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ENERGY OF GRAPHS AND DIGRAPHS.

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CERTIFICATE

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

Professor S. Pirzada.
Supervisor

ABSTRACT

In Chapter 1, we present a brief introduction of spectra of graphs and some definitions. Chapter 2 is a brief review of energy of graphs and digraphs. We study the problem of real numbers which cannot be the energy of a digraph. In Chapter 3, we study the problem of minimal energy in unicyclic signed graphs. We also construct pairs of equienergetic signed graphs. In Chapter 4, we have introduced the concept of energy in signed digraphs. We characterize unicyclic signed digraphs with minimal and maximal energy. We extend the concept of non extended p-sum (NEPS) to signed digraphs and study its spectra. We obtain upper bounds for the energy of signed digraphs. We also construct pairs of non cospectral equienergetic signed digraphs. In Chapter 5, we obtain a sufficient condition for the even coefficients of the characteristic polynomial of a bipartite signed digraph to alternate in sign and in this case we show it is possible to compare the energy of bipartite signed digraphs by means of a quasi-order relation defined on coefficients. We also obtain a sufficient condition for all the even coefficients of a bipartite signed digraph to be nonnegative. We construct integral, real and Gaussian signed digraphs and qausi-cospectral digraphs.

DECLARATION

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

Mushtaq Ahmad Bhat

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CHAPTER 1

Introduction

1.1 Background

Spectral graph theory (Algebraic graph theory) which emerged in 1950s and 1960s is the study of properties of a graph in relationship to the characteristic polynomial, eigenvalues and eigenvectors of matrices associated to the graph. The major source of research in spectral graph theory has been the study of relationship between the structural and spectral properties of graphs. Another source has research in quantam chemistry. The 1980 monograph 'spectra of graphs' by Cvetković, Doob and Sach [14] summarised nearly all research to date in the area. In 1988 it was updated by the survey 'Recent results in the theory of graph spectra'. The third edition of spectra of graphs (1995) contains a summary of the further contributions to the subject. Since then the theory has been developed to a greater extend and many research papers have been published. It is important to mention that spectral graph theory has a wide range of applications to other areas of mathematics and to other areas of sciences which include Computer Science, Physics, Chemistry, Biology, Statistics etc.

One of the richest theories in spectral graph theory is the energy of graphs. The concept of energy of a graph is formulated from the pioneering work of Hückel [27, 42] who made certain simplification of Schrodinger's wave equations [14]. Chemists are interested in finding the wave functions and energy levels of a given molecule. The wave functions ϕ are the solutions of Schrodinger's wave equation $(H - E)\phi = 0$, where H is the energy operator and E is the electron energy. In order to solve this equation for molecules, Hückel [42] replaced the Schrodinger's wave function by the speculation equation $|(H - ES)| = 0$, where $H = \alpha I + \beta A$ and $S = I + \sigma A$. Here α (the Coulomb integral for carbon atom), β (the resonance integral for two carbon atoms) and σ are all constants. If we normalize the system so that $\alpha = 0$ (the zero energy reference point) and $\beta = 1$ (the energy unit), then H is the adjacency matrix $A(G)$ of the associated graph G. The wave functions ϕ are then eigenvalues of $A(G)$. Both wave functions and energy levels can be measured experimentally and accord well with the predictions of Hückel theory.

The spectra of graphs can be used to calculate the energy levels of a conjugated hydrocarbon as calculated with Hückel Molecular Orbital (HMO) method. The details of Hückel theory and how it is related to spectral graph theory can be found in [14].

To study the energy levels of general class of graphs certainly help us in determining the energy levels of various classes of conjugated hydrocarbons in chemistry. Considerable work on this aspect has been done from Hückel [42] till today.

Conjugated hydrocarbons are of great importance for both science and technology. A conjugated hydrocarbon can be characterized as a molecule composed entirely of carbon and hydrogen atoms, every carbon atom having exactly three neighbours (which may be either carbon or hydrogen atoms). For example benzene is a conjugated hydrocarbon. There are theoretical reasons [27, 76] to associate a graph with a conjugated hydrocarbon according to the following rule:

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

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

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

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

Gutman [29] in 1978 defined the concept of energy for graphs. This concept became so popular that more than 300 papers have been published in this direction till date. At the begining some chemical problems were given graph theoretical shape and were solved using spectral graph theory. One such problem can be seen in [31]. Upper and lower bounds for energy were obtained for different classes of graphs which can be used to estimate the total π-electron energy of molecular graphs. Pẽna and Rada [62] in 2007 extended energy to digraphs and defined the energy of a digraph as the sum of the absolute values of real parts of eigenvalues of the digraph. They obtained Coulson's integral formula for energy of digraphs and also characterized unicyclic digraphs with minimal and maximal energy.

Germina, Hameed and Zaslavsky [23] in 2011 extended the concept of energy

to signed graphs. They defined the energy of a signed graph as the sum of the absolute values of eigenvalues of a signed graph. They studied the eigenvalues and energy and laplacian energy for different products of signed graphs. We extend the concept of energy to signed digraphs in a similar way as graph energy was extended to energy of digraphs and obtain Coulson's integral formula for energy of signed digraphs. We characterize unicyclic signed digraphs with minimal and maximal energy and also obtain upper bounds for the energy of signed digraphs. We study the problem of equienergetic signed digraphs.
Here are some definitions.

1.2 Basic Definitions

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

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

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

Definition 1.2.4. *Subgraph of a graph.* Let $G = (V, \mathscr{E})$ be a graph, $H = (U, \mathscr{E}')$ is the subgraph of G whenever $U \subseteq V$ and $\mathscr{E}' \subseteq \mathscr{E}$. If $U = V$ the subgraph is said to be spanning.

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

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

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

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

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

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

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

Definition 1.2.12. *Cartesian product.* The Cartesian product of two graphs $G_1(V_1,\mathscr{E}_1)$ and $G_2(V_2,\mathscr{E}_2)$ denoted by $G_1 \times G_2$ is the graph $(V,\mathscr{E})$, where $V = V_1 \times V_2$ and $((x_1, x_2), (y_1, y_2)) \in \mathscr{E}$ if either $x_1 = y_1$ and $(x_2, y_2) \in \mathscr{E}_2$ or $(x_1, y_1) \in \mathscr{E}_1$ and $x_2 = y_2$.

Definition 1.2.13. *Kronecker product.* The Kronecker product of two graphs $G_1(V_1,\mathscr{E}_1)$ and $G_2(V_2,\mathscr{E}_2)$ denoted by $G_1 \otimes G_2$ is the graph $(V,\mathscr{E})$, where $V = V_1 \times V_2$ and $((x_1, x_2), (y_1, y_2)) \in \mathscr{E}$ if $(x_1, y_1) \in \mathscr{E}_1$ and $(x_2, y_2) \in \mathscr{E}_2$.

Definition 1.2.14. (i)*Elementary figure.* We call a graph to be an elementary figure if it is either K_2 or a cycle C_p, $p \geq 3$.
(ii)*Basic figure.* A graph whose components are elementary figures is called a basic figure.

Definition 1.2.15. *Digraph (or directed graph).* A digraph D is a pair $(V,\mathscr{A})$, where V is a nonempty set of objects called vertices and $\mathscr{A}$ is a subset of $V^{(2)}$, (the set of ordered pairs of distinct elements of V). The elements of $\mathscr{A}$ are called arcs of D.

Definition 1.2.16. *Multidigraph.* A multidigraph D is a pair $(V,\mathscr{A})$, where V is a nonempty set of vertices and $\mathscr{A}$ is a multiset of arcs (directed edges). The number of times an arc occurs in D is called its multiplicity and arcs with multiplicity greater than one are called multiple arcs.

Definition 1.2.17. *General digraph.* A general digraph D is a pair $(V, \mathscr{A})$, where V is a non empty set of vertices and $\mathscr{A}$ is a multiset of arcs. We denote by (u, v) an arc from vertex u to vertex v. An arc of the form (u, u), where $u \in V$, is called the loop of D and arcs which are not loops are called the proper arcs. The number of times a loop occurs is called its multiplicity. A loop with multiplicity greater than one is called a multiple loop.

Definition 1.2.18. *Subdigraph of a digraph.* Let $D = (V, \mathscr{A})$ be a digraph, $H = (U, \mathscr{A}')$ is the subdigraph of D whenever $U \subseteq V$ and $\mathscr{A}' \subseteq \mathscr{A}$. If $U = V$ the subdigraph is said to be spanning.

Definition 1.2.19. *Outdegree and indegree.* In a digraph $D = (V, \mathscr{A})$, the out-degree of a vertex v is the number of vertices to which the vertex v is adjacent, it is denoted by $d^+(v)$ or d_v^+. Similarly the indegree of a vertex v in a digraph D is the number of vertices from which v is adjacent and it is denoted by $d^-(v)$ or d_v^-. If $d_v^+ = d_v^- = k$, then the digraph is said to be k-regular. A vertex v is said to be isolated if $d_v^+ = d_v^- = 0$.

Definition 1.2.20. Two digraphs D_1 and D_2 are said to be *isomorphic* if their underlying graphs are isomorphic and the direction of arcs are same and we write $D_1 \cong D_2$.

Definition 1.2.21. *Complement of a Digraph.* The complement of digraph $D = (V, \mathscr{A})$ is denoted by $\bar{D}$. It has a vertex set V and $(u, v) \in \bar{\mathscr{A}}$ if and only if $(u, v) \notin \mathscr{A}$. $\bar{D}$ is the relative complement of D in K_n^*, where K_n^* is a complete symmetric digraph, i.e., a digraph in which for every pair of vertices there is a directed arc from one to other.

Definition 1.2.22. *Self complementary digraph.* A digraph D is said to be self complementary if $D \cong \bar{D}$, and D is said to be self converse if $D \cong D'$.

Definition 1.2.23. *Directed Path.* A path of length $n - 1$ $(n \geq 2)$, denoted by P_n, is a digraph with n vertices $v_1, v_2, \cdots, v_n$ and with $n - 1$ arcs (v_i, v_{i+1}), where $i = 1, 2, \cdots, n - 1$.

Definition 1.2.24. *Directed cycle.* A cycle of length n, denoted by C_n, is the digraph with vertex set $v_1, v_2, \cdots, v_n$ having arcs (v_i, v_{i+1}), $i = 1, 2, \cdots, n - 1$ and (v_n, v_1). A digraph is acyclic if it has no cycles.

Definition 1.2.25. *Strong connectedness.* A digraph D is called strongly connected if for any two vertices there is a path from one to other. The strong components of a digraph are the maximally strongly connected subdigraphs.

Definition 1.2.26. *Oriented graph.* An oriented graph is a digraph with no symmetric pairs of directed arcs and without loops.

Definition 1.2.27. *Signed graph.* A signed graph is defined to be a pair $S = (G, \sigma)$, where $G = (V, \mathscr{E})$ is the underlying graph and $\sigma : \mathscr{E} \to \{-1, 1\}$ is the signing function. The sets of positive and negative edges of S are respectively denoted by $\mathscr{E}^+$ and $\mathscr{E}^-$.

Definition 1.2.28. *Signed digraph.* A signed digraph is defined to be a pair $S = (D, \sigma)$ where $D = (V, \mathscr{A})$ is the underlying digraph and $\sigma : \mathscr{A} \to \{-1, 1\}$ is the signing function. The sets of positive and negative arcs of S are respectively denoted by $\mathscr{A}^+$ and $\mathscr{A}^-$.

CHAPTER 2

On the energy of graphs and digraphs

In this Chapter, we study the energy of graphs and digraphs and present some well known results on energy of graphs and digraphs. We study the problem of the real numbers that cannot be the energy of a digraph. We also obtain a sharp lower bound for the energy of a strongly connected digraph.

2.1 Introduction

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

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

The characteristic polynomial $|xI - A(G)|$ of the adjacency matrix $A(G)$ of G is called the characteristic polynomial of G and is denoted by $\phi_G(x)$. The eigenvalues of $A(G)$ are called the eigenvalues of G. The set of distinct eigenvalues of G together with their multiplicities is called the spectrum of G. If G has k distinct eigenvalues $x_1, x_2, \cdots, x_k$ with respective multiplicities $m_1, m_2, \cdots, m_k$, then we write the spectrum of G as $spec(G) = \{x_1^{(m_1)}, x_2^{(m_2)}, \cdots, x_k^{(m_k)}\}$.

The following result relates the coefficients of the characteristic polynomial of a graph with the structure of the graph and is also known as Sach's Theorem [14].

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

$$\phi_G(x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + \cdots + a_{n-1} x + a_n.$$

Then

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

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

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

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

The even coefficients of a bipartite graph alternate in sign [14] i.e., $(-1)^j a_{2j} \geq 0$ for all j. Therefore

$$\phi_B(x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j} x^{n-2j}, \tag{2.1}$$

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

2.2 Energy of graphs

Definition 2.2.1. *Energy of a graph.* Let G be a graph of order n with eigenvalues $x_1, x_2, \cdots, x_n$. The energy of G is defined as

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

This concept was first introduced in 1978 by Gutman [29]. The following is the integral representation for the energy of a graph (also known as the Coulson's integral formula).

Theorem 2.2.2. *Let G be a graph with n vertices having characteristic polynomial*

$\phi_G(x)$. Then

$$E(G) = \sum_{j=1}^{n} |x_j| = \frac{1}{\pi} \int_{-\infty}^{\infty} (n - \frac{\iota x \phi'_G(\iota x)}{\phi_G(\iota x)}) dx,$$

where $x_1, x_2, \cdots, x_n$ are the eigenvalues of graph G, $\iota = \sqrt{-1}$ and $\int_{-\infty}^{\infty} F(x)dx$ denotes the principle value of the respective integral.

The following observations [30] follow from Coulson's integral formula.

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

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

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

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{\infty} \log |\frac{\phi_{G_1}(\iota x)}{\phi_{G_2}(\iota x)}| dx.$$

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

Combining (2.1) and Theorem 2.2.3, the energy of a bipartite graph B is given as under [33].

Theorem 2.2.5. *If B is a bipartite graph on n vertices, then*

$$E(B) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log[1 + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} b_{2j} x^{2j}] dx,$$

where $b_{2j} \geq 0$.

From this energy expression, we see that the energy of a bipartite graph is an increasing function of the coefficients b_{2j}. Given bipartite graphs B_1 and B_2 (not of same order), we say $B_1 \preceq B_2$ if and only if $b_{2j}(B_1) \leq b_{2j}(B_2)$. If for some j, $b_{2j}(B_1) < b_{2j}(B_2)$, then we say $B_1 \prec B_2$. Thus the relation $\preceq$ is a quasi-order relation and energy increases with respect to this relation. That is, if $B_1 \prec B_2$ then $E(B_1) < E(B_2)$.

2.3 Bounds for the energy of a graph

Several upper and lower bounds for the energy are known. The following upper and lower bound of energy of a graph in terms of order n, size m and determinant of adjacency matrix is due to McClelland [57].

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

$$\sqrt{2m + n(n-1)|A(G)|^{\frac{n}{2}}} \leq E(G) \leq \sqrt{2mn}. \tag{2.2}$$

An immediate consequence of Theorem 2.3.1 is the following observation.

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

The graph energy as a function of the number of edges satisfies the following inequalities [15].

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

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

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

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

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

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

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

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

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

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

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

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

The following result due to Koolen and Moulton [47] improves the McClelland upper bound for the graphs with $\frac{2m}{n} \geq 1$, where n is the number of vertices and

m is the number of edges of the graph.

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

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - (\frac{2m}{n})^2]} \tag{2.3}$$

holds. Moreover, equality holds in (2.3) *if and only if* G *is either* $\frac{n}{2}K_2$ *or* K_n *or a non-complete connected strongly regular graph with two non trivial eigenvalues both with absolute value* $\sqrt{\frac{(2m-(\frac{2m}{n})^2)}{(n-1)}}$.

Since a graph G with n vertices has at most $\frac{n(n-1)}{2}$ edges, it follows from McClelland's bound (2.2) that

$$E(G) \leq n\sqrt{n-1} \tag{2.4}$$

must hold.

