ when $h \equiv 0 \pmod{2}$.

Theorem 3.24. *The iota energy increases over $S_{n,h}^2$ with respect to the quasi-order relation when $h \equiv 0 \pmod{2}$, that is, if $S_1 \preceq S_2$ then $E_c(S_1) \leq E_c(S_2)$ where $S_1, S_2 \in S_{n,h}^2$.*

Proof. Let $S \in S_{n,h}^2$. Then by Theorem 3.23 the characteristic polynomial of S is given by:

$$\phi_S^c(x) = x^n + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} i^{kh} c(S, kh) x^{n-kh}. \quad (3.20)$$

This gives

$$\begin{aligned}
\phi_S^c\left(\frac{i}{x}\right) &= \left(\frac{i}{x}\right)^n + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} (i)^{kh} c(S, kh) \left(\frac{i}{x}\right)^{n-kh} \\
&= \frac{i^n}{x^n} \left(1 + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} c(S, kh) x^{kh}\right) \\
&= \frac{i^n}{x^n} \left(1 + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} c(S, kh) x^{kh}\right).
\end{aligned}$$

By using Corollary 3.17, we get

$$\begin{aligned}
E_c(S) &= \frac{1}{\pi} p.v \int_{-\infty}^{\infty} \frac{1}{x^2} \log \left| x^n \frac{i^n}{x^n} \left(1 + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} c(S, kh) x^{kh}\right) \right| dx \\
&= \frac{1}{\pi} p.v \int_{-\infty}^{\infty} \frac{1}{x^2} \log \left(\left(1 + \sum_{k=1}^{\lfloor \frac{n}{h} \rfloor} c(S, kh) x^{kh}\right) \right) dx.
\end{aligned}$$

The last equality is obtained by using $\frac{1}{\pi} p.v. \int_{-\infty}^{\infty} \log(i^n) \frac{dx}{x^2} = 0$. It is easy from the above iota energy expression that iota energy increases with respect to quasi-order relation \preceq over $S_{n,h}^2$. \square

In the following example it is shown that the assertion of Theorem 3.24 does not hold when $h \equiv 1 \pmod{2}$.

Example 3.25. Consider sidigraphs $S_7, S_8 \in S_{22,6}^2$ shown in Fig. 3.7. By Theorem 3.23 the characteristic polynomials of S_7 and S_8 are

$$\begin{aligned}
\phi_{S_7}(x) &= x^{10} + 4x^7 + 3x^4 + x, \\
\phi_{S_8}(x) &= x^{10} + 4x^7 + 4x^4 + x.
\end{aligned}$$

Here $c(S_7, kh) \leq c(S_8, kh)$ and the iota energy of S_7 and S_8 are $E_c(S_7) = 10.9816$ and $E_c(S_8) = 5.3759$. It can easily be seen that $E_c(S_7) > E_c(S_8)$. Thus, the iota energy does not possess increasing property with respect to the quasi-order relation defined over $S_{n,h}^2$ when $h \equiv 1 \pmod{2}$.

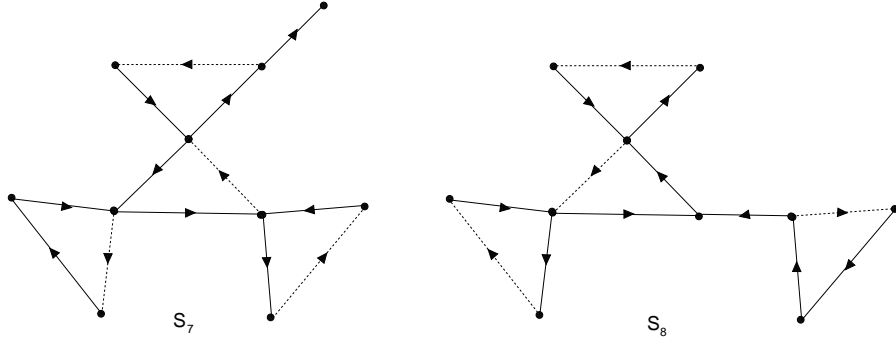


Figure 3.7: $S_7, S_8 \in S_{10,3}^2$

3.4 Upper bounds for the iota energy of sidigraphs

Let S be a sidigraph of order n with adjacency matrix A . Then it is shown in [21] that power of $A(S)$ counts the number of walks in signed manner. An alternating sequence of vertices and signed edges is called a signed walk. If the sign of the edges is removed and a direction is assigned to each edge then the resulting walk is called a directed walk. Recall that the number of m -length positive directed closed walks are denoted by c_m^+ and the number of m -length negative directed closed walks are denoted by c_m^- .