The following result shows that inequality (2.3) allows to improve the bound given by (2.5)

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

$$E(G) \leq \frac{n}{2}(1+\sqrt{n}) \tag{2.5}$$

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

Koolen and Moulton in [46] conjectured that for a given $\epsilon > 0$, there exists a graph G of order n such that for almost all $n \geq 1$,

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

which was later proved by Nikiforov [59]. For energy bounds about bipartite graphs see [47, 68].

2.4 Equienergetic graphs

Two graphs G_1 and G_2 are said to be cospectral if they have same spectrum and non cospectral, otherwise. Isomorphic graphs are cospectral, since adjacency matrices of isomorphic graphs are similar by means of a permutation matrix. There exist non isomorphic cospectral graphs [14]. Cospectral graphs are obviously equienergetic, therefore problem of equienergetic graphs reduces to the problem of construction of non cospectral equienergetic graphs.

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

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

Equienergetic graphs were first constructed by Ramane et al. [72]. The following result shows that for a regular graph, the energy of second iterated line graph depends only on degree and number of vertices.

Theorem 2.4.2. *If G is an r-regular graph of order n, then*

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

From Theorem 2.4.2 and noting that iterated line graphs of non cospectral regular graphs are non cospectral, the following result [72] yields the existence of non cospectral equienergetic graphs.

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

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

The following result due to Ramanne et al. [75] gives a method of construction of equienergetic complement graphs.

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

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

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

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

An inductive argument gives the following result.

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

Balakrishnan [6] proved that for a non trivial graph Q, if $G = C_4$ and $H = K_2 \otimes K_2$, then $Q \otimes G$ and $Q \otimes H$ are non cospectral and equienergetic. Bonifacio et al. [11] have given conditions on an arbitrary pair G and H of equienergetic non cospectral graphs to make assertion true for any non trivial connected graph Q.

Theorem 2.4.7. *Let G and H be two equienergetic non cospectral graphs such that there is an eigenvalue x of G for which $x > |y|$, for all eigenvalues y of H. If Q is a non trivial connected graph, then $Q \otimes G$ and $Q \otimes H$ are equienergetic non cospectral graphs.*

The following result due to Bonifacio et al. [11] characterizes a graph G for which $G \otimes K_2$ and $G \times K_2$ are non cospectral and equienergetic.

Theorem 2.4.8. *Let G be a connected graph with eigenvalues $x_1, x_2, \cdots, x_n$. Then $G \otimes K_2$ and $G \times K_2$ are equienergetic non cospectral graphs if and only if $|x_i| \geq 1$, for all $i = 1, 2, \cdots, n$.*

Liu and Liu [50] proved that there exist a pair of equienergetic graphs on p vertices for all $p \geq 10$. Indulal and Vijaykumar [43] constructed self complementary graphs on p vertices for every $p = 4k$, where $k \geq 2$ and $p = 24t + 1$, where $t \geq 3$. For more about equienergetic graphs see [45, 78].

2.5 Hyperenergetic graphs

From Theorem 2.3.1, a graph G with n vertices and m edges satisfies the upper bound $E(G) \leq \sqrt{2mn}$. This bound depends only on m and n. As among all n-vertex graphs, the complete graph K_n has maximum number of edges which is $\frac{n(n-1)}{2}$. This motivated Gutman to conjecture that among all n-vertex graphs, the complete graph K_n has maximum energy which is equal to $2(n-1)$. Later Godsil [26] in 1980's proved that there exists graphs of order n with energy greater than $2(n-1)$. This motivated the following definition.

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

Gutman et al. [34] proved that no Hückel graph (molecular graph) is hyperenergetic. Pirzada [63] proved that Frutch graph is not hyperenergetic. Panigrahi and Mohapatra [60] proved all primitive strongly regular graphs except SRG$(5, 2, 0, 1)$, SRG$(9, 4, 1, 2)$, SRG$(10, 3, 0, 1)$and SRG$(16, 5, 0, 2)$ are hyperenergetic. Balakrishnan posed an open problem in [6] that $K_n - H$ is non-hyperenergetic for $n \geq 4$, where H is a Hamiltonian cycle of K_n. Stevanović and Stanković [79] proved that $K_n - H$ is indeed hyperenergetic, where H is the Hamiltonian cycle of K_n. In fact, they proved the following stronger result.

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

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

2.6 Energy of digraphs

Pẽna and Rada [62] extended the concept of energy to digraphs in such a way that Coulson's integral formula remains valid. Before defining energy of a digraph, we give a brief introduction of spectra of digraphs.

Let D be a digraph with n vertices $v_1, v_2, \cdots, v_n$. The adjacency matrix of D is the $n \times n$ matrix $A(D) = (a_{ij})$, where

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

Unlike graphs the adjacency matrix of a digraph need not be real symmetric, so eigenvalues can be complex numbers. We denote the characteristic polynomial $|xI - A(D)|$ of the adjacency matrix $A(D)$ by $\phi_D(x)$. If $z_1, z_2, \ldots, z_n$ are eigenvalues of digraph D, we label them so that $\Re z_1 \geq \Re z_2 \geq \cdots \geq \Re z_n$, where $\Re z_j$ denotes the real part of complex number z_j. By Perron Frobenius theorem $\Re z_1$ is an eigenvalue of D with largest absolute value and is called spectral radius of D. It is denoted by ρ. A linear subdigraph of a digraph D is a subdigraph with indegree and outdegree of each vertex equal to one. Consequently, a linear subdigraph is either a cycle or disjoint union of cycles. The following result due to Sach [14] relates the coefficients of the characteristic polynomial of a digraph with its structure.

Theorem 2.6.1. *If D is a digraph of order n with characteristic polynomial*

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

then

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

where $\pounds_j$ is the set of all linear subdigraphs of D of order j and $p(L)$ denotes the number of components of L.

The following is the definition of the energy of a digraph as given by Pẽna and Rada [62].

Definition 2.6.2. Let D be a digraph on n vertices with eigenvalues $z_1, z_2, \cdots, z_n$. The energy of D is defined as

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

where $\Re z_j$ denotes the real part of the complex number z_j. This definition was motivated by following integral formula.

Theorem 2.6.3. *(Coulson's integral formula). If D is a digraph on n vertices and with characteristic polynomial $\phi_D(x)$, then*

$$E(D) = \sum_{j=1}^{n} |\Re z_j| = \frac{1}{\pi} \int_{-\infty}^{\infty} (n - \frac{\iota x \phi'_D(\iota x)}{\phi_D(\iota x)}) dx,$$

where $z_1, z_2, \cdots, z_n$ are eigenvalues of D, $\iota = \sqrt{-1}$ and $\int_{-\infty}^{\infty} F(x)dx$ stands for the principal value of the respective integral.

The following result is an immediate consequence of Coulson's integral formula.

Theorem 2.6.4. *If D is a digraph with n vertices, then*

$$E(D) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log |x^n \phi_D(\frac{\iota}{x})| dx.$$

2.7 Bounds for the energy of digraphs

Recall that a digraph is said to be symmetric if $(u, v) \in \mathscr{A}$, then $(v, u) \in \mathscr{A}$, where $u, v \in V$. A one to one correspondence between graphs and symmetric digraphs is given by $G \rightsquigarrow \overleftrightarrow{G}$, where $\overleftrightarrow{G}$ has the same vertex set as the graph G and each edge (u, v) is replaced by a pair of symmetric arcs (u, v) and (v, u). Under this identification, a graph can be regarded as a symmetric digraph.

Gudiño and Rada [28] extended the Koolen and Moulton bound for graph energy to energy of digraphs. The following extends the upper bound (2.3) of graph energy to digraphs.

Theorem 2.7.1. *If D is a digraph with n vertices, a arcs and c_2 closed walks of length 2, then*

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

Equality holds if and only if D is the empty digraph (i.e., n isolated vertices) or $D = \overleftrightarrow{G}$, where G is one of the following:
(i) $G = \frac{n}{2}K_2$, (ii) $G = K_n$, (iii) G is a non-complete connected strongly regular graph with two non trivial eigenvalues both with absolute value $\sqrt{\frac{(a-(\frac{c_2}{n})^2)}{(n-1)}}$.

Definition 2.7.2. Let D be a digraph with a arcs and c_2 closed walks of length 2. The *symmetry index* of D, denoted by s, is defined as $s = a - c_2$. Clearly, $0 \leq s \leq n(n-1)$ for every digraph D. Also note that a digraph D is symmetric if and only if $s = 0$.

The following result extends bound (2.5) of graph energy to digraphs.

Theorem 2.7.3. *If D is a digraph with n vertices and symmetry index s, then*

$$E(D) \leq \frac{n}{2}(1 + \sqrt{n + \frac{4s}{n}}).$$

Equality hods if and only if $D = \overleftrightarrow{G}$, where G is a strongly regular graph with *parameters* $(n, \frac{(n+\sqrt{n})}{2}, \frac{(n+2\sqrt{n})}{4}, \frac{(n+2\sqrt{n})}{4})$.

The following result due to Tian and Cui [80] improves in some cases the upper bound in Theorem 2.7.1.

Theorem 2.7.4. *Let D be a digraph with n vertices and a arcs. Also let $(c_2^{(1)}, c_2^{(2)}, \ldots, c_2^{(n)})$ be the closed walk sequence of length 2 of D. Then*

$$E(D) \leq \sqrt{\frac{\sum_{j=1}^{n}(c_2^{(j)})^2}{n}} + \sqrt{(n-1)(a - \frac{\sum_{j=1}^{n}(c_2^{(j)})^2}{n})}.$$

The equality holds if and only if $D = \overleftrightarrow{G}$, where G is either $\frac{n}{2}K_2$ or K_n or a non-complete strongly regular graph with two non trivial eigenvalues both with absolute value $\sqrt{\frac{(a - \frac{\sum_{j=1}^{n}(c_2^{(j)})^2}{n})}{(n-1)}}$ or nK_1.

Ayyaswamy, Balachandran and Gutman [5] obtained the following upper bounds for the energy of strongly connected digraphs.

Theorem 2.7.5. *If D is a strongly connected digraph on n vertices and a arcs, such that $\Re(z_1) \geq \frac{(a+c_2)}{2n} \geq 1$, then the inequality*

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

Equality holds if and only if $D = \overleftrightarrow{G}$ is either $\frac{n}{2}K_2$ or K_n or a non complete strongly regular graph with two non trivial eigenvalues both with absolute value $\sqrt{\frac{\frac{a+c_2}{2} - (\frac{a+c_2}{2n})^2}{(n-1)}}$.

Suppose that D is a digraph on n vertices with adjacency matrix $A(D)$. We say D is *strongly regular digraph* with parameters (n, k, t, λ, μ) if $0 < t < k$ and A satisfies the following matrix equations.

$$JA(D) = A(D)J = kJ$$

and

$$A^2(D) = tI + \lambda A(D) + \mu(J - I - A),$$

where J is the matrix whose all elements are equal to unity.

The following result [19] connects parameters of a strongly regular digraph.

Lemma 2.7.6. *For a strongly regular digraph with parameters (n, k, t, λ, μ), the following holds.*

$$0 \leq \lambda < t < k$$

and

$$0 < \mu \leq t < k.$$

The following result [19] gives the spectrum of a strongly regular digraph.

Lemma 2.7.7. *Let $A(D)$ be the adjacency matrix of a strongly regular digraph with parameters (n, k, t, λ, μ). Then $A(D)$ has integer eigenvalues $\theta_0 = k$, $\theta_1 = \frac{\lambda-\mu+\delta}{2}$, $\theta_2 = \frac{\lambda-\mu-\delta}{2}$ with multiplicities $m_0 = 1$, $m_1 = -\frac{k+\theta_2(n-1)}{\theta_1-\theta_2}$ and $m_2 = \frac{k+\theta_1(n-1)}{\theta_1-\theta_2}$ respectively, provided $\delta = \sqrt{(\mu-\lambda)^2 + 4(t-\mu)}$ is a positive integer.*

The following result [5] gives the upper bound for energy of strongly connected digraphs in terms of number of vertices.

Theorem 2.7.8. *Let D be a strongly connected digraph on n vertices and a arcs, such that $\Re z_1 \geq \frac{(a+c_2)}{2n} \geq 1$. Then*

$$E(D) \leq \frac{n(1+\sqrt{n})}{2}$$

with equality if and only if D is a strongly regular digraph with parameters $(n, \frac{n+\sqrt{n}}{2}, \frac{3n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8})$.

The following result [70] gives a lower bound for the energy of a digraph.

Theorem 2.7.9. *If D is a digraph with c_2 closed walks of length 2, then*

$$E(D) \geq \sqrt{2c_2}.$$

Further, $E(D) = \sqrt{2c_2}$ if and only if D is acyclic or $spec(D) = \{-\sqrt{\frac{c_2}{2}}, 0^{(n-2)}, \sqrt{\frac{c_2}{2}}\}$, where n is the number of vertices of D.

For more about bounds for energy of digraphs see [18].

2.8 Real numbers that cannot be the energy of a digraph

We recall from [10] that every rational algebraic integer is an integer and sum and product of algebraic integers is an algebraic integer. We have the following observation.

Lemma 2.8.1. *Let $A = (a_{ij})$ be a square matrix of order n having integral entries and zero trace and let $z_1, z_2, \cdots, z_n$ be its eigenvalues. Put $\alpha = \sum_{j=1}^{n} |\Re z_j|$, then α cannot be of the form (i) $(2^t s)^{\frac{1}{h}}$ with $h \geq 1,\ 0 \leq t < h$ and s odd (ii) $(\frac{m}{n})^{\frac{1}{r}}$, where $\frac{m}{n}$ is non-integral rational and r is a positive integer.*

Proof. We note that $\alpha = 2 \sum_{\Re z_j \geq 0} z_j$. Put $z = \sum_{\Re z_j \geq 0} z_j$, then z being sum of algebraic integers is an algebraic integer.

(i) Assume $\alpha = (2^t s)^{\frac{1}{h}}$, so that $2z = (2^t s)^{\frac{1}{h}}$. Simplifying gives $z^h = \frac{s}{2^l}$, where $l = h - t \geq 1$. As s is odd, therefore we see z^h is non-integral rational algebraic integer, a contradiction.

(ii) As in part (i), assume $\alpha = (\frac{m}{n})^{\frac{1}{r}}$, so that $2z = (\frac{m}{n})^{\frac{1}{r}}$. This gives, $z^r = \frac{m}{n2^r}$. As $\frac{m}{n}$ is non-integral rational, so is $\frac{m}{n2^r}$, i.e., z^r is a non-integral rational algebraic integer, a contradiction. $\square$

Bapat and Pati [7] proved that the energy of a graph cannot be an odd integer. Later Pirzada and Gutman [64] proved that energy of a graph cannot be the square root of an odd integer. We next extend these results to digraphs.

Theorem 2.8.2. *Energy of a digraph cannot be of the form (i) $(2^t s)^{\frac{1}{h}}$ with $h \geq 1,\ 0 \leq t < h$ and s odd (ii) $(\frac{m}{n})^{\frac{1}{r}}$, where $\frac{m}{n}$ is non-integral rational num-*

ber and $r \geq 1$.

Proof. Let D be a digraph with adjacency matrix $A(D)$. Apply Lemma 2.8.1 to $A(D)$ and note that $E(D) = \sum_{j=1}^{n} |\Re z_j|$, the result follows. □

The following result gives a sharp lower bound for the energy of strongly connected digraphs.

Theorem 2.8.3. *If D is a strongly connected digraph of order n, then $E(D) \geq 2$, with equality if and only if $D = C_r$, $r = 2, 3, 4$.*

Proof. Let D be a strongly connected digraph with n vertices $v_1, v_2, \cdots, v_n$, therefore $d^+_{v_i} \geq 1$ for all $i = 1, 2, \cdots, n$. Now it is well known that the spectral radius $\rho \geq \min\ (d^+_{v_1}, d^+_{v_2}, \cdots, d^+_{v_n})$ which implies that $\rho \geq 1$. Hence

$$E(D) = 2 \sum_{\Re z_j \geq 0} z_j \geq 2\rho \geq 2.$$

If $E(D) = 2$, then $\rho = 1$. Since D is a strongly connected digraph, then from [6], D is a cycle, say $D = C_r$. It is shown in [62] that $E(C_r) > 2$ for all $r \geq 5$. Consequently $r = 2, 3$ or 4. □

In [69] it was shown that a digraph is acyclic if and only if its energy is zero. Also energy of a digraph is the sum of the energies of its strong components [62]. With these arguments and Theorem 2.8.3, we have the following result.

Theorem 2.8.4. *No Positive real number less than two can be the energy of a digraph.*

CHAPTER 3

On the energy of signed graphs

In this Chapter, we characterize unicyclic signed graphs with minimal energy. We show that for each positive integer $n \geq 3$, there exists a pair of connected, non-cospectral and equienergetic unicyclic signed graphs on n vertices with one constituent balanced and other constituent unbalanced. It is shown that for each positive integer $n \geq 4$, there exists a pair of connected, non-cospectral and equienergetic signed graphs of order n with both constituents unbalanced.

3.1 Introduction

A *signed graph* is defined to be a pair $S = (G, \sigma)$, where $G = (V, \mathscr{E})$ is the underlying graph and $\sigma : \mathscr{E} \to \{-1, 1\}$ is the signing function. The sets of positive and negative edges of S are respectively denoted by $\mathscr{E}^+$ and $\mathscr{E}^-$. Thus $\mathscr{E} = \mathscr{E}^+ \cup \mathscr{E}^-$. Our signed graphs have simple underlying graphs. A signed graph is said to be homogeneous if all of its edges have either positive sign or negative sign and heterogeneous, otherwise. A graph can be considered to be a homogeneous signed graph with each edge positive; thus signed graphs become a generalization of graphs. Throughout this Chapter bold lines denote positive edges and dotted lines denote negative edges. The sign of a signed graph is defined as the product of signs of its edges. A signed graph is said to be positive (respectively, negative) if its sign is positive (respectively, negative) i.e., it contains an even (respectively, odd) number of negative edges. A signed graph is said to be all-positive (respectively, all-negative) if all of its edges are positive (respectively, negative). A signed graph is said to be balanced if each of its cycles is positive and unbalanced, otherwise. We denote by $-S$ the signed graph obtained by negating each edge of S and call it the negative of S. We call balanced cycle a positive cycle and an unbalanced cycle a negative cycle and respectively denote them by C_n and $\mathbf{C}_n$, where n is number of vertices.

The adjacency matrix of a signed graph S whose vertices are $v_1, v_2, \cdots, v_n$ is the $n \times n$ matrix $A(S) = (a_{ij})$, where

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

Clearly, $A(S)$ is real symmetric and so all its eigenvalues are real. The characteristic polynomial $|xI - A(S)|$ of the adjacency matrix $A(S)$ of signed graph S is called the characteristic polynomial of S and is denoted by $\phi_S(x)$. The eigenvalues of $A(S)$ are called the eigenvalues of S. The set of distinct eigenvalues of S together with their multiplicities is called the spectrum of S. Let S be a signed graph of order n with distinct eigenvalues $x_1, x_2, \cdots, x_k$ and let their respective multiplicities be $m_1, m_2, \cdots, m_k$. Then we write the spectrum of S as $spec(S) = \{x_1^{(m_1)}, x_2^{(m_2)}, \cdots, x_k^{(m_k)}\}$.

The following is the coefficient Theorem for signed graphs [1].

Theorem 3.1.1. *If S is a signed graph with characteristic polynomial*

$$\phi_S(x) = x^n + a_1 x^{n-1} + \cdots + a_{n-1}x + a_n,$$

then

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

for all $j = 1, 2, \cdots, n$, where $\pounds_j$ is the set of all basic figures L of S of order j, $p(L)$ denotes number of components of L, $c(L)$ denotes the set of all cycles of L and $s(Z)$ the sign of cycle Z.

From this result, it is clear that the spectrum of a signed graph remains invariant by changing the signs of non cyclic edges. Here we note that whenever we need to compare the energy of two signed graphs we use $a_j(S)$ for j-th coefficient of characteristic polynomial of S instead of a_j.

The spectral criterion for balance of signed graphs given by Acharya [1] is as follows.

Theorem 3.1.2. *A signed graph is balanced if and only if it is cospectral with the underlying unsigned graph.*

The *Cartesian product* of two signed graphs $S_1 = (V_1, \mathscr{E}_1, \sigma_1)$ and $S_2 = (V_2, \mathscr{E}_2, \sigma_2)$ denoted by $S_1 \times S_2$ is the signed graph $(V_1 \times V_2, \mathscr{E}, \sigma)$, where the edge set is that of the Cartesian product of underlying unsigned graphs and the sign function is defined by

$$\sigma((u_i, v_j), (u_k, v_l)) = \begin{cases} \sigma_1(u_i, u_k), & \text{if } j = l, \\ \sigma_2(v_j, v_l), & \text{if } i = k. \end{cases}$$

The *Kronecker product* of two signed graphs $S_1 = (V_1, \mathscr{E}_1, \sigma_1)$ and $S_2 = (V_2, \mathscr{E}_2, \sigma_2)$ denoted by $S_1 \otimes S_2$ is the signed graph $(V_1 \times V_2, \mathscr{E}, \sigma)$, where edge set is that of the Kronecker product of underlying unsigned graphs and the sign function is defined by $\sigma((u_i, v_j), (u_k, v_l)) = \sigma_1(u_i, u_k)\sigma_2(v_j, v_l)$.

Let S be a signed graph with vertex set V. Switching S by set $X \subset V$, means reversing the signs of all edges between X and its complement.

Another way to define switching is by means of a function $\theta : V \to \{+1, -1\}$, called a switching function. Switching S by θ means changing σ to σ^θ defined by

$$\sigma^\theta(u, v) = \theta(u)\sigma(u, v)\theta(v).$$

We denote switched graph by S^θ. Two signed graphs are said to be switching equivalent if one can be obtained from the other by switching. Switching equivalence is an equivalence relation on the signings of a fixed graph. An equivalence class is called a switching class. A switching class of S is denoted by $[S]$. If S' is isomorphic to a switching of S, we say S and S' are switching isomorphic.

The concept of energy was extended to signed graphs by Germina, Hameed and Zaslavsky [23]. They defined the energy of a signed graph S to be the sum of absolute values of eigenvalues of S.

A connected signed graph of order n is said to be unicyclic if the number of its edges is also n. The girth of signed graph is the length of its smallest cycle and we denote it by g. Let S_n^g, $n \geq g \geq 3$ (respectively, $\mathbf{S}_n^g$) denote the balanced (respectively, unbalanced) unicyclic signed graph of order n obtained by identifying the root vertex of a signed star on $n - g + 1$ vertices with a vertex of a positive (respectively, negative) cycle of order g (see Fig. 3.1) and let $S(n, g)$ denote the set of all unicyclic signed graphs with n vertices and girth $g \leq n$. For unicyclic graphs with minimal energy see [38, 53]. Caprossi et al. [15] posed the following conjecture based upon the results attained with the computer system AutoGraphix.

Conjecture 3.1.3. *Among all connected graphs G with $n \geq 6$ vertices and $n - 1 \leq m \leq 2(n - 2)$ edges, the graph with minimum energy are stars with $m - n + 1$ additional edges all connected to the same vertex for $m \leq n + \lfloor \frac{(n-7)}{2} \rfloor$, and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side, otherwise.*

For $m = n - 1$ and $m = 2(n - 2)$ Caprossi et al. [15] proved the conjecture. The following result of Hou [38] proves conjecture for $m = n$.

Theorem 3.1.4. *Let G be a unicyclic graph with $n \geq 6$ vertices and $G \neq \mathscr{S}_n^3$. Then $E(\mathscr{S}_n^3) < E(G)$, where $\mathscr{S}_n^3$ is the graph obtained from the star graph with n vertices by adding an edge.*

We show for $m = n$, a signed analogue of the conjecture is true, that is, among all unicyclic signed graphs with $n \geq 6$ vertices and n edges, all signed graphs in $[S_n^3]$ and $[\mathbf{S_n^3}]$ have the minimal energy.

3.2 Switching in signed graphs

The following result can be seen in [85].

Lemma 3.2.1. *A signed graph is balanced if and only if it switches to an all-positive signing.*

The following result shows that there are only two switching classes on signings of unicyclic graph.

Theorem 3.2.2. *There exists only two switching classes on the signings of fixed unicyclic graph.*

Proof. Let G be a unicyclic graph. By Lemma 3.2.1, all balanced unicyclic signed graphs on G comprise one switching class. We show that all unbalanced signed graphs on G are switching equivalent to an unbalanced signed graph with exactly one negative cyclic edge and all other edges positive. Let S be any unbalanced signed graph on G. Choose a negative edge $e = (u, v)$. Then $S - e$ is balanced and hence by Lemma 3.2.1, $S - e$ switches to an all positive signed graph. Now return edge e in the all positive signed graph of $S - e$. Again, by Lemma 3.2.1, with this switching e must be a negative edge. Thus S is switching equivalent to an unbalanced signed graph with exactly one negative cyclic edge and all other edges positive. □

The following result shows that adjacency matrices of switching equivalent signed graphs are similar by means of a signature matrix.

Theorem 3.2.3. *Signed graphs S_1 and S_2 with same underlying graph are switching equivalent if and only if their adjacency matrices satisfy $A(S_2) = D^{-1}A(S_1)D$ for some $(0, \pm 1)$-matrix D whose diagonal has no zeroes.*

Theorem 3.2.3 shows that switching equivalent signed graphs are always cospectral. It is not known whether the converse is true or not. However, we have examples of cospectral unbalanced signed graphs whose underlying graphs are non-isomprphic (Signed graphs S_1 and S_2 in Fig. 3.1). It is shown in Remark 3.3.8 (i) that all unbalanced signed graphs on a fixed unicyclic graph are cospectral. Thus there are only two cospectral classes on the signings of a fixed unicyclic graph, one for balanced and one for unbalanced. Therefore, by Theorem 3.2.2, the following result is true for unicyclic signed graphs.

Theorem 3.2.4. *Two unicyclic signed graphs with the same underlying graph are cospectral if and only if they are switching equivalent.*

3.3 Integral representation for energy of signed graphs and its applications

First we obtain Coulson's integral formula and then discuss its consequences for signed graphs.

Theorem 3.3.1. *Let S be a signed graph with n vertices having characteristic polynomial $\phi_S(x)$. Then*

$$E(S) = \sum_{j=1}^{n} |x_j| = \frac{1}{\pi}\int_{-\infty}^{\infty} (n - \frac{\iota x \phi'_S(\iota x)}{\phi_S(\iota x)})dx,$$

where $x_1, x_2, \cdots, x_n$ are the eigenvalues of signed graph S, $\iota = \sqrt{-1}$ and $\int_{-\infty}^{\infty} F(x)dx$ denotes principle value of the respective integral.

Proof. Let $x_1, x_2, \ldots, x_n$ be the zeroes of polynomial $\phi_S(x)$. Then $\phi_S(x) = \prod_{j=1}^{n}(x - x_j)$ and $\phi'_S(x) = \sum_{j=1}^{n}\prod_{k\neq j}(x - x_k)$, so that $\frac{\phi'_S(x)}{\phi_S(x)} = \sum_{j=1}^{n}\frac{1}{x-x_j}$.
Using the integrals $\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{x_j^2}{(x_j^2+x^2)}dx = |x_j|$ and $\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{x_j^2 x}{(x_j^2+x^2)}dx = 0$, we have

$$\begin{aligned}
|x_j| = |x_j| + \iota 0 &= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{x_j^2}{(x_j^2 + x^2)}dx + \iota\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{x_j^2 x}{(x_j^2 + x^2)}dx \\
&= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{x_j^2 + \iota x_j x}{(x_j^2 + x^2)}dx = \frac{1}{\pi}\int_{-\infty}^{\infty}(1 - \frac{\iota x}{\iota x - x_j})dx.
\end{aligned}$$

Therefore, $E(S) = \sum_{j=1}^{n}|x_j| = \frac{1}{\pi}\int_{-\infty}^{\infty}\sum_{j=1}^{n}(1 - \frac{\iota x}{\iota x - x_j})dx = \frac{1}{\pi}\int_{-\infty}^{\infty}(n - \frac{\iota x\phi'_S(\iota x)}{\phi_S(\iota x)})dx.$ □

The following result is a consequence of Coulson's integral formula.

Theorem 3.3.2. *If S is a signed graph on n vertices, then*

$$E(S) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1}{x^2}\log|x^n\phi_S(\frac{\iota}{x})|dx.$$

Proof. By Theorem 3.3.1, we have

$$\begin{aligned}E(S) &= \frac{1}{\pi}\int\limits_{-\infty}^{\infty}(n - \frac{\iota x\phi_S'(\iota x)}{\phi_S(\iota x)})dx \\ &= \frac{1}{\pi}\int\limits_{-\infty}^{0}(n - \frac{\iota x\phi_S'(\iota x)}{\phi_S(\iota x)})dx + \frac{1}{\pi}\int\limits_{0}^{\infty}(n - \frac{\iota x\phi_S'(\iota x)}{\phi_S(\iota x)})dx\end{aligned}$$

Put $x = \frac{1}{y}$, so that

$$E(S) = \frac{1}{\pi}\int\limits_{-\infty}^{\infty}(n - \frac{\iota\frac{1}{y}\phi_S'(\iota\frac{1}{y})}{\phi_S(\iota\frac{1}{y})})\frac{1}{y^2}dy.$$

Now, integrating by parts and taking $u = \frac{1}{y}$ and $dv = (\frac{n}{y} - \frac{\iota\frac{1}{y^2}\phi_S'(\iota\frac{1}{y})}{\phi_S(\iota\frac{1}{y})})$, so that $du = -\frac{1}{y^2}dy$ and $v = \log|y^n\phi_S(\frac{\iota}{y})|$.
Therefore

$$\begin{aligned}E(S) &= \frac{1}{\pi}(\frac{1}{y}\log|y^n\phi_S(\frac{\iota}{y})|)_{-\infty}^{\infty} + \frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{1}{y^2}\log|y^n\phi_S(\frac{\iota}{y})|dy \\ &= \frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{1}{y^2}\log|y^n\phi_S(\frac{\iota}{y})|dy.\end{aligned}$$

Using change of variable, the result follows. □

Theorem 3.3.3. *If S is a signed graph on n vertices with characteristic polynomial $\phi_S(x) = x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n$, then*

$$E(S) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\frac{1}{x^2}\log[(\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j}x^{2j})^2 + (\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j+1}x^{2j+1})^2]dx.$$

Proof. Let $\psi(x) = (-\iota x)^n\phi_S(\frac{\iota}{x})$ and note that

$$\psi(x) = \sum_{j=0}^{n}a_j(-\iota x)^j = \sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j}x^{2j} - \iota\sum_{j=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^j a_{2j+1}x^{2j+1},$$

where $a_0 = 1$ and $a_j = 0$ for $j > n$. By Theorem 3.3.2, $E(S) = \frac{1}{\pi} \int\limits_{-\infty}^{\infty} \frac{1}{x^2} \log |\psi(x)|$. Substituting the value for $\psi(x)$, the result follows. $\square$

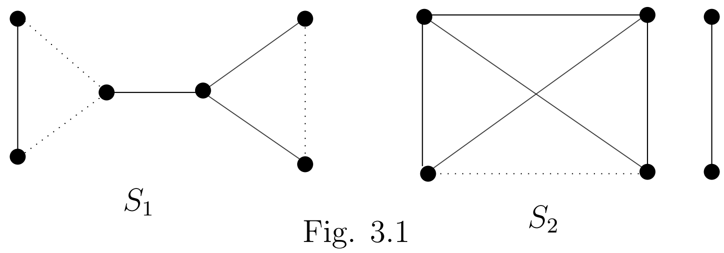


Fig. 3.1

We know from [[14], Theorem 3.11] that a graph containing at least one edge is bipartite if and only if its spectrum, considered as a set of points on the real axis, is symmetric with respect to the origin. This is not true for signed graphs. There exists non bipartite signed graphs whose spectrum is symmetric about origin. Signed graphs S_1 and S_2 in Fig. 3.1 are clearly non bipartite, but $spec(S_1) = spec(S_2) = \{-\sqrt{5}, -1^{(2)}, 1^{(2)}, \sqrt{5}\}$. We say a signed graph has a pairing property if its spectrum is symmetric about the origin. We denote by Δ_n, the set of all signed graphs on n vertices with pairing property. The next result shows that all the odd coefficients of the characteristic polynomial of a signed graph in Δ_n are zero and all the even coefficients alternate in sign.