Next theorem is analogue of Theorem 2.19. We give upper bound of iota energy of sidigraphs in this theorem. The proofs of both theorems are almost similar. However, for the sake of self-containment, we include it.

Theorem 3.26. *Let S be a sidigraph having n vertices and $a = a^+ + a^-$ arcs and let z_1, \dots, z_n be its eigenvalues. Then*

$$E_c(S) \leq \sqrt{\frac{1}{2}n(a - c_2^+ + c_2^-)}.$$

and equality holds if $S = \frac{n}{2}C_2^-$, n is even or S is any symmetric sidigraph of order n .

Proof. Adding part (1) and (2) of the Lemma 2.18, we get

$$\sum_{j=1}^n (\operatorname{Re}(z_j))^2 \leq \frac{1}{2}(a + c_2^+ - c_2^-). \quad (3.21)$$

Also from part (1) of Lemma 2.18, we obtain

$$\sum_{j=1}^n (\operatorname{Im}(z_j))^2 = \sum_{j=1}^n (\operatorname{Re}(z_j))^2 - c_2^+ + c_2^-. \quad (3.22)$$

Using cauchy-schwarz inequality we get

$$\begin{aligned} E_c(S) &= \sum_{j=1}^n |\operatorname{Im}(z_j)| \\ &\leq \sqrt{n} \sqrt{\sum_{j=1}^n |\operatorname{Im}(z_j)|^2}. \end{aligned}$$

Using (3.21) and (3.22), we get

$$\begin{aligned} E_c(S) &= \sqrt{n} \sqrt{\sum_{j=1}^n (\operatorname{Re}(z_j))^2 - c_2^+ + c_2^-} \\ &\leq \sqrt{n} \sqrt{\frac{1}{2}(a + c_2^+ - c_2^-) - c_2^+ + c_2^-} \\ &= \sqrt{n} \sqrt{\frac{1}{2}(a) - \frac{1}{2}(c_2^+) + \frac{1}{2}(c_2^-)} \\ &\leq \sqrt{\frac{1}{2}n(a - c_2^+ + c_2^-)}. \end{aligned}$$

The proof is complete. \square

Using Theorem 2.10, we see that a symmetric digraph on two vertices is the positive directed cycle of length 2. We extend Theorem 2.20 for iota energy.

Theorem 3.27. *Let a sidigraph S has a arcs then $E_c(S) \leq a$ with equality if and only if $S = \frac{a}{2}C_2^-$ plus some isolated vertices.*

Proof. Proof is analogue to the proof of Theorem 2.20. \square

3.5 Equienergetic sidigraphs

Two positive (respectively, negative) sidigraphs are said to be isomorphic if their underlying digraphs are isomorphic. Two sidigraphs having same A_c -spectrum are called

A_c -cospectral, otherwise non A_c -cospectral. Any two sidigraphs which have same order and iota energy are called equienergetic sidigraphs. Obviously, two A_c -cospectral sidigraphs having same order are always equienergetic. In this section, we are interested to construct some families of equienergetic A_c -noncospectral sidigraphs. We extend theorem 2.21 for iota energy. It gives a sidigraph whose iota energy is equal to the number of its vertices.

Theorem 3.28. *Let S be a sidigraph of order n having eigenvalues z_1, \dots, z_n such that $|\operatorname{Im}(z_j)| \leq 1$ for every $j = 1, 2, \dots, n$. Then*

$$E_c(S \times C_2^-) = 2n.$$

Proof. Let z_1, \dots, z_m be eigenvalues with non-negative imaginary parts and z_{m+1}, \dots, z_n be those with negative imaginary parts, where $1 \leq m \leq n$. Eigenvalues of the cartesian product of $S \times C_2^-$ are $z_1 \pm i, z_2 \pm i, \dots, z_m \pm i, z_{m+1} \pm i, \dots, z_n \pm i$. Therefore

$$E_c(S \times C_2^-) = \sum_{j=1}^m (|\operatorname{Im}(z_j) + 1| + |\operatorname{Im}(z_j) - 1|) + \sum_{j=m+1}^n (|\operatorname{Im}(z_j) + 1| + |\operatorname{Im}(z_j) - 1|)$$