Lemma 3.3.4. *Let $S \in \Delta_n$, then $\phi_S(x) = x^n + \sum\limits_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j} x^{n-2j}$, where $b_j = |a_j|$ and a_j is the j-th coefficient of characteristic polynomial for $j = 1, 2, \cdots, n$.*

Proof. Assume $S \in \Delta_n$. Let $\alpha_1, \alpha_2, \cdots, \alpha_p$ be the positive eigenvalues of S, where $p \leq \lfloor \frac{n}{2} \rfloor$. Then

$$\phi_S(x) = x^\delta \prod_{j=1}^{p} (x^2 - {\alpha_j}^2) = x^\delta \psi(x^2),$$

where $\psi(x^2) = \prod\limits_{j=1}^{p} (x^2 - {\alpha_j}^2)$ is a polynomial in x^2 and $\delta \geq 0$ is a non negative integer. Using the fact that if the zeroes of a polynomial are real and positive then its coefficients alternate in sign, we see that the coefficients of $\psi(x^2)$ and hence $\phi_S(x)$ alternate in sign. Therefore the result follows. $\square$

Remark 3.3.5. Let S be a bipartite signed graph. Then S has no odd cycles and consequently no basic figure of odd order. By Theorem 3.1.1, we see that the characteristic polynomial of S is of the form $\phi_S(x) = x^{\delta}\psi(x^2)$, where $\delta = 0$ or 1 and $\psi(x^2)$ is a polynomial in x^2. This shows that S has the pairing property, i.e., $S \in \Delta_n$.

We now define a quasi-order relation for signed graphs in Δ_n and show it is possible to compare energy of signed graphs in Δ_n.

Given signed graphs S_1 and S_2 in Δ_n, by Theorem 3.3.4, for $i = 1, 2$, we have

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

where $b_{2j}(S_i)$ are non negative integers for all $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$. If $b_{2j}(S_1) \leq b_{2j}(S_2)$ for all $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, then we define $S_1 \preceq S_2$. If in addition $b_{2j}(S_1) < b_{2j}(S_2)$ for some $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, then we write $S_1 \prec S_2$. Clearly $\preceq$ is a quasi-order relation. The following result which is a consequence of Theorem 3.3.3 shows that the energy increases with respect to this quasi-order relation.

Theorem 3.3.6. *If $S \in \Delta_n$, then*

$$E(S) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log[1 + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(S) x^{2j}] dx.$$

In particular, if $S_1, S_2 \in \Delta_n$ and $S_1 \prec S_2$ then $E(S_1) < E(S_2)$.

Put $b_j = |a_j|$, $j = 1, 2, \cdots, n$. Note $b_1 = 0, b_2 =$number of edges of signed graph S and so on. We denote by $m(S, j)$ the number of matchings of S of size j. This number is independent of signing. We use the convention that $m(S, 0) = 1$. The following result shows that the even and odd coefficients of the characteristic polynomial of a unicyclic signed graph alternate in sign.

Theorem 3.3.7. *Let $S \in S(n, g)$. Then $(-1)^j a_{2j} \geq 0$ for all $j \geq 0$ irrespective of S is balanced or unbalanced and g is odd or even. Moreover, if $g = 2r + 1$, $r \geq 1$, then $(-1)^j a_{2j+1} \geq 0$ (respectively, (≤ 0)) for all $j \geq 0$ if either r is odd and S is* *balanced or r is even and S is unbalanced (respectively, if either r is even and S is balanced or r is odd and S is unbalanced).*

Proof. If g is even, then S is bipartite. By Remark 3.3.5, $a_{2j+1} = 0$ for all $j \geq 0$ and $a_{2j} = (-1)^j b_{2j}$. This gives $(-1)^j a_{2j} = b_{2j} \geq 0$. Also if g is odd, say $g = 2r+1$, then S is non bipartite. Now, $a_{2j} = (-1)^j m(S,j)$ which gives $(-1)^j a_{2j} = m(S,j) \geq 0$. The odd coefficients in balanced and unbalanced case are respectively given by

$$a_{2j+1} = \begin{cases} 0, & \text{if } 2j+1 < g, \\ -2(-1)^{j-r} m(S - C_g, j-r), & \text{if } 2j+1 \geq g. \end{cases}$$

and

$$a_{2j+1} = \begin{cases} 0, & \text{if } 2j+1 < g, \\ 2(-1)^{j-r} m(S - \mathbf{C}_g, j-r), & \text{if } 2j+1 \geq g. \end{cases}$$

From this, the result follows. □

Remark 3.3.8.(i) From the above result, it follows that all unbalanced signed graphs on a fixed unicyclic graph are cospectral.
(ii) It is now possible to compare the energy in unicyclic signed graphs of odd girth as well by means of a quasi-order relation defined on b_j's.

Given two unicyclic signed graphs S_1 and S_2, by Theorem 3.3.7, for $i = 1, 2$, we have

$$\phi_{S_i(x)} = \sum_{j \geq 0} \{(-1)^j b_{2j}(S_i) x^{n-2j} + (-1)^{j+[s]} b_{2j+1}(S_i) x^{n-(2j+1)}\},$$

where $[s] = 1$ if the girth g_i of S_i satisfies $g_i = 2r_i + 1$ with either r_i is even and S_i is balanced or r_i is odd and S_i is unbalanced, otherwise $[s] = 0$. If $b_j(S_1) \leq b_j(S_2)$ for all $j \geq 0$, then we define $S_1 \preceq S_2$. If in addition $b_j(S_1) < b_j(S_2)$ for some j, then we write $S_1 \prec S_2$. The following result is a consequence of Theorem 3.3.3

and it shows that the energy increases with respect to this quasi-order relation.

Theorem 3.3.9. *Let S be a unicyclic signed graph of order n. Then*

$$E(S) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{x^2}\log[(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(S)x^{2j})^2 + (\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j+1}(S)x^{2j+1})^2]dx.$$

In particular, if S_1 and S_2 are unicyclic signed graphs and $S_1 \prec S_2$, then $E(S_1) < E(S_2)$.

We now show that all signed graphs on a unicyclic graph of odd girth are equienergetic.

Corollary 3.3.10. *For each positive integer $n \geq 3$, there exists a pair of connected, non cospectral and equienergetic unicyclic signed graphs of order n with one constituent balanced and other constituent unbalanced.*

Proof. Let G be a unicyclic graph of order n and odd girth g. Let S be any balanced signed graph on G and T be any unbalanced signed graph on G. Then S and T are non cospectral by Theorem 3.1.2. The coefficients of signed graphs S and T are related as follows

$a_{2j+1}(S) = -a_{2j+1}(T)$ for all $j = 0, 1, 2, \cdots \lfloor \frac{n}{2} \rfloor$ and $a_{2j}(S) = a_{2j}(T)$ for all $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$. Thus $b_j(S) = b_j(T)$ for all $j = 1, 2, \cdots, n$. By Theorem 3.3.9 $E(S) = E(T)$.

Now we use Theorem 3.3.9 to compare the energies of signed graphs obtained from a unicyclic bipartite graph.

Theorem 3.3.11. *Let G be a unicyclic graph of order n and even girth g i.e., bipartite unicyclic graph, and let S be any balanced signed graph on G and T be any unbalanced one. Then*

(i)$E(S) < E(T)$ if and only if $g \equiv 0 \pmod 4$;

(ii)$E(S) > E(T)$ if and only if $g \equiv 2 \pmod 4$.

Proof. Let G be a unicyclic graph of order n and even girth $g \geq 4$ and let S and T respectively be any balanced signed graph and any unbalanced signed graph on

G. The coefficients of S are given by
$a_{2j}(S) = m(S,j)$ for all $j = 1, 2, \ldots, \frac{g}{2} - 1$; $a_{g+2j}(S) = -2(-1)^j m(S - C_g, j) + (-1)^{\frac{g}{2}+j} m(S, \frac{g}{2} + j)$ for all $j = 0, 1, \cdots, \lfloor \frac{n-g}{2} \rfloor$ and $a_{2j+1}(S) = 0$ for all $j = 0, 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$.
whereas the coefficients of T are given by
$a_{2j}(T) = m(T,j)$ for all $j = 1, 2, \ldots, \frac{g}{2} - 1$; $a_{g+2j}(T) = 2(-1)^j m(T - \mathbf{C}_g, j) + (-1)^{\frac{g}{2}+j} m(T, \frac{g}{2} + j)$ for all $j = 0, 1, \cdots, \lfloor \frac{n-g}{2} \rfloor$ and $a_{2j+1}(T) = 0$ for all $j = 0, 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$.
Two cases arise here (i) $g \equiv 0 \pmod 4$ and (ii) $g \equiv 2 \pmod 4$.
Case (i) $g \equiv 0 \pmod 4$. We have $b_{2j+1}(S) = b_{2j+1}(T) = 0$ for all $j = 0, 1, \cdots, \lfloor \frac{n}{2} \rfloor$; $b_{2j}(S) = b_{2j}(T)$ for all $j = 1, 2, \ldots, \frac{g}{2} - 1$; $b_{g+2j}(S) = |-2m(S - C_g, j) + m(S, \frac{g}{2} + j)|$ for all $j = 0, 1, \cdots, \lfloor \frac{n-g}{2} \rfloor$ and $b_{g+2j}(T) = |2m(T - \mathbf{C}_g, j) + m(T, \frac{g}{2} + j)|$ for all $j = 0, 1, \cdots, \lfloor \frac{n-g}{2} \rfloor$.
Clearly, $b_j(S) \leq b_j(T)$ for all $j = 1, 2, \cdots, n$. In particular $b_g(S) < b_g(T)$. Therefore $S \prec T$ and by Theorem 3.3.9, $E(S) < E(T)$.
The proof of case (ii) follows on similar lines. $\square$

3.4 Unicyclic signed graphs with minimal energy

Gill and Acharya [24] obtained the following recurrence formula for the characteristic polynomial of a signed graph.

Lemma 3.4.1. *Let S be a signed graph and v be its arbitrary vertex. Then*

$$\phi_S(x) = x\phi_{(S-v)}(x) - \sum_{(w,v)\in\mathscr{E}} \phi_{(S-v-w)}(x) - 2\Big[\sum_{Z\in C^+(v)} \phi_{(S-V(Z))}(x) - \sum_{Z\in C^-(v)} \phi_{(S-V(Z))}(x)\Big],$$

where $C^+(v)$ and $C^-(v)$ denote the set of positive and negative cycles containing vertex v.

Now we have the following result.

Lemma 3.4.2. *Let $S \in S(n,g)$ be unbalanced, and let (u,v) be the pendant edge of S with pendant vertex v. Then*

$$b_j(S) = b_j(S-v) + b_{j-2}(S-v-u).$$

Proof. Since S is unicyclic and v is a pendant vertex, Lemma 3.4.1 takes the form

$$\phi_S(x) = x\phi_{(S-v)}(x) - \phi_{(S-v-u)}(x)$$

which gives

$$a_j(S) = a_j(S-v) - a_{j-2}(S-v-u).$$

We now claim that the coefficients $a_j(S-v)$ and $a_{j-2}(S-v-u)$ are of opposite signs. In case S is bipartite, then all is clear by Remark 3.3.5. Assume S is non bipartite and both the signed graphs $S-v$ and $S-v-u$ contain the odd cycle $\mathbf{C}_g$, then claim follows by Theorem 3.3.7. Finally, suppose only $S-v-u$ is acyclic; for odd j, $a_j(S-v-u) = 0$, so $a_j(S-v) = -a_{j-2}(S-v-u)$ and same holds for even j, since basic figures are only matchings. This proves our claim.

Now $b_j(S) = |a_j(S)| = |a_j(S-v) - a_{j-2}(S-v-u)| = |a_j(S-v)| + |a_{j-2}(S-v-u)| = b_j(S-v) + b_{j-2}(S-v-u)$. $\square$

The following result shows that among all unbalanced unicyclic signed graphs in $S(n,g)$, $\mathbf{S}_n^g$ has minimal energy.

Theorem 3.4.3. *Let $S \in S(n,g)$ be unbalanced and $S \neq \mathbf{S}_n^g$. Then $\mathbf{S}_n^g \prec S$ and $E(\mathbf{S}_n^g) < E(S)$.*

Proof. We prove the result by induction on $n-g$. If $n-g=0$, the result is vacuously true. Let $p \geq 1$ and suppose the result is true for $n-g<p$. We show it holds for $n-g=p$. Since S is unicyclic and $n>g$, so S is not a cycle and hence it must have a pendant vertex, say v, and v is adjacent to a unique vertex say u. By Lemma 3.4.2, we have

$$b_j(S) = b_j(S-v) + b_{j-2}(S-v-u),$$
$$b_j(\mathbf{S}_n^g) = b_j(\mathbf{S}_{n-1}^g) + b_{j-2}(P_{g-1}).$$

By induction hypothesis,

$$b_j(S-v) \geq b_j(\mathbf{S}_{n-1}^g) \tag{3.1}$$

for all $j \geq 0$.

As

$$b_{j-2}(P_{g-1}) = \begin{cases} 0, & \text{if } j \text{ is odd or if } j \text{ is even and } j > g+1; \\ m(P_{g-1}, \frac{j-2}{2}), & \text{if } j \text{ is even and } j \leq g+1. \end{cases}$$

Since $S - v - u$ contains the signed path P_{g-1} as its subgraph, therefore if j is odd or $j > l+1$, then $b_{j-2}(S-u-v) \geq b_{j-2}(P_{g-1})$. If j is even and $j \leq g+1$, then $b_{j-2}(S-v-u) = m(S-v-u, \frac{(j-2)}{2}) \geq m(P_{g-1}, \frac{(j-2)}{2})$. Therefore, we have

$$b_{j-2}(S-v-u) \geq b_{j-2}(P_{g-1}) \tag{3.2}$$

From (3.1) and (3.2), we see $b_j(S) \geq b_j(\mathbf{S}_n^g)$. Also if $S \neq \mathbf{S}_n^g$, then $b_2(S - v - u) > g-2 = b_2(P_{g-1})$. Hence $b_4(\mathbf{S}_n^g) < b_4(S)$. The second part follows by Theorem 3.3.9. □

The following result shows that $\mathbf{S}_n^4$ has minimal energy among all unicyclic signed graphs $\mathbf{S}_n^g$, where $n \geq g$, $n \geq 6$ and $g \geq 4$.

Theorem 3.4.4. *Let $n \geq g$, where $n \geq 6$ and $g \geq 5$. Then $\mathbf{S}_n^4 \prec \mathbf{S}_n^g$ and $E(\mathbf{S}_n^4) < E(\mathbf{S}_n^g)$.*

Proof. We use induction on $n-g$ for $n \geq g$, where $n \geq 6$ and $g \geq 5$. By Theorem 3.1.1, we have

$$\phi_{\mathbf{S}_n^4}(x) = x^{n-4}\{x^4 - nx^2 + 2(n-2)\}. \tag{3.3}$$

It is enough to show that $b_4(\mathbf{S}_n^4) < b_4(\mathbf{S}_n^g)$. If $n-g=0$, then $\mathbf{S}_n^g = \mathbf{C}_n$. Note that $b_4(\mathbf{C}_n) = \frac{n}{2}(n-3)$ and $b_4(\mathbf{S}_n^4) = 2(n-2)$. Clearly $b_4(\mathbf{S}_n^4) < b_4(\mathbf{C}_n)$ for all $n \geq 6$.

By Lemma 3.4.2, we have
$b_4(\mathbf{S}_n^g) = b_4(\mathbf{S}_{n-1}^g) + b_2(P_{g-1}) = b_4(\mathbf{S}_{n-1}^g) + g - 2 = 2(n-1-2) + g - 2 = 2(n-2) + g - 4 > 2(n-2)$, for $g \geq 5$. □

Now we determine unicyclic unbalanced signed graphs with minimal energy.

Theorem 3.4.5. *Let S be an unbalanced unicyclic signed graph with $n \geq 6$ vertices and $S \neq \mathbf{S}_n^3$. Then $E(\mathbf{S}_n^3) < E(S)$.*

Proof. In view of Theorems 3.4.3 and 3.4.4, it suffices to prove that $E(\mathbf{S}_n^3) < E(\mathbf{S}_n^4)$ for all $n \geq 6$. By Theorem 3.1.1, we have

$$\phi_{\mathbf{S}_n^3}(x) = x^{n-4}\{x^4 - nx^2 + 2x + (n-3)\}. \tag{3.4}$$

From equations (3.3) and (3.4) and Theorem 3.3.9, we have

$$E(\mathbf{S}_n^4) - E(\mathbf{S}_n^3) = \frac{1}{\pi}\int_0^\infty \frac{1}{x^2}\log\frac{[(1+nx^2+2(n-2)x^4)]^2}{[(1+nx^2+(n-3)x^4)^2+4x^6]}dx.$$

Let $f(x) = [1+nx^2+2(n-2)x^4]^2$ and $g(x) = [(1+nx^2+(n-3)x^4)^2+4x^6]$. Then

$$\begin{aligned} f(x) - g(x) &= [1+nx^2+2(n-2)x^4]^2 - [(1+nx^2+(n-3)x^4)^2+4x^6] \\ &= 2(n-1)x^4 + 2(n-2)(n+1)x^6 + (3n-7)(n-1)x^8 > 0, \end{aligned}$$

for all $n \geq 6$. Therefore, $E(\mathbf{S}_n^3) < E(\mathbf{S}_n^4)$ for all $n \geq 6$. $\square$

The following result characterizes unicyclic signed graphs with minimal energy.

Theorem 3.4.6. *Among all unicyclic signed graphs with $n \geq 6$ vertices, all signed graphs in $[S_n^3]$ and $[\mathbf{S}_n^3]$ have minimal energy. Moreover, for $n = 3, 4$ and 5 all signed graphs in $[S]$ have minimal energy, where S is one of the signed graphs C_3 or $\mathbf{C_3}$ or C_4 or S_5^4.*

Proof. A manual calculation shows that for $m = 3, 4$ and 5 all signed graphs in $[S]$ have minimal energy, where S is one of the signed graphs C_3 or $\mathbf{C_3}$ or C_4 or S_5^4. As in Theorem 3.3.10, $E(S_n^3) = E(\mathbf{S}_n^3)$. By Theorems 3.1.4 and 3.4.5 and noting that all graphs in a switching class are equienergetic, the result follows. $\square$

3.5 Equienergetic signed graphs

Two signed graphs are said to be isomorphic if their underlying graphs are isomorphic such that the signs are preserved. Any two isomorphic signed graphs are obviously cospectral. There exist unbalanced non isomorphic cospectral signed graphs, e.g., signed graphs S_1 and S_2 in Fig. 3.1. Two signed graphs S_1 and S_2 of same order are said to be equienergetic if $E(S_1) = E(S_2)$. Cospectral signed graphs are obviously equienergetic, therefore in view of Theorem 3.1.2, the problem of equienergetic signed graphs reduces to problem of construction of non cospectral pairs of equienergetic signed graphs such that for every pair not both signed graphs are balanced. In this regard, we have shown for each positive integer $n \geq 3$, there exists a pair of connected, non cospectral and equienergetic unicyclic signed graphs on n vertices with one constituent balanced and the other unbalanced.

We note that the spectral radius of S, $\rho(S) = max_{1\leq k\leq n}|x_k|$ is an eigenvalue of S for every $S \in \Delta_n$. The following Lemma gives the spectrum of Cartesian and Kronecker product of two signed graphs in terms of that of the corresponding signed graphs [22].

Lemma 3.5.1. *Let S_1 and S_2 be two signed graphs with respective eigenvalues $\xi_1, \xi_2, \cdots, \xi_{n_1}$ and $\zeta_1, \zeta_2, \cdots, \zeta_{n_2}$. Then*
(i) the eigenvalues of $S_1 \times S_2$ are $\xi_i + \zeta_j$, for all $i = 1, 2, \cdots, n_1$ and $j = 1, 2, \cdots, n_2$;
(ii) the eigenvalues of $S_1 \otimes S_2$ are $\xi_i\zeta_j$, for all $i = 1, 2, \cdots, n_1$ and $j = 1, 2, \cdots, n_2$.

We have the following result.

Lemma 3.5.2. *(i) $E(S_1 \otimes S_2) = E(S_1)E(S_2)$*
(ii) For each $n \geq 3$, $(K_n, -K_n)$ is a pair of non cospectral and equienergetic signed graphs with one constituent balanced and the other unbalanced.
(iii) For all positive integers $m, n \geq 2$, the signed graphs $S = -K_m \times -K_n$ and $T = -K_m \otimes -K_n$ are non cospectral equienergetic signed graphs with S unbalanced and T balanced.
Proof. Let $x_1, x_2, \ldots, x_{n_1}$ be eigenvalues of S_1 and $y_1, y_2, \cdots, y_{n_2}$ be eigenvalues of S_2. By Lemma 3.5.1, eigenvalues of $S_1 \otimes S_2$ are x_iy_j, where $i = 1, 2, \ldots, n_1$ and

$j = 1, 2, \ldots, n_2$. Therefore, $E(S_1 \otimes S_2) = \sum\limits_{i,j} |x_i y_j| = \sum\limits_{i=1}^{n_1} |x_i| \sum\limits_{j=1}^{n_2} |y_j| = E(S_1)E(S_2)$. This proves part (i).

(ii) We know that for each positive integer $n \geq 3$, $spec(K_n) = \{-1^{(n-1)}, n-1\}$ so that $spec(-K_n) = \{1-n, 1^{(n-1)}\}$. Therefore, $E(K_n) = E(-K_n) = 2(n-1)$. Note that K_n is balanced whereas $-K_n$ is unbalanced.

(iii) We have, $Spec(S) = \{2-m-n, (2-m)^{(n-1)}, (2-n)^{(m-1)}, 2^{(m-1)(n-1)}\} \neq \{(1-m)(1-n), (1-m)^{(n-1)}, (1-n)^{(m-1)}, 1^{(m-1)(n-1)}\} = spec(T)$. Therefore S and T are non cospectral.

Also, $E(S) = |2-m-n| + (n-1)|2-m| + (m-1)|2-n| + (m-1)(n-1)|2| = 4(m-1)(n-1)$. By part (i), $E(T) = E(-K_m \otimes -K_n) = E(-K_m)E(-K_n) = 4(m-1)(n-1)$. Therefore S and T are equienergetic. S is unbalanced and T is balanced follows from Theorem 3.1.2.

The following result characterizes a signed graph S in Δ_n for which the Cartesian product and Kronecker product of S with K_2 are unbalanced, non cospectral and equienergetic.

Theorem 3.5.3. *Let S be an unbalanced signed graph in Δ_n with at least one edge having eigenvalues $x_1, x_2, \cdots, x_n$. Then $S \times K_2$ and $S \otimes K_2$ are unbalanced, noncospectral and equienergetic if and only if $|x_j| \geq 1$, for all $j = 1, 2, \cdots, n$.*

Proof. By Theorem 3.1.2, it is clear that $S \in \Delta_n$ is unbalanced if and only if both $S \times K_2$ and $S \otimes K_2$ are unbalanced. We first suppose that $|x_j| \geq 1$ for all $j = 1, 2, \ldots, n$. Let $x_1 \geq x_2 \geq \cdots \geq x_n$. Assume $x_1, x_2, \ldots, x_k$ are positive and $x_{k+1}, x_{k+2} \ldots, x_n$ are negative.

Also

$$E(S \times K_2) = \sum_{j=1}^{k} (|x_j + 1| + |x_j - 1|) + \sum_{j=k+1}^{n} (|x_j + 1| + |x_j - 1|).$$

As $|x_j| \geq 1$ for all $j = 1, 2, \ldots, n$, we have

$$
\begin{aligned}
E(S \times K_2) &= \sum_{j=1}^{k}(|x_j| + 1 + |x_j| - 1) + \sum_{j=k+1}^{n}(|x_j| - 1 + |x_j| + 1) \\
&= 2\sum_{j=1}^{k}|x_j| + 2\sum_{j=k+1}^{n}|x_j| = 2\sum_{j=1}^{n}|x_j| = 2E(S) \\
&= E(S)E(K_2) = E(S \otimes K_2).
\end{aligned}
$$

Note that $x_1 + 1 \in spec(S \times K_2)$ but $x_1 + 1 \notin spec(S \otimes K_2)$, therefore $S \times K_2$ and $S \otimes K_2$ are non cospectral.

Conversely, suppose $|x_s| < 1$ for some s. Because of pairing property, we can assume $x_s \geq 0$. Choose a real number α_s such that $x_s + \alpha_s = 1$. Therefore, $|x_s + 1| + |x_s - 1| = 1 + x_s + \alpha_s = 2 > 2|x_s|$. Suppose $|x_j| \geq 1$ for $j = 1, 2, \ldots, k$ and $|x_j| < 1$ for $j = k+1, k+2, \ldots, n$. Then as before $\sum_{j=1}^{k}(|x_j + 1| + |x_j - 1|) = 2\sum_{j=1}^{k}|x_j|$ and $\sum_{j=k+1}^{n}(|x_j + 1| + |x_j - 1|) > 2\sum_{j=k+1}^{n}|x_j|$.

Therefore $E(S \times K_2) = \sum_{j=1}^{k}(|x_j+1|+|x_j-1|) + \sum_{j=k+1}^{n}(|x_j+1|+|x_j-1|) > 2\sum_{j=1}^{n}|x_j| = E(S \otimes K_2)$, a contradiction. □

Example 3.5.4. Consider signed graphs S_1 and S_2 in Fig. 3.1. Clearly, eigenvalues of S_1 and S_2 have absolute value at least 1, therefore by Theorem 3.5.3, $S_i \times K_2$ and $S_i \otimes K_2$ are unbalanced, non cospectral and equienergetic for $i = 1, 2$.

We know from [22] the eigenvalues of a positive and negative cycles with n vertices are given by the following result

Lemma 3.5.5. *The eigenvalues of C_n and $\mathbf{C_n}$ are respectively given by $x_k = 2\cos\frac{2k\pi}{n}, \quad k = 0, 1, \cdots, n-1$ and $x_k = 2\cos\frac{(2k+1)\pi}{n}, \quad k = 0, 1, \cdots, n-1$.*

From Lemma 3.5.5 one can derive the following energy formulae. For proof see Theorem 4.3.1

$$E(C_n) = \begin{cases} 4\cot\frac{\pi}{n}, & \text{if } n = 4k, \\ 4\csc\frac{\pi}{n}, & \text{if } n = 4k+2, \\ 2\csc\frac{\pi}{2n}, & \text{if } n = 2k+1. \end{cases}$$

and

$$E(\mathbf{C_n}) = \begin{cases} 4\csc\frac{\pi}{n}, & \text{if } n = 4k, \\ 4\cot\frac{\pi}{n}, & \text{if } n = 4k+2, \\ 2\csc\frac{\pi}{2n}, & \text{if } n = 2k+1. \end{cases}$$

From energy formulae we see that for each odd $n \geq 3$, $E(C_n) = E(\mathbf{C_n})$, where C_n is balanced and $\mathbf{C_n}$ is unbalanced as already proved in Theorem 3.3.10 but here we have exact formulae for energy.

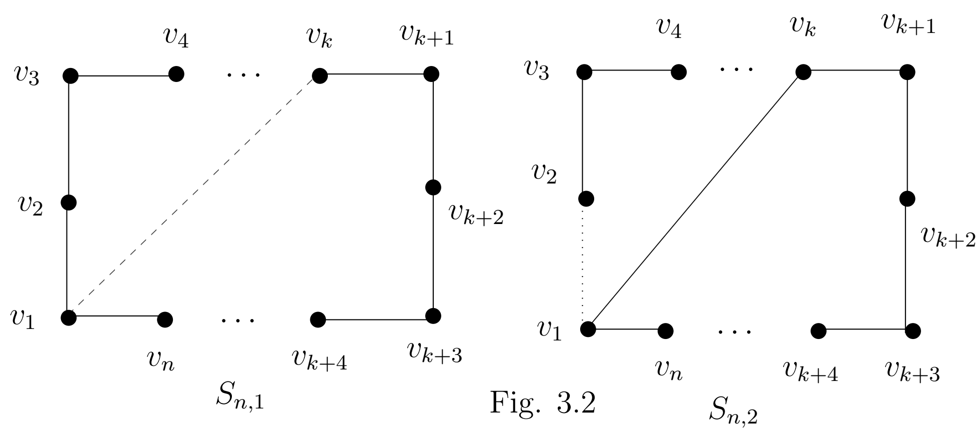


Fig. 3.2

It is easy to see that there does not exist a pair of non cospectral and equienergetic signed graphs on 3 vertices with both constituents unbalanced. The following result proves the existence of a pair of connected, non cospectral and equienergetic signed graphs on $n \geq 4$ vertices with both the constituents unbalanced.

Theorem 3.5.6. *For each positive integer $n \geq 4$, there exists a pair of connected, non cospectral equienergetic signed graphs of order n with both constituents unbalanced.*

Proof. Case 1. When n is odd. Assume $n \geq 5$ is an odd integer. Consider the signed graphs $S_{n,1}$ and $S_{n,2}$ with vertex and edge sets given by

$$V(S_{n,1}) = V(S_{n,2}) = \{v_1, v_2, \cdots, v_n\},$$

$$\mathscr{E}(S_{n,1}) = \{(v_1, v_2), (v_2, v_3), \cdots, (v_k, v_{k+1}), \cdots, (v_n, v_1), [v_1, v_k]\}$$

and

$$\mathscr{E}(S_{n,2}) = \{[v_1, v_2], (v_2, v_3), \cdots, (v_k, v_{k+1}), \cdots, (v_n, v_1), (v_1, v_k)\},$$

where (u, v) means edge from vertex u to v is positive and $[u, v]$ means edge from u to v is negative and we choose vertex v_k such that the positive integer k is even. The signed graphs so constructed are shown in Fig. 3.2.

As both the signed graphs have only one even cycle $\mathbf{C_k}$ and their underlying graphs are same, it follows by Theorem 3.1.1 that $a_{2j}(S_{n,1}) = a_{2j}(S_{n,2})$, for all $j = 1, 2, \cdots, \frac{n-1}{2}$.