As $|\operatorname{Im}(z_j)| \leq 1$ for all $j = 1, 2, \dots, n$, it follows that

$$\begin{aligned} E_c(S \times C_2^-) &= \sum_{j=1}^m (\operatorname{Im}(z_j) + 1 + 1 - \operatorname{Im}(z_j)) + \sum_{j=m+1}^n (1 - \operatorname{Im}(z_j) + \operatorname{Im}(z_j) + 1) \\ &= \sum_{j=1}^m 2 + \sum_{j=m+1}^n 2 \\ &= 2m + 2(n - m) = 2n. \end{aligned}$$

This completes the proof. □

We can easily see that eigenvalues of C_n^+ and C_n^- meet the requirement of Theorem 3.28. Moreover $1 + i \in \operatorname{Spec}(C_n^+ \times C_2^-)$ but $1 + i \notin \operatorname{Spec}(C_n^- \times C_2^-)$. Thus we have the following corollary.

Corollary 3.29. *For $n \geq 2$, we have*

$$E_c(C_n^- \times C_2^-) = E_c(C_n^+ \times C_2^-)$$

Moreover, $C_n^- \times C_2^-$ and $C_n^+ \times C_2^-$ are A_c -noncospectral sidigraphs.

Theorem 3.30. *Let S be a sidigraph of order n having eigenvalues z_1, \dots, z_n such that $|\operatorname{Im}(z_k)| \leq 1$ for every $k = 1, \dots, n$ then*

$$E_c(S \times C_2^+) = 2E_c(S).$$

Proof. Proof is parallel to the proof of Theorem 3.28. □

We note that $\operatorname{Spec}(C_n^-) = -\operatorname{Spec}(C_n^+)$ and $1 \notin \operatorname{Spec}(C_n^-)$ but $1 \in \operatorname{Spec}(C_n^+)$, when $n \equiv 1 \pmod{2}$. Thus we have the following corollary of Theorem 3.30.

Corollary 3.31. *If $n \equiv 1 \pmod{2}$ then $C_n^- \times C_2^+$ and $C_n^+ \times C_2^+$ are A_c -noncospectral equienergetic sidigraphs.*

Chapter 4

Extremal iota energy of bicyclic signed digraphs

Extremal energy and iota energy of unicyclic signed digraphs is known. In this chapter, we find sidigraphs with extremal iota energy among vertex disjoint bicyclic signed digraphs of fixed order.

4.1 Iota energy of bicyclic signed digraphs

The following lemma will be helpful in proving a few results.

Lemma 4.1 (Khan et al. [13]). *Suppose z, p, q are real numbers such that $z \geq p > 0$ and $q > 0$. Then*

$$\frac{2z\pi}{qz^2 - \pi^2} \leq \frac{2p\pi}{qp^2 - \pi^2}.$$

For any real number z the following inequalities are satisfied for $0 < z < \frac{\pi}{2}$ such that $z \in \mathcal{R}$, where \mathcal{R} is the set of real numbers.

$$\sin z \leq z, \quad \sin z \geq z - \frac{z^3}{3!}, \quad \cos z \geq 1 - \frac{z^2}{2} \tag{4.1}$$

$$\cot z \leq \frac{1}{z}, \quad \cot z \geq \frac{1}{z} - 0.429z. \tag{4.2}$$

In the following lemma, we give lower bounds for the sum of iota energies of two vertex disjoint directed cycles C_{k-2}^- and C_2^- , where $k \geq 8$.