Also, the odd coefficients of $S_{n,1}$ are given by

$a_{2j-1}(S_{n,1}) = 0$ for all $j = 1, 2, \cdots, \frac{n-k+1}{2}$

and

$$a_{n-k+2+2j}(S_{n,1}) = \begin{cases} 2(-1)^{(j+2)} m(S_{n,1} - \mathbf{C}_{n-k+2}, j), & \text{if } j = 0, 1, 2, \cdots, \frac{k-4}{2}, \\ 2\{(-1)^{\frac{k+2}{2}} m(S_{n,1} - \mathbf{C}_{n-k+2}, \frac{k-2}{2}) - 1\}, & \text{if } j = \frac{k-2}{2}, \end{cases}$$

whereas the odd coefficients of $S_{n,2}$ are given by

$a_{2j-1}(S_{n,2}) = 0$ for all $j = 1, 2, \cdots, \frac{n-k+1}{2}$

and

$$a_{n-k+2+2j}(S_{n,2}) = \begin{cases} 2(-1)^{(j+1)} m(S_{n,2} - C_{n-k+2}, j), & \text{if } j = 0, 1, 2, \cdots, \frac{k-4}{2}, \\ 2\{(-1)^{\frac{k}{2}} m(S_{n,2} - C_{n-k+2}, \frac{k-2}{2}) + 1\}, & \text{if } j = \frac{k-2}{2}. \end{cases}$$

It is clear that $a_{2j}(S_{n,1}) = a_{2j}(S_{n,2})$, for all $j = 1, 2, \cdots, \frac{n-1}{2}$ and $a_{2j-1}(S_{n,1}) = -a_{2j-1}(S_{n,2})$ for all $j = 1, 2, \cdots, \frac{n+1}{2}$. Thus $S_{n,1}$ and $S_{n,2}$ are non cospectral. From the relation between coefficients of these two signed graphs, it follows that $\phi_{S_{n,1}}(-x) = -\phi_{S_{n,2}}(x)$ which gives $spec(S_{n,1}) = -spec(S_{n,2})$. Thus $E(S_{n,1}) = E(S_{n,2})$.

Case 2. When n is even. Assume $n \geq 6$ is even. Consider the signed graphs $S_{n,3}$ and $S_{n,4}$ with vertex and edge sets given by

$$V(S_{n,3}) = V(S_{n,4}) = \{v_1, v_2, \cdots, v_n\},$$

$$\mathscr{E}(S_{n,3}) = \{(v_1, v_2), (v_2, v_3), \cdots, (v_k, v_{k+1}), \cdots, (v_{n-1}, v_1), [v_1, v_k], (v_k, v_n)\},$$

and

$$\mathscr{E}(S_{n,4}) = \{[v_1, v_2], (v_2, v_3), \cdots, (v_k, v_{k+1}), \cdots, (v_{n-1}, v_1), (v_1, v_k)(v_k, v_n)\},$$

where k is even. The signed graphs so constructed are shown in Fig. 3.3. As in Case 1, it is easy to check that $S_{n,3}$ and $S_{n,4}$ are two non cospectral equienergetic signed graphs. Clearly, all the signed graphs are unbalanced.

For $n = 4$, consider the signed graphs S_1 and S_2 as shown in Fig. 3.4. By Theorem 3.1.1, the characteristic polynomials of S_1 and S_2 are $\phi_{S_1}(x) = x^4 - 5x^2 + 4$ and $\phi_{S_2}(x) = x^4 - 6x^2 + 8x - 3$ so that $spec(S_1) = \{-2, -1, 1, 2\}$ and $spec(S_2) = \{-3, 1^{(3)}\}$. That is, S_1 and S_2 are non cospectral. Also $E(S_1) = E(S_2) = 6$ and S_1 and S_2 are unbalanced. □

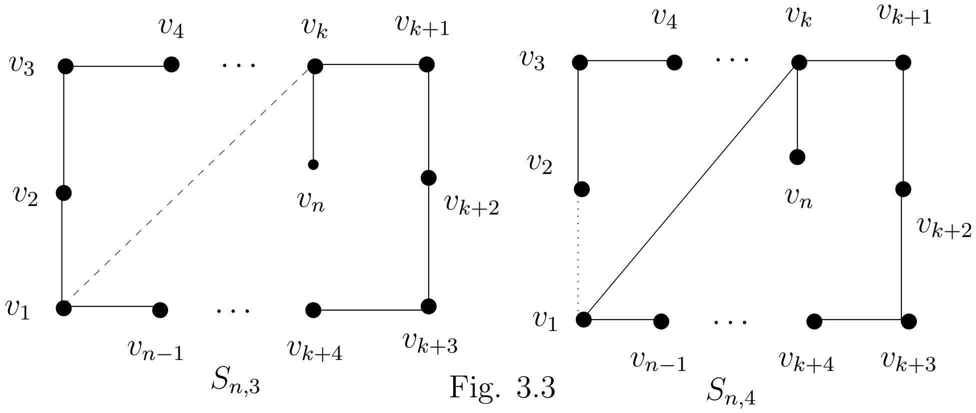


Fig. 3.3

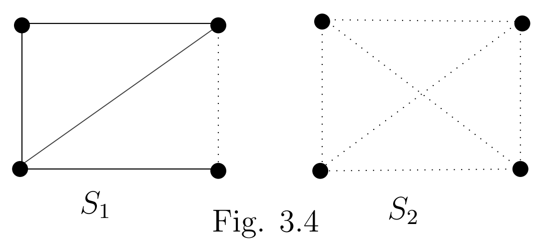


Fig. 3.4

3.6 Conclusion

We conclude this Chapter with the following open problem.

Problem 3.6.1. *Characterize signed graphs having pairing property.*

CHAPTER 4

Energy of signed digraphs

In this Chapter, we extend the concept of energy to signed digraphs and we obtain Coulson's integral formula for the energy of signed digraphs. We characterize unicyclic signed digraphs with minimal and maximal energy. We extend the concept of non complete extended p sum (or briefly, NEPS) to signed digraphs. We construct pairs of non cospectral equienergetic signed digraphs. Moreover, we extend McClelland's inequality to signed digraphs and also obtain sharp upper bound for energy of signed digraph in terms of the number of arcs.

4.1 Introduction

A *signed digraph* is defined to be a pair $S = (D, \sigma)$ where $D = (V, \mathscr{A})$ is the underlying digraph and $\sigma : \mathscr{A} \to \{-1, 1\}$ is the signing function. The sets of positive and negative arcs of S are respectively denoted by $\mathscr{A}^+$ and $\mathscr{A}^-$. Thus $\mathscr{A} = \mathscr{A}^+ \cup \mathscr{A}^-$. A signed digraph is said to be homogeneous if all of its arcs have either positive sign or negative sign and heterogeneous, otherwise.

Two vertices are adjacent if they are connected by an arc. A path of length $n-1$ ($n \geq 2$), denoted by P_n, is a signed digraph on n vertices $v_1, v_2, \cdots, v_n$ with $n-1$ signed arcs (v_i, v_{i+1}), $i = 1, 2, \ldots, n-1$. A cycle of length n is a signed digraph having vertices $v_1, v_2, \cdots, v_n$ and signed arcs (v_i, v_{i+1}), $i = 1, 2, \cdots, n-1$ and (v_n, v_1). The sign of a signed digraph is defined as the product of signs of its arcs. A signed digraph is said to be positive (respectively, negative) if its sign is positive (respectively, negative) i.e., it contains an even (respectively, odd) number of negative arcs. A signed digraph is said to be all-positive (respectively, all-negative) if all its arcs are positive (respectively, negative). A signed digraph is said to be cycle balanced if each of its cycles is positive, otherwise non cycle balanced. Throughout this Chapter, we call cycle balanced cycle a positive cycle and non cycle balanced cycle a negative cycle and respectively denote them by C_n and $\mathbf{C}_n$, where n is the number of vertices. Further dotted arcs denote the negative arcs and bold arcs denote the positive arcs. A linear signed subdigraph of a signed digraph is a subdigraph with indegree and outdegree of each vertex equal to one.

The adjacency matrix of a signed digraph S whose vertices are $v_1, v_2, \cdots, v_n$ is the $n \times n$ matrix $A(S) = (a_{ij})$, where

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

The characteristic polynomial $|xI - A(S)|$ of the adjacency matrix $A(S)$ of signed digraph S is called the characteristic polynomial of S and is denoted by $\phi_S(x)$. The eigenvalues of $A(S)$ are called the eigenvalues of S.

A signed digraph is said to be symmetric if $(u, v) \in \mathscr{A}^+$ or $\mathscr{A}^-$, then $(v, u) \in \mathscr{A}^+$ or $\mathscr{A}^-$, where $u, v \in V$. A one to one correspondence between signed graphs and symmetric signed digraphs is given by $S \rightsquigarrow \overleftrightarrow{S}$, where $\overleftrightarrow{S}$ has the same vertex set as that of signed graph S, and each signed edge (u, v) is replaced by a pair of symmetric arcs (u, v) and (v, u) both with same sign as that of edge (u, v). Under this correspondence a signed graph can be identified with a symmetric signed digraph. A signed digraph is said to be skew symmetric if its adjacency matrix is skew symmetric. We denote a skew symmetric signed digraph of order n by $\mathbf{S}_n$.

The weighted directed graph S of an $n \times n$ matrix $M = (m_{ij})$ of reals consists of n vertices with vertex i joined to vertex j by a directed arc with weight m_{ij} if and only if m_{ij} is non-zero. In case the matrix consists of entries $-1, 0$ and 1, then we get a signed digraph. Thus there is a one to one correspondence between the set of integral $(-1, 0, 1)$-matrices of order n and the set of signed digraphs of order n.

The following is the coefficient Theorem for signed digraphs [2].

Theorem 4.1.1. *If S is a signed digraph with characteristic polynomial*

$$\phi_S(x) = x^n + a_1 x^{n-1} + \cdots + a_{n-1} x + a_n,$$

then

$$a_j = \sum_{L \in \pounds_j} (-1)^{p(L)} \prod_{Z \in c(L)} s(Z),$$

for all $j = 1, 2, \cdots, n$, *where* $\pounds_j$ *is the set of all linear signed subdigraphs* L *of* S *of order* j, $p(L)$ *denotes number of components of* L *and* $c(L)$ *denotes the set of all cycles of* L *and* $s(Z)$ *the sign of cycle* Z.

Remark 4.1.2. For undirected signed graph (when considered as symmetric signed digraph) Theorem 4.1.1 takes the form of Theorem 3.1.1.

The spectral criterion for cycle balance of signed digraphs given by Acharya [1] is as follows.

Theorem 4.1.3. *A signed digraph is cycle balanced if and only if it is cospectral with the underlying unsigned digraph.*

4.2 Energy of signed digraphs

In this section, we extend the concept of energy to signed digraphs in a similar way as graph energy has been extended to energy of digraphs in [62]. Unlike signed graphs the adjacency matrix of a signed digraph need not be real symmetric, so eigenvalues can be complex numbers.

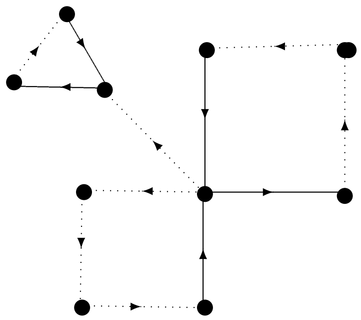
Definition 4.2.1. Let S be a signed digraph of order n having eigenvalues $z_1, z_2, \cdots, z_n$. The energy of S is defined as

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

where $\Re z_j$ denotes the real part of complex number z_j.

If S is a signed graph and $\overleftrightarrow{S}$ be its symmetric signed digraph, then clearly $A(S) = A(\overleftrightarrow{S})$ and so $E(S) = E(\overleftrightarrow{S})$. In this way, definition 4.2.1 generalizes the concept of energy of undirected signed graphs.

Example 4.2.2. Let S be a signed digraph shown in Figure 4.1. Clearly, S is non cycle balanced signed digraph. By Theorem 4.1.1, the characteristic polynomial of S is $\phi_S(x) = x^{10} + x^7 = x^7(x^3 + 1)$. The spectrum of S is $spec(S) = \{-1, 0^7, \frac{1-\sqrt{3}\iota}{2}, \frac{1+\sqrt{3}\iota}{2}\}$, where $\iota = \sqrt{-1}$, so $E(S) = 2$.



S

Figure 4.1

Example 4.2.3. Let S be an acyclic signed digraph. Then by Theorem 4.1.1, the characteristic polynomial of S is $\phi_S(x) = x^n$, so that $spec(S) = \{0^n\}$ and hence $E(S) = 0$.

Example 4.2.4. Consider $\mathbf{S}_n$, the skew symmetric signed digraph on $n \geq 2$ vertices, then eigenvalues are of the form $\pm\iota\alpha$, where $\alpha \in \mathbb{R}$ and therefore $E(S) = 0$.

Example 4.2.5. If S is the signed directed cycle on n vertices, then the characteristic polynomial of S is $\phi_S(x) = x^n + (-1)^{[s]}$, where the symbol $[s]$ is defined as $[s] = 1$ or 0 according as S is positive or negative. If $S = C_n$, then $spec(S) = \{e^{\frac{2\iota j\pi}{n}},\ j = 0, 1, \cdots, n-1\}$ so that $E(S) = \sum_{j=0}^{n-1} |\cos(\frac{2j\pi}{n})|$. If $S = \mathbf{C}_n$, then $spec(S) = \{e^{\frac{\iota(2j+1)\pi}{n}},\ j = 0, 1, \cdots, n-1\}$ so that $E(S) = \sum_{j=0}^{n-1} |\cos(\frac{(2j+1)\pi}{n})|$. In particular if $S = \mathbf{C}_4$, then $spec(S) = \{\frac{1-\iota}{\sqrt{2}}, \frac{1+\iota}{\sqrt{2}}, \frac{-1-\iota}{\sqrt{2}}, \frac{-1+\iota}{\sqrt{2}}\}$ and $E(S) = 2\sqrt{2}$.

Example 4.2.6. Let S be a signed digraph having n vertices and unique cycle of length r, where $2 \leq r \leq n$. Then by Theorem 4.1.1, $\phi_S(x) = x^n + (-1)^{[s]}x^{n-r} = x^{n-r}(x^r + (-1)^{[s]})$, where the symbol $[s]$ is defined as $[s] = 1$ or 0 according as S is cycle balanced or non cycle balanced. Clearly, energy equals to the energy of the unique cycle.

Given t signed digraphs $S_1, S_2, \cdots S_t$, their direct sum denoted by $S_1 \oplus S_2 \oplus \cdots \oplus S_t$ is the signed digraph with $V(S_1 \oplus S_2 \oplus \cdots \oplus S_t) = \bigcup\limits_{j=1}^{t} V(S_j)$ and arc set $\mathscr{A}(S_1 \oplus S_2 \oplus \cdots \oplus S_t) = \bigcup\limits_{j=1}^{t} \mathscr{A}(S_j)$.

Now we have the following result.

Theorem 4.2.7. Let S be a signed digraph on n vertices and $S_1, S_2, \cdots, S_k$ be its strong components. Then $E(S) = \sum\limits_{j=1}^{k} E(S_j)$.

Proof. Let $Y = \{a \in \mathscr{A} : a \notin c(S)\}$, where $c(S)$ is the set of all cycles of S. By Theorem 4.1.1, $\phi_S(x) = \phi_{S-Y}(x)$, where $S-Y$ is the signed digraph obtained from S by deleting the non-cyclic arcs. Clearly, $S - Y = S_1 \oplus S_2 \oplus \cdots \oplus S_k$ and adjacency matrix of signed digraph $S-Y$ is in block diagonal form with diagonal blocks as the adjacency matrices of strong components (isolated vertex is considered as strong component of order one). Therefore $\phi_{S-Y}(x) = \phi_{S_1}(x)\phi_{S_2}(x) \cdots \phi_{S_k}(x)$ and so $E(S) = \sum\limits_{j=1}^{k} E(S_j)$. $\square$

Remark 4.2.8. From Theorem 4.1.1, $a_j = \sum\limits_{L \in \pounds_j} (-1)^{p(L)} s(L)$, for $j = 1, 2, \cdots, n$, where $s(L) = \prod\limits_{Z \in c(L)} s(Z)$. Clearly, this sum contains positive and negative ones. Clearly
+1 arises if and only if
(a) Number of components of $L \in \pounds_j$ is odd and $s(L) < 0$. We call such linear signed digraphs as type a linear signed digraphs.
(b) Number of components of $L \in \pounds_j$ is even and $s(L) > 0$. We call such linear signed digraphs as type b.
−1 will occur if and only if
(c) Number of components of $L \in \pounds_j$ is odd and $s(L) > 0$. We call such linear signed digraphs as type c.
(d) Number of components of $L \in \pounds_j$ is even and $s(L) < 0$. We call such linear signed digraphs as type d.

From the above remark, we observe that $a_j = 0$ if and only if either S is acyclic or in S, for each j, number of linear signed digraphs of order j of type a or type b or both types is equal to the number of linear signed digraphs of order j of type c or type d or both types.

An immediate consequence of the Remark 4.2.8 is the following Lemma.

Lemma 4.2.9. *An integral $(-1, 0, 1)$-matrix is nilpotent if and only if its underlying signed digraph S is either acyclic or in S, for each $j = 1, 2, \cdots, n$, the number of linear signed digraphs of order j of type a or type b or both types is equal to number of linear signed digraphs of order j of type c or type d or both types.*

Unlike unsigned strong component, energy of a signed directed strong component can be zero, for example, signed digraph S_1 in Figure 4.2. Now we have the following result.

Theorem 4.2.10. *Let S be a signed digraph of order n. Then $E(S) = 0$ if S satisfies one of the following conditions (i) S is acyclic or (ii) each strong component of S is skew symmetric or (iii) for each $j = 1, 2, \cdots, n$, the number of linear signed digraphs of order j of type a or type b or both types is equal to number of linear signed digraphs of order j of type c or type d or both types.*

Proof. Let S be a signed digraph of order n. If S is acyclic or satisfies (iii), then by Lemma 4.2.9, $\phi_S(x) = x^n$ and so $E(S) = 0$. If S satisfies (ii), then the eigenvalues of S are of the form $\pm\iota\alpha$, where $\alpha \in \mathbb{R}$, therefore $E(S) = 0$. $\square$

Here we note that Lemma 4.2.9 characterizes signed digraphs with zero as the only eigenvalue. Skew-symmetric signed digraphs have eigenvalues of the form $\pm\iota\alpha$, where $\alpha \in \mathbb{R}$. But there are signed digraphs with eigenvalues of the form $\pm\iota\alpha$, where $\alpha \in \mathbb{R}$, which are not skew symmetric. For example, consider the signed digraph S obtained by joining two copies of $\mathbf{S_2}$, a skew symmetric signed digraph of order two, by an arc (sign being immaterial). The spectrum of S is $spec(S) = \{\iota^{(2)}, -\iota^{(2)}\}$, where $\iota = \sqrt{-1}$. But S is not skew symmetric digraph as $A(S)$ is not a skew symmetric matrix. Therefore characterization of signed digraphs with energy zero reduces to the problem of characterizing signed digraphs with eigenvalues of the form $\pm\iota\alpha$, where $\alpha \in \mathbb{R}$.

4.3 Computation of energy of signed directed cycles

We first give energy formulae for positive cycles. Let C_n be a positive cycle on $n \geq 2$ vertices. The characteristic polynomial of C_n is $\phi_{C_n}(x) = x^n - 1$, so that $spec(C_n) = \{e^{\frac{2\pi \iota j}{n}}, j = 0, 1, \cdots, n-1\}$, where $\iota = \sqrt{-1}$. Consequently energy of C_n is

$$E(C_n) = \sum_{j=0}^{n-1} |\cos \frac{2j\pi}{n}|.$$

Given a positive integer n, it has one of the forms $4k$, or $2k+1$, or $4k+2$, where $k \geq 0$.

If $n = 4k$, then

$$\begin{aligned} E(C_n) &= \sum_{j=0}^{4k-1} |\cos \frac{2j\pi}{4k}| = \sum_{j=0}^{4k-1} |\cos \frac{j\pi}{2k}| = 2 \sum_{j=0}^{2k-1} |\cos \frac{j\pi}{2k}| \\ &= 2 + 4 \sum_{j=1}^{k-1} \cos \frac{j\pi}{2k} = 2 + 4\{\frac{-1}{2} + \frac{\sin \frac{(k-\frac{1}{2})\pi}{2k}}{2 \sin \frac{\pi}{4k}}\} = 2 \cot \frac{\pi}{n}. \end{aligned}$$

If $n = 2k+1$, then

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

If $n = 4k+2$, then

$$\begin{aligned} E(C_n) &= \sum_{j=0}^{4k+1} |\cos \frac{2j\pi}{4k+2}| = \sum_{j=0}^{4k+1} |\cos \frac{j\pi}{2k+1}| = 2 \sum_{j=0}^{2k} |\cos \frac{j\pi}{2k+1}| \\ &= 2 + 4 \sum_{j=1}^{k} \cos \frac{j\pi}{2k+1} = 2 + 4\{\frac{-1}{2} + \frac{\sin \frac{(k+\frac{1}{2})\pi}{2k+1}}{2 \sin \frac{\pi}{4k+2}}\} = 2 \csc \frac{\pi}{n}. \end{aligned}$$

We now give exact formulae for the energy of negative cycles of length n. Let $\mathbf{C}_n$ denote the negative cycle with n vertices. Then $\phi_{\mathbf{C}_n}(x) = x^n + 1$ and so

$Spec(\mathbf{C}_n) = \{e^{\frac{(2j+1)\pi\iota}{n}}, j = 0, 1, \cdots, n-1\}$, where $\iota = \sqrt{-1}$. Therefore the energy is given by

$$E(\mathbf{C}_n) = \sum_{j=0}^{n-1} |\cos\frac{(2j+1)\pi}{n}|.$$

If $n = 4k$, then

$$\begin{aligned} E(\mathbf{C}_n) &= \sum_{j=0}^{4k-1} |\cos\frac{(2j+1)\pi}{4k}| = 2\sum_{j=0}^{2k-1} |\cos\frac{(2j+1)\pi}{4k}| = 4\sum_{j=0}^{k-1} \cos\frac{(2j+1)\pi}{4k} \\ &= 4\{\cos\frac{\pi}{4k} + \cos\frac{3\pi}{4k} + \cdots + \cos\frac{(2k-1)\pi}{4k}\} \\ &= 4\frac{\cos(\frac{\pi}{4k} + \frac{k-1}{2}\frac{2\pi}{4k})\sin k\frac{2\pi}{8k}}{\sin\frac{2\pi}{8k}} = 2\csc\frac{\pi}{n}. \end{aligned}$$

If $n = 4k+2$, then

$$\begin{aligned} E(\mathbf{C}_n) &= \sum_{j=0}^{4k+1} |\cos\frac{(2j+1)\pi}{4k+2}| = 4\sum_{j=0}^{k-1} \cos\frac{(2j+1)\pi}{4k+2} \\ &= 4\{\cos\frac{\pi}{4k+2} + \cos\frac{3\pi}{4k+2} + \cdots + \cos\frac{(2k-1)\pi}{4k+2}\} = 2\cot\frac{\pi}{n}. \end{aligned}$$

If $n = 2k+1$, then since -1 is the eigenvalue of $\mathbf{C}_n$, we have $spec(\mathbf{C}_n) = -spec(C_n)$, and so $E(\mathbf{C}_n) = E(C_n)$.

Summarizing, all the above cases can be written as follows:

$$E(C_n) = \begin{cases} 2\cot\frac{\pi}{n}, & \text{if } n = 4k, \\ 2\csc\frac{\pi}{n}, & \text{if } n = 4k+2, \\ \csc\frac{\pi}{2n}, & \text{if } n = 2k+1. \end{cases}$$

and

$$E(\mathbf{C_n}) = \begin{cases} 2\csc\frac{\pi}{n}, & \text{if } n = 4k, \\ 2\cot\frac{\pi}{n}, & \text{if } n = 4k+2, \\ \csc\frac{\pi}{2n}, & \text{if } n = 2k+1. \end{cases}$$

Pẽna and Rada [62] proved that the energy of directed unsigned cycles increases monotonically with respect to order $n \geq 4$. From energy formulae for positive and negative signed directed cycles, the following two results are immediate.

Theorem 4.3.1. *Energy of negative cycles increases monotonically with respect to the order. Among all non cycle balanced unicyclic signed digraphs on n vertices, the cycle has the largest energy. Moreover, the minimal energy is attained in unicyclic signed digraph with unique cycle* $\mathbf{C}_2$.

Theorem 4.3.2. *Energy of positive and negative cycles satisfy the following:*
(i) *Energy of positive cycle of odd order equals energy of negative cycle of same order.*
(ii) *Energy of negative cycle of even order is greater than energy of positive cycle of same order if and only if* $n = 4k$.
(iii) *Energy of negative cycle of even order is less than energy of positive cycle of same order if and only if* $n = 4k + 2$.

We now obtain Coulson's integral formula for energy of signed digraphs.

Theorem 4.3.3. *Let S be a signed digraph with n vertices having characteristic polynomial $\phi_S(x)$. Then*

$$E(S) = \sum_{j=1}^{n} |\Re z_j| = \frac{1}{\pi} \int_{-\infty}^{\infty} (n - \frac{\iota x \phi'_S(\iota x)}{\phi_S(\iota x)}) dx,$$

where $z_1, z_2, \cdots, z_n$ are the eigenvalues of signed digraph S and $\int_{-\infty}^{\infty} F(x)dx$ denotes principle value of the respective integral.

Proof. Consider the function

$$f(z) = n - \frac{z\phi'_S(z)}{\phi_S(z)},$$

where $\phi_S(z)$ is the characteristic polynomial of S and $z_j = a_j + \iota b_j$, $j = 1, 2, \ldots, n$ are its zeros.

Then

$$f(z) = n - \sum_{j=1}^{n} \frac{z}{z - z_j} = \sum_{j=1}^{n} \frac{z_j}{z_j - z}$$

implying that

$$\frac{1}{\pi}\int_{-\infty}^{\infty} (n - \frac{\iota y \phi'_S(\iota y)}{\phi_S(\iota y)})dy = \frac{1}{\pi}\int_{-\infty}^{\infty} f(\iota y)dy = \frac{1}{\pi}\sum_{j=1}^{n}\int_{-\infty}^{\infty} \frac{z_j}{z_j - \iota y}dy.$$

Using the integrals $\int\limits_{-\infty}^{\infty} \frac{a}{(y-b)^2+a^2}dy = \pi.sgn(a)$ and $\int\limits_{-\infty}^{\infty} \frac{y-b}{(y-b)^2+a^2}dy = 0$, where a and b are real numbers and $sgn(a)$ denotes the sign of real number a, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{z_j}{z_j - \iota y}dy &= \int_{-\infty}^{\infty} \frac{a_j + \iota b_j}{a_j - \iota(y - b_j)}dy \\
&= \int_{-\infty}^{\infty} \frac{a_j^2 - b_j(y - b_j) + [a_j(y - b_j) + a_j b_j]\iota}{(y - b_j)^2 + a_j^2}dy \\
&= \pi a_j.sgn(a_j) + \pi b_j.sgn(a_j)\iota = \pi.sgn(a_j)(a_j + \iota b_j) \\
&= \pi.sgn(a_j)z_j.
\end{aligned}$$

Therefore

$$\frac{1}{\pi}\int_{-\infty}^{\infty} (n - \frac{\iota y \phi'_S(\iota y)}{\phi_S(\iota y)})dy = \frac{1}{\pi}\sum_{j=1}^{n} \pi.sgn(a_j)z_j = \sum_{j=1}^{n} sgn(\Re z_j)z_j = \sum_{j=1}^{n} |\Re z_j| = E(S).$$

□

The Coulson's integral formula given above is another motivation to define the energy of a signed digraph as the sum of absolute values of real parts of eigenvalues.

Example 4.3.4. Consider the cycle $\mathbf{C}_4$, the characteristic polynomial is $\phi_{\mathbf{C}_4}(x) = x^4 + 1$ and hence

$$E(\mathbf{C}_4) = \frac{1}{\pi}\int_{-\infty}^{\infty} [4 - \frac{4\iota x(\iota x)^3}{(\iota x)^4 + 1}]dx = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{4}{x^4 + 1}dx = \frac{4}{\pi}\frac{\pi}{2\sin\frac{\pi}{4}} = 2\sqrt{2},$$

as calculated in example 4.2.5.

An immediate consequence of Coulson's integral formula is the following observation, the proof being similar to the proof of Theorem 3.3.2 for signed graphs.

Theorem 4.3.5. *If S is a signed digraph on n vertices, then*

$$E(S) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log |x^n \phi_S(\frac{\iota}{x})| dx.$$

4.4 NEPS in signed digraphs

We recall that [41] Kronecker product of two matrices $A = (a_{ij})_{r\times s}$ and $B = (b_{ij})_{t\times u}$ denoted by $A \otimes B$ is a matrix of order $rt \times su$ obtained by replacing each entry a_{ij} of A by a block $a_{ij}B$. Thus $A \otimes B$ consists of all $rtsu$ possible products of an entry of A with an entry of B. The Kronecker product is a component wise operation, i.e., $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$, provided the products AC and BD exist. This operation is also associative, so we can define the multiple product $A_1 \otimes A_2 \otimes \cdots \otimes A_m$. Let order of A_i be $r_i \times s_i$. We index elements of A_i by $a_{i;jk}$ and those of multiple product by a pair of $m-$tuples, a row index $j = (j_1, j_2, \cdots, j_m)$ and a column index $k = (k_1, k_2, \cdots, k_m)$, where $1 \leq j_i \leq r_i$ and $1 \leq k_i \leq s_i$. The element a_{jk} of the product matrix is $a_{jk} = a_{1;j_1k_1} a_{2;j_2k_2} \cdots a_{m;j_mk_m}$.

Lemma 4.4.1. *[23]. Let A_i, for $i = 1, 2, \cdots, m$, be a square matrix of order n_i and ξ_{ij}, for $j = 1, 2, \cdots, n_i$ be its eigenvalues. If $k_1, k_2, \cdots, k_m$ are non-negative integers, then the $n_1n_2 \cdots n_m$ eigenvalues of the matrix $A_1^{k_1} \otimes \cdots \otimes A_m^{k_m}$ are $\xi_{j_1j_2\cdots j_m} = \xi_{1j_1}^{k_1} \cdots \xi_{mj_m}^{k_m}$ for $1 \leq j_i \leq n_i$. Let $k_p = (k_{p1}, k_{p2}, \cdots, k_{pm})$, for $p = 1, 2, \cdots, q$, be vectors of non-negative integers. Then the $n_1n_2 \cdots n_m$ eigenvalues of $\sum\limits_{p=1}^{q} A_1^{k_{p1}} \otimes \cdots \otimes A_m^{k_{pm}}$ are $\xi_{j_1j_2\cdots j_m} = \sum\limits_{p=1}^{q} \xi_{1j_1}^{k_{p1}} \cdots \xi_{mj_m}^{k_{pm}}$.*

For NEPS in graphs see [14]. The following definition extends this concept to signed digraphs.

Definition 4.4.2. Let $\mathscr{B}$ be a set of binary $n-$tuples called basis for the product. The non-complete extended $p-$sum (or simply called NEPS) of signed digraphs $S_1, S_2, \cdots, S_n$ with basis $\mathscr{B}$ denoted by NEPS$(S_1, S_2, \cdots, S_n; \mathscr{B})$ is a signed digraph with vertex set $V(S_1) \times V(S_2) \times \cdots \times V(S_n)$. There is an arc from vertex $(u_1, u_2, \cdots, u_n)$ to $(v_1, v_2, \cdots, v_n)$ if and only if there exists $(\beta_1, \beta_2, \cdots, \beta_n) \in \mathscr{B}$ such that $(u_i, v_i) \in A(S_i)$ whenever $\beta_i = 1$ and $u_i = v_i$ whenever $\beta_i = 0$. The sign of the arc is given by

$$\sigma((u_1, u_2, \cdots, u_n), (v_1, v_2, \cdots, v_n)) = \prod_{i=1}^{n} \sigma_i(u_i, v_i)^{\beta_i} = \prod_{i:\beta_i=1} \sigma_i(u_i, v_i).$$

Assume that the basis $\mathscr{B}$ has $r \geq 1$ elements, i.e., $\mathscr{B} = \{\beta_1, \beta_2, \cdots, \beta_r\} \subseteq \{0,1\}^n \backslash \{(0, 0, \cdots, 0)\}$, we define

$$NEPS(S_1, S_2, \cdots, S_n; \mathscr{B}) = \bigcup_{\beta \in \mathscr{B}} NEPS(S_1, S_2, \cdots, S_n; \beta).$$

Example 4.4.3. The Kronecker product $S_1 \otimes S_2 \otimes \cdots \otimes S_n$ of signed digraphs $S_1, S_2, \cdots, S_n$ is the NEPS of these signed digraphs with basis $\mathscr{B} = \{(1, 1, \cdots, 1)\}$; the Cartesian product $S_1 \times S_2 \times \cdots \times S_n$ is NEPS with basis $\mathscr{B} = \{e_i\}$, $i = 1, 2, \cdots, n$, where e_i is $n-$tuple with 1 at ith position and 0 otherwise.