Lemma 4.2. *If $k \geq 8$ then we have the following:*

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq \begin{cases} \frac{2k}{\pi} - \frac{4}{\pi} + 2 & \text{if } k \equiv 0(\text{mod}2) \\ \frac{2k}{\pi} - \frac{4}{\pi} + 2 - \frac{0.429\pi}{2(k-2)} & \text{if } k \equiv 1(\text{mod}2). \end{cases} \quad (4.3)$$

Proof. We know that $E(C_2^-) = 2$. If $k \equiv 0(\text{mod}2)$ then using (3.9) and (4.1), we find:

$$\begin{aligned} E_c(C_{k-2}^-) + E_c(C_2^-) &= 2 \csc \frac{\pi}{k-2} + 2 \\ &\geq 2 \left(\frac{1}{\frac{\pi}{k-2}} + 1 \right) \\ &= \frac{2k}{\pi} - \frac{4}{\pi} + 2. \end{aligned}$$

Next, if $k \equiv 1(\text{mod}2)$ then (3.9) and (4.2) imply that:

$$\begin{aligned} E_c(C_{k-2}^-) + E_c(C_2^-) &= \cot \frac{\pi}{2(k-2)} + 2 \\ &\geq \frac{1}{\frac{\pi}{2(k-2)}} - \frac{0.429\pi}{2(k-2)} + 2 \\ &= \frac{2k}{\pi} - \frac{4}{\pi} + 2 - \frac{0.429\pi}{2(k-2)}. \end{aligned}$$

This completes the proof. □

Next two lemmas give different upper bounds for the sum of iota energies of vertex disjoint directed cycles.

Lemma 4.3. *If $k \equiv 0(\text{mod} 2)$ and $l, k-l \geq 2$ then we have the following:*

(1)

$$E_c(C_{k-l}^+) + E_c(C_l^+) \leq \begin{cases} \frac{2k}{\pi} & \text{if } l \equiv 0(\text{mod}2) \\ \frac{2k}{\pi} & \text{if } l \equiv 1(\text{mod}2). \end{cases}$$

(2)

$$E_c(C_{k-l}^+) + E_c(C_l^-) \leq \begin{cases} \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} & \text{if } l \equiv 0(\text{mod}2) \\ \frac{2k}{\pi} & \text{if } l \equiv 1(\text{mod}2). \end{cases}$$

(3)

$$E_c(C_{k-l}^-) + E_c(C_l^+) \leq \begin{cases} \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

(4)

$$E_c(C_{k-l}^-) + E_c(C_l^-) \leq \begin{cases} \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

Proof. (1) Let $l \equiv 0 \pmod{2}$. Then $k-l \equiv 0 \pmod{2}$. By using (3.5) and (4.2) we get:

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^+) &= 2 \cot \frac{\pi}{k-l} + \cot \frac{\pi}{l} \\ &\leq 2 \frac{1}{\frac{\pi}{k-l}} + 2 \frac{1}{\frac{\pi}{l}} \\ &= \frac{2k}{\pi}. \end{aligned}$$

Next, if $l \equiv 1 \pmod{2}$ then $k-l \equiv 1 \pmod{2}$. Using (3.5) and (4.2), we find that:

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^+) &= \cot \frac{\pi}{2(k-l)} + \cot \frac{\pi}{2l} \\ &\leq \frac{1}{\frac{\pi}{2(k-l)}} + \frac{1}{\frac{\pi}{2l}} \\ &= \frac{2k}{\pi}. \end{aligned}$$

(2) If $l \equiv 0 \pmod{2}$ then $k-l \equiv 0 \pmod{2}$. From (3.5) and (3.9) we get:

$$E_c(C_{k-l}^+) + E_c(C_l^-) = 2 \cot \frac{\pi}{(k-l)} + 2 \csc \frac{\pi}{l}.$$

Applying (4.1) and (4.2), we obtain:

$$\begin{aligned} 2 \cot \frac{\pi}{(k-l)} + 2 \csc \frac{\pi}{l} &\leq 2 \left(\frac{1}{\frac{\pi}{k-l}} \right) + 2 \left(\frac{1}{\frac{\pi}{l} (1 - \frac{\pi^2}{6l^2})} \right) \\ &= 2 \left(\frac{k-l}{\pi} \right) + 2 \left(\frac{1}{\frac{\pi}{l} + \frac{l\pi}{6l^2 - \pi^2}} \right) \\ &= \frac{2k-2l}{\pi} + \frac{2l}{\pi} + \frac{2l\pi}{6k^2 - \pi^2} \\ &= \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2}. \end{aligned}$$

Thus

$$E_c(C_{k-l}^+) + E_c(C_l^-) \leq \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2}.$$

Next, if $l \equiv 1 \pmod{2}$ then $k - l \equiv 1 \pmod{2}$. Using (3.5), (3.9) and (4.2), we obtain:

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^-) &= \cot \frac{\pi}{2(k-l)} + \cot \frac{\pi}{2l} \\ &\leq \frac{2k}{\pi}. \end{aligned}$$

(3) If $l \equiv 0 \pmod{2}$ then $k - l \equiv 0 \pmod{2}$. From (3.5) and (3.9), we get

$$E_c(C_{k-l}^-) + E_c(C_l^+) = 2 \csc \frac{\pi}{k-l} + 2 \cot \frac{\pi}{l}.$$

Using inequalities (4.1) and (4.2), we obtain:

$$\begin{aligned} 2 \csc \frac{\pi}{k-l} + 2 \cot \frac{\pi}{l} &\leq \left(\frac{1}{\frac{\pi}{k-l} \left(1 - \frac{\pi^2}{6(k-l)^2}\right)} \right) + 2 \left(\frac{1}{\frac{\pi}{l}} \right) \\ &= 2 \left(\frac{1}{\frac{\pi}{k-l} \left(1 - \frac{\pi^2}{6(k-l)^2}\right)} \right) + \frac{2l}{\pi} \\ &= 2 \left(\frac{1}{\frac{\pi}{k-l}} + \frac{\frac{\pi}{6(k-l)}}{1 - \frac{\pi^2}{6(k-l)^2}} \right) + \frac{2l}{\pi} \\ &= \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2}. \end{aligned}$$

Thus

$$E_c(C_{k-l}^-) + E_c(C_l^+) = \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2}.$$

Next, if $l \equiv 1 \pmod{2}$ then using (3.5), (3.9) and (4.2), we have

$$\begin{aligned} E_c(C_{k-l}^-) + E_c(C_l^+) &= \cot \frac{\pi}{2(k-l)} + \cot \frac{\pi}{2l} \\ &\leq \frac{2k}{\pi}. \end{aligned}$$

(4) If $l \equiv 0 \pmod{2}$ then by using (3.9) and (4.1), we obtain

$$\begin{aligned}
E_c(C_{k-l}^-) + E_c(C_l^-) &= 2 \csc \frac{\pi}{k-l} + 2 \csc \frac{\pi}{l} \\
&\leq 2 \left(\frac{1}{\frac{\pi}{k-l} \left(1 - \frac{\pi^2}{6(k-l)^2}\right)} \right) + 2 \left(\frac{1}{\frac{\pi}{l} \left(1 - \frac{\pi^2}{6l^2}\right)} \right) \\
&= \frac{2(k-l)}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} + \frac{2l}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} \\
&= \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} + \frac{2l\pi}{6l^2 - \pi^2}.
\end{aligned}$$

If $l \equiv 1 \pmod{2}$ then (3.9) and (4.2) imply that

$$\begin{aligned}
E_c(C_{k-l}^-) + E_c(C_l^-) &= \cot \frac{\pi}{2(k-l)} + \cot \frac{\pi}{2l} \\
&\leq \frac{2k}{\pi}.
\end{aligned}$$

This gives the required result. □

Lemma 4.4. *If $k \equiv 1 \pmod{2}$ and $k, k-l \geq 2$ then we have the following:*

(1)

$$E_c(C_{k-l}^+) + E_c(C_l^+) \leq \begin{cases} \frac{2k}{\pi} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

(2)

$$E_c(C_{k-l}^+) + E_c(C_l^-) \leq \begin{cases} \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

(3)

$$E_c(C_{k-l}^-) + E_c(C_l^+) \leq \begin{cases} \frac{2k}{\pi} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

(4)

$$E_c(C_{k-l}^-) + E_c(C_l^-) \leq \begin{cases} \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} & \text{if } l \equiv 0 \pmod{2} \\ \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2} & \text{if } l \equiv 1 \pmod{2}. \end{cases}$$

Proof. **(1)** Let $l \equiv 0 \pmod{2}$. Then $k - l \equiv 1 \pmod{2}$. By using (3.5) and (4.2) we get:

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^+) &= \cot \frac{\pi}{2(k-l)} + 2 \cot \frac{\pi}{l} \\ &\leq \frac{1}{\frac{\pi}{2(k-l)}} + 2 \left(\frac{1}{l} \right) \\ &= \frac{2k}{\pi}. \end{aligned}$$

Next, if $l \equiv 1 \pmod{2}$ then $k - l \equiv 0 \pmod{2}$. By (3.5) and (4.2), we see that:

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^+) &= 2 \cot \frac{\pi}{(k-l)} + \cot \frac{\pi}{2l} \\ &\leq 2 \frac{1}{\frac{\pi}{(k-l)}} + \frac{1}{\frac{\pi}{2l}} \\ &= \frac{2k}{\pi}. \end{aligned}$$

(2) If $l \equiv 0 \pmod{2}$ then $k - l \equiv 1 \pmod{2}$. From (3.5) and (3.9) we get:

$$E_c(C_{k-l}^+) + E_c(C_l^-) = \cot \frac{\pi}{2(k-l)} + 2 \csc \frac{\pi}{l}.$$

Applying the inequalities (4.1) and (4.2), we obtain

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^-) &\leq 2 \left(\frac{1}{\frac{\pi}{2(k-l)}} \right) + 2 \left(\frac{1}{\frac{\pi}{l} \left(1 - \frac{\pi^2}{6l^2} \right)} \right) \\ &= \frac{2k - 2l}{\pi} + \frac{2l}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} \\ &= \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2}. \end{aligned}$$

Next if $l \equiv 1 \pmod{2}$ then $k - l \equiv 0 \pmod{2}$. From (3.5), (3.9) and (4.2), we get

$$\begin{aligned} E_c(C_{k-l}^+) + E_c(C_l^-) &= 2 \cot \frac{\pi}{k-l} + \cot \frac{\pi}{2l} \\ &\leq \frac{2k}{\pi} \end{aligned}$$

(3) If $l \equiv 0 \pmod{2}$ then $k - l \equiv 1 \pmod{2}$. From (3.5), (3.9) and (4.2), we obtain

$$\begin{aligned} E_c(C_{k-l}^-) + E_c(C_l^+) &= \cot \frac{\pi}{2(k-l)} + 2 \cot \frac{\pi}{l} \\ &\leq \left(\frac{1}{\frac{\pi}{2(k-l)}} \right) + 2 \left(\frac{1}{l} \right) \\ &= \frac{2k}{\pi}. \end{aligned}$$

Next if $l \equiv 1 \pmod{2}$ then (3.5) and (3.9) imply that

$$E_c(C_{k-l}^-) + E_c(C_l^+) = 2 \csc \frac{\pi}{k-l} + \cot \frac{\pi}{2l}.$$

By using inequalities (4.1) and (4.2), we find that:

$$\begin{aligned} E_c(C_{k-l}^-) + E_c(C_l^+) &\leq 2 \left(\frac{1}{\frac{\pi}{k-l} \left(1 - \frac{\pi^2}{6(k-l)^2}\right)} \right) + \frac{1}{2l} \\ &= \frac{2(k-l)}{\pi} + 2 \left(\frac{\pi(k-l)}{6(k-l)^2 - \pi^2} \right) + \frac{2l}{\pi} \\ &= \frac{2k}{\pi} + \frac{2\pi(k-l)}{6(k-l)^2 - \pi^2}. \end{aligned}$$

(4) If $l \equiv 0 \pmod{2}$ then by using (3.9), (4.1) and (4.2), we obtain

$$\begin{aligned} E_c(C_{k-l}^-) + E_c(C_l^-) &= 2 \cot \frac{\pi}{2(k-l)} + 2 \csc \frac{\pi}{l} \\ &\leq \frac{1}{\frac{\pi}{2(k-l)}} + 2 \left(\frac{1}{\frac{\pi}{l} \left(1 - \frac{\pi^2}{6l^2}\right)} \right) \\ &= \frac{2(k-l)}{\pi} + \frac{2l}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} \\ &= \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2}. \end{aligned}$$

If $l \equiv 1 \pmod{2}$ then by (3.9), (4.1) and (4.2), it holds that

$$\begin{aligned} E_c(C_{k-l}^-) + E_c(C_l^-) &= 2 \csc \frac{\pi}{k-l} + \cot \frac{\pi}{2l} \\ &\leq 2 \left(\frac{1}{\frac{\pi}{k-l} \left(1 - \frac{\pi^2}{6(k-l)^2}\right)} \right) + \frac{1}{2l} \\ &\leq \frac{2k}{\pi} + \frac{2(k-l)\pi}{6(k-l)^2 - \pi^2}. \end{aligned}$$

This completes the proof. □

Lemma 4.5. *Let $l \in \{2, 3\}$ or $k-l \in \{2, 3\}$ such that $k \geq 4$ then following inequalities hold for vertex disjoint directed cycles:*

(1) *If $k \equiv 0 \pmod{2}$ then*

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l).$$

(2) If $k \equiv 1 \pmod{2}$ then

$$E_c(C_{k-2}) + E_c(C_2^+) \geq E_c(C_{k-l}) + E_c(C_l).$$

Proof. (1). If $l \in \{2, 3\}$ then (3.5) and (3.9) imply

$$E_c(C_2^-) \geq E_c(C_l). \quad (4.4)$$

Also $k - 2 \geq k - l$. By Theorem 3.13, we obtain

$$E_c(C_{k-2}^-) \geq E_c(C_{k-l}). \quad (4.5)$$

By combining inequalities (4.4) and (4.5), we get

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l).$$

We can similarly get the above inequality if $k - l \in \{2, 3\}$. Part (2) can be proved analogously. \square

Lemma 4.6. For $l, k - l \geq 4$, the following inequalities hold for vertex disjoint cycles:

(1) If $k \equiv 0 \pmod{2}$ then

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l). \quad (4.6)$$

(2) If $k \equiv 1 \pmod{2}$ then

$$E_c(C_{k-2}) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l). \quad (4.7)$$

Proof. (1). Let $k \equiv 0 \pmod{2}$. In this case $k - 2 \geq 6$. Using Lemma 4.2 we have

$$\begin{aligned} E_c(C_{k-2}^-) + E_c(C_2^-) &\geq \frac{2k}{\pi} - \frac{4}{\pi} + 2 \\ &= \frac{2k}{\pi} + 0.72. \end{aligned} \quad (4.8)$$

On the other hand, assume that $l \equiv 0 \pmod{2}$. Then $l, k - 4 \geq 4$. Lemma 4.3 implies

$$E_c(C_{k-l}^+) + E_c(C_l^+) \leq \frac{2k}{\pi}. \quad (4.9)$$

Futhermore, applying Lemma 4.3 and Lemma 4.1, we obtain

$$\begin{aligned}
E_c(C_{k-l}^+) + E_c(C_l^-) &\leq \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} \\
&\leq \frac{2k}{\pi} + \frac{8\pi}{6(4)^2 - \pi^2} \\
&= \frac{2k}{\pi} + 0.29.
\end{aligned} \tag{4.10}$$

Similarly, we obtain

$$E_c(C_{k-l}^-) + E_c(C_l^+) \leq \frac{2k}{\pi} + 0.29, \tag{4.11}$$

$$E_c(C_{k-l}^-) + E_c(C_l^-) \leq \frac{2k}{\pi} + 0.59. \tag{4.12}$$

Then the required inequality (4.6) follows from (4.8)–(4.12).

Next, let $l \equiv 1 \pmod{2}$. Then $l \geq 5$ and $k - l \geq 7$. Lemma 4.3 implies that

$$E_c(C_{k-l}) + E_c(C_l) \leq \frac{2k}{\pi}. \tag{4.13}$$

The required inequality (4.6) follows from (4.8) and (4.13)

(2). Let $k \equiv 1 \pmod{2}$. In this case $k - 2 \geq 7$. Using Lemma 4.2 we have

$$\begin{aligned}
E_c(C_{k-2}) + E_c(C_2^-) &\geq \frac{2k}{\pi} - \frac{4}{\pi} + 2 - \frac{0.429\pi}{2(k-2)} \\
&= \frac{2k}{\pi} + 0.63.
\end{aligned}$$

On the other hand if $l \equiv 0 \pmod{2}$ then $k - l \geq 5$. Lemma 4.4 implies that

$$E_c(C_{k-l}^+) + E_c(C_l^-) \leq \frac{2k}{\pi}. \tag{4.14}$$

Furthermore, applying Lemma 4.4 and Lemma 4.1, we obtain

$$\begin{aligned}
E_c(C_{k-l}^+) + E_c(C_l^-) &\leq \frac{2k}{\pi} + \frac{2l\pi}{6l^2 - \pi^2} \\
&\leq \frac{2k}{\pi} + \frac{2(5)\pi}{6(5)^2 - \pi^2} \\
&= \frac{2k}{\pi} + 0.22.
\end{aligned} \tag{4.15}$$

Analogously, we can show the following inequalities:

$$E_c(C_{k-l}^-) + E_c(C_l^+) \leq \frac{2k}{\pi}, \quad (4.16)$$

$$E_c(C_{k-l}^-) + E_c(C_l^-) \leq \frac{2k}{\pi} + 0.22. \quad (4.17)$$

Inequality (4.7) follows from (4.14)–(4.17).

If $l \equiv 1 \pmod{2}$ then $k - l \equiv 0 \pmod{2}$. In this case we have $l \geq 5$ and $k - l \geq 4$.

Lemma 4.4 gives us:

$$E_c(C_{k-l}^+) + E_c(C_l^+) \leq \frac{2k}{\pi}. \quad (4.18)$$

Furthermore, applying Lemma 4.1 and Lemma 4.4, we get

$$E_c(C_{k-l}^+) + E_c(C_l^-) \leq \frac{2k}{\pi}, \quad (4.19)$$

$$E_c(C_{k-l}^-) + E_c(C_l^+) \leq \frac{2k}{\pi} + 0.22, \quad (4.20)$$

$$E_c(C_{k-l}^-) + E_c(C_l^-) \leq \frac{2k}{\pi} + 0.22. \quad (4.21)$$

Inequality (4.7) follows from (4.14) and (4.18)–(4.21). \square

Combining Lemma 4.5 and Lemma 4.6, we get the following theorem.

Theorem 4.7. *For $k, k - l \geq 2$, the following hold for vertex disjoint directed cycles.*

(1) *If $k \equiv 0 \pmod{2}$ then*

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l).$$

(2) *If $k \equiv 0 \pmod{2}$ then*

$$E_c(C_{k-2}) + E_c(C_2^-) \geq E_c(C_{k-l}) + E_c(C_l).$$

We finally give our main theorem.

Theorem 4.8. *Let $S \in S_k$ with signed directed cycles C_{j_1} and C_{j_2} , where $2 \leq j_1, j_2 \leq k-2$.*

(1) *S has smallest iota energy when $C_{j_1} = C_{j_2} = C_2^+$.*

(2) If $k \equiv 0 \pmod{2}$ then S has largest iota energy when $C_{j_1} = C_{k-2}^-$ and $C_{j_2} = C_2^-$.

(3) If $k \equiv 1 \pmod{2}$ then S has largest iota energy when $C_{j_1} = C_{k-2}$ and $C_{j_2} = C_2^-$.

Proof. Let $S \in S_k$ with signed directed cycles C_{j_1} and C_{j_2} , where $2 \leq j_1, j_2 \leq k-2$. It follows from Theorem 2.3 that

$$E_c(S) = E_c(C_{j_1}) + E_c(C_{j_2}). \quad (4.22)$$

(1) We know that $E(C_2^+) = 0$. Thus (4.22) shows that S has smallest iota energy when $C_{j_1} = C_{j_2} = C_2^+$.

(2) If $k \equiv 0 \pmod{2}$ then let $C_{j_1} = C_{k-2}^-$ and $C_{j_2} = C_2^-$. We take a sidigraph $H \in S_k$ with signed directed cycles C_{m_1} and C_{m_2} , where $2 \leq m_1, m_2 \leq n-2$. Then

$$E_c(S) = E_c(C_{k-2}^-) + E_c(C_2^-), \quad (4.23)$$

$$E_c(H) = E_c(C_{m_1}) + E_c(C_{m_2}). \quad (4.24)$$

By Theorem 4.7, we find that

$$E_c(C_{k-2}^-) + E_c(C_2^-) \geq E_c(C_{m_1}) + E_c(C_{m_2}).$$

By above inequality, we see that $E_c(S) \geq E_c(H)$. Thus S has largest iota energy among all sidigraphs of S_k .

(3) can be obtained analogously.

□

4.2 Conclusion

In this chapter, we considered a specific class S_k of vertex disjoint bicyclic sidigraphs of fixed order $n \geq 4$. We find sidigraphs with smallest and largest iota energy in S_k . One is compelled to work on a more general class of bicyclic sidigraphs and find sidigraphs with extremal iota energy in this general class. We leave this problem to future work.

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