The following result shows that two different basis vectors give disjoint arc sets. Proof is similar to signed graphs [23].

Lemma 4.4.4. *If $S = NEPS\,(S_1, S_2, \cdots, S_n; \beta)$ and $S' = NEPS\,(S_1, S_2, \cdots, S_n; \beta')$, $\beta \neq \beta'$, then $\mathscr{A}(S) \cap \mathscr{A}(S') = \emptyset$.*

The following result gives adjacency matrix and spectra of NEPS in terms of the constituent factor signed digraphs.

Theorem 4.4.5. *If S =NEPS$(S_1, S_2, \cdots, S_n; \mathscr{B})$, then the adjacency matrix is given by $A(S) = \sum\limits_{\beta \in \mathscr{B}} A_1^{\beta_1} \otimes \cdots \otimes A_n^{\beta_n}$, and eigenvalues are given by $z_{j_1 j_2 \cdots j_n} = \sum\limits_{\beta \in \mathscr{B}} z_{1j_1}^{\beta_1} \cdots z_{nj_n}^{\beta_n}$, where $1 \leq j_i \leq |V(S_i)|$, $i = 1, 2, \cdots, n$.*

Proof. Let $u = (u_{1j_1}, u_{2j_2}, \cdots, u_{nj_n})$ and $v = (v_{1k_1}, v_{2k_2}, \cdots, v_{nk_n})$, where $1 \leq$

$j_i, k_i \leq |V(S_i)|$, for $i = 1, 2, \cdots, n$, be any two vertices of S. Then

$$\begin{aligned}
[A(S)]_{uv} &= \sum_{\beta \in \mathscr{B}} (A_1^{\beta_1})_{u_{1j_1} v_{1k_1}} (A_2^{\beta_2})_{u_{2j_2} v_{2k_2}} \cdots (A_n^{\beta_n})_{u_{nj_n} v_{nk_n}} \\
&= \sigma_1(u_{1j_1}, v_{1k_1})^{\beta_1} \sigma_2(u_{2j_2}, v_{2k_2})^{\beta_2} \cdots \sigma_n(u_{nj_n}, v_{nk_n})^{\beta_n} \\
&= a_{1;j_1k_1}^{\beta_1} a_{2;j_2k_2}^{\beta_2} \cdots a_{n;j_nk_n}^{\beta_n} = [\sum_{\beta \in \mathscr{B}} A_1^{\beta_1} \otimes \cdots \otimes A_n^{\beta_n}]_{uv}.
\end{aligned}$$

The second part of the result follows by Lemma 4.4.1. □

We note two special cases of Theorem 4.4.5.
(i) The Kronecker product $S_1 \otimes S_2 \otimes \cdots \otimes S_n$ has eigenvalues $z_{j_1 j_2 \cdots j_n} = z_{1j_1} z_{2j_2} \cdots z_{nj_n}$, for $1 \leq j_i \leq |V(S_i)|, i = 1, 2, \cdots, n$.
(ii) The Cartesian product $S_1 \times S_2 \times \cdots \times S_n$ has eigenvalues $z_{j_1 j_2 \cdots j_n} = z_{1j_1} + z_{2j_2} + \cdots + z_{nj_n}$, $1 \leq j_i \leq |V(S_i)|$, for $i = 1, 2, \cdots, n$.

Germina, Hameed and Zaslavsky [23] considered the problem of balance in NEPS of signed graphs. It is natural to consider the problem of cycle balance for signed digraphs. The next result gives sufficient but not necessary condition for cycle balance of NEPS and the proof follows on same lines as that in undirected case.

Theorem 4.4.6. *NEPS$(S_1, S_2, \cdots, S_n; \mathscr{B})$ is balanced if $S_1, S_2, \cdots, S_n$ are cycle balanced.*

Remark 4.4.7. (i) Theorem 4.4.6 does not have a general converse. A counter example is $S =$ NEPS$(-C_3, -\overleftrightarrow{K_2}, \{(1,1)\})$, where $-C_3$ denotes all negative directed cycle of order 3 and $-\overleftrightarrow{K_2}$ is symmetric signed digraph of order 2 with both arcs negative. S is all positive and hence cycle balanced. However $-C_3$ is non cycle balanced.
(ii) In view of Theorem 4.1.3, the converse of Theorem 4.4.6 is always true if basis $\mathscr{B} = \{e_i\}, i = 1, 2, \cdots, n$.
Now we have the following result.

Theorem 4.4.8. *The following statements are equivalent about Cartesian product $S = S_1 \times S_2 \times \cdots \times S_n$.*

(i) S is cycle balanced.
(ii) All of $S_1, S_2, \cdots, S_n$ are cycle balanced.
(iii) S and S^u are cospectral.
Proof. Theorem 4.1.3 implies equivalence of (i) and (iii). Also (ii) of Remark 4.4.7 implies equivalence of (i) and (ii). $\square$

4.5 Upper bounds for the energy of signed digraphs

Let S be a signed digraph of order n with adjacency matrix $A(S) = (a_{ij})$. The powers of $A(S)$ count the number of walks in signed manner. Let $w_{ij}^{+}(l)$ and $w_{ij}^{-}(l)$ respectively denote the number of positive and negative walks of length l from v_i to v_j. The following result relates the integral powers of the adjacency matrix with the number of positive and negative walks.

Theorem 4.5.1. *If A is an adjacency matrix of a signed digraph on n vertices, then $[A^l]_{ij} = w_{ij}^{+}(l) - w_{ij}^{-}(l)$.*
Proof. We prove the result by induction on l. For $l = 1$, the result is vacuously true. For $l = 2$, let n_{ij}^{+} denote the number of positive neighbours of distinct vertices v_i and v_j, and let n_{ij}^{-} the number of their common negative neighbours and $n_{ij}^{\pm}$ be the number of neighbours that are positive to one vertex and negative to other. The (i, i) entry of A^2 equals $w_{ii}^{+}(2) - w_{ii}^{-}(2)$. For (i, j), $i \neq j$, $n_{ij}^{+} + n_{ij}^{-} = w_{ij}^{+}(2)$ and $n_{ij}^{\pm} = w_{ij}^{-}(2)$, so that (i, j)th entry$= w_{ij}^{+}(2) - w_{ij}^{-}(2)$. Now assume the result to be true for $l = m$.

We have, $[A^{m+1}]_{ij} = [A^m A]_{ij} = \sum\limits_{k=1}^{n} [A^m]_{ik}[A]_{kj} = w_{ij}^{+}(m+1) - w_{ij}^{-}(m+1)$, by induction hypothesis. Therefore, the result follows. $\square$

In the signed digraph S, let c_m^{+} denote the number of positive closed walks of length m and c_m^{-} the number of negative closed walks of length m. In view of the fact that sum of eigenvalues of a matrix equals to its trace, we have the following observation.

Corollary 4.5.2. *If $z_1, z_2, \cdots, z_n$ are the eigenvalues of a signed digraph S, then $\sum\limits_{j=1}^{n} z_j^m = c_m^{+} - c_m^{-}$.*

Now we extend the results of [76] to signed digraphs.

Lemma 4.5.3. *Let S be a signed digraph having n vertices and a arcs and let $z_1, z_2, \cdots, z_n$ be its eigenvalues. Then*
(i) $\sum\limits_{j=1}^{n}(\Re z_j)^2 - \sum\limits_{j=1}^{n}(\Im z_j)^2 = c_2^+ - c_2^-$, *(ii)* $\sum\limits_{j=1}^{n}(\Re z_j)^2 + \sum\limits_{j=1}^{n}(\Im z_j)^2 \leq a = a^+ + a^-$.

Proof. By Corollary 4.5.2, we have

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

Equating real and imaginary parts proves (i).

By Schur's unitary triangularization, there exists a unitary matrix U such that the adjacency matrix A of the signed digraph S is unitarily similar to an upper triangular matrix $T = (t_{jk})$ with $t_{jj} = z_j$ for each $j = 1, 2, \cdots, n$. Then $\sum\limits_{j,k=1}^{n} |a_{jk}|^2 = \sum\limits_{j,k=1}^{n} |t_{jk}|^2$. As A is $(-1, 0, 1)-$matrix, we have

$$a = \sum_{j,k=1}^{n} |\sigma(v_j, v_k)| = \sum_{j,k=1}^{n} |a_{jk}| = \sum_{j,k=1}^{n} |a_{jk}|^2 = \sum_{j,k=1}^{n} |t_{jk}|^2 \geq \sum_{j=1}^{n} |t_{jj}|^2$$

$$= \sum_{j=1}^{n} |z_j|^2 = \sum_{j=1}^{n} \Re z_j^2 + \sum_{j=1}^{n} \Im z_j^2.$$

thereby proving (ii). □

Theorem 4.5.4. *Let S be a signed digraph with n vertices and $a = a^+ + a^-$ arcs, and let $z_1, z_2, \cdots, z_n$ be its eigenvalues. Then $E(S) \leq \sqrt{\frac{1}{2} n(a + c_2^+ - c_2^-)}$.*

Proof. Subtracting part (i) of Lemma 4.5.3 from (ii), we see that

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

Applying Cauchy-Schwarz inequality to vectors $(|\Re z_1|, |\Re z_2|, \cdots, |\Re z_n|)$ and $(1, 1, \cdots, 1)$, we have

$$E(S)=\sum_{j=1}^{n}|\Re z_j|\le \sqrt{n}\sqrt{\sum_{j=1}^{n}(\Re z_j)^2}=\sqrt{n}\sqrt{(c_2^+-c_2^-)+\sum_{j=1}^{n}(\Im z_j)^2}$$

$$\le \sqrt{n}\sqrt{(c_2^+-c_2^-)+\frac{1}{2}(a-(c_2^+-c_2^-))}=\sqrt{\frac{1}{2}n(a+c_2^+-c_2^-)}.$$

$\square$

Remark 4.5.5. (i). The upper bound in Theorem 4.5.4 is attained by signed digraphs $S_1=(\frac{n}{2}\overleftrightarrow{K_2},+)$, $S_2=(\frac{n}{2}\overleftrightarrow{K_2},-)$, (where $(\overleftrightarrow{K}_2,+)$ and $(\overleftrightarrow{K}_2,-)$ respectively denote symmetric digraphs obtained from $+K_2$ and $-K_2$) and skew symmetric signed digraph of order n. Note that $spec(S_1)=spec(S_2)=\{-1^{(\frac{n}{2})},+1^{(\frac{n}{2})}\}$ and eigenvalues of skew symmetric signed digraph of order n are of the form $\pm\iota\alpha$, where $\alpha\in\mathbb{R}$.
(ii). The Above result extends McClleland's inequality for signed graphs [35] which states that $E(S)\le\sqrt{2pq}$, holds for every signed graph with p vertices and q edges. Let $\overleftrightarrow{S}$ be the symmetric signed digraph of signed graph S, then in $\overleftrightarrow{S}$, $a=2q=c_2^+=c_2^+-c_2^-$. By Theorem 4.5.4, $E(S)=E(\overleftrightarrow{S})\le\sqrt{\frac{1}{2}p(2q+2q)}=\sqrt{2pq}$.

Note that if S is strongly connected, then $d_{v_j}^+\ge 1$(respectively, $d_{v_j}^-\ge 1$) for all $j=1,2,\ldots,n$. Therefore, $a=\sum\limits_{j=1}^{n}d_{v_j}^+\ge n$. Also, for any signed digraph S, $a\ge c_2^+-c_2^-$.

The following result gives the sharp upper bound of energy of signed digraphs in terms of the number of arcs.

Theorem 4.5.6. *Let S be a signed digraph with a arcs. Then $E(S)\le a$ with equality if and only if $S=(\frac{a}{2}\overleftrightarrow{K_2},+)$ or $S=(\frac{a}{2}\overleftrightarrow{K_2},-)$ plus some isolated vertices.*
Proof. If S is acyclic, then the result is obvious. Assume S is strongly connected, then by Theorem 4.5.4, we have

$$E(S)\le\sqrt{\frac{1}{2}n(a+c_2^+-c_2^-)}\le\sqrt{na}\le\sqrt{a^2}=a. \tag{4.1}$$

In general, let $S_1, S_2, \ldots, S_k$ be strong components of S and let the number of vertices and arcs of S_j respectively be n_j and a_j. By Theorem 4.2.7, we have

$$E(S) = \sum_{j=1}^{k} E(S_j) \leq \sum_{j=1}^{k} a_j \leq a. \tag{4.2}$$

It is easy to see that if $S = (\frac{a}{2}\overleftrightarrow{K_2}, +)$ or $(\frac{a}{2}\overleftrightarrow{K_2}, -)$ plus some isolated vertices, then $E(S) = a$. Conversely, if S is strongly connected and $E(S) = a$, then all inequalities in (4.1) are equalities. From (4.1), $na = a^2$, which gives $a = 0$ or $a = n$. If $a = 0$, then S is a vertex, otherwise $a = n$. Also from (4.1), $\frac{1}{2}n(a + c_2^+ - c_2^-) = na$, which gives $c_2^+ - c_2^- = a = n$, which is possible only if $S = (\overleftrightarrow{K_2}, +)$ or $(\overleftrightarrow{K_2}, -)$. In general case, all inequalities in (4.2) are equalities. Also, from $E(S_j) \leq a_j$, we conclude that $E(S_j) = a_j$ for $j = 1, 2, \ldots, k$. Then as earlier $S_j = (\overleftrightarrow{K_2}, +)$ or $(\overleftrightarrow{K_2}, -)$ or a vertex. So, in this case $S = (\frac{a}{2}\overleftrightarrow{K_2}, +)$ or $S = (\frac{a}{2}\overleftrightarrow{K_2}, -)$ plus some isolated vertices. $\square$

Remark 4.5.7. Theorem 4.5.6 extends the result for signed graphs [35], which states that $E(S) \leq 2q$ for every signed graph with q edges with equality if and only if $S = (\frac{q}{2}K_2, +)$ or $S = (\frac{q}{2}K_2, -)$ plus some isolated vertices.

4.6 Equienergetic signed digraphs

Two signed digraphs are said to be isomorphic if their underlying digraphs are isomorphic such that the signs are preserved. Any two isomorphic signed digraphs are obviously cospectral. There exist non isomorphic signed digraphs which are cospectral, e.g., consider the signed digraphs S_1 and S_2 shown in Figure 4.2. Clearly, S_1 and S_2 are nonisomorphic, but *spec* $S_1 = \{0^{(5)}\} =$ *spec* S_2.

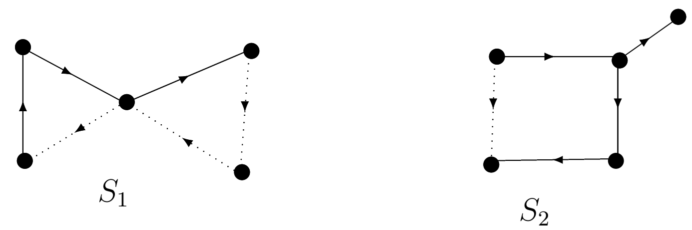


Figure 4.2

Two nonisomorphic signed digraphs S_1 and S_2 of same order are said to be equienergetic if $E(S_1) = E(S_2)$. Rada [76] proved the existence of pairs of non-symmetric and non cospectral equienergetic digraphs. Cospectral signed digraphs are obviously equienergetic, therefore the problem of equienergetic signed digraphs reduces to the problem of construction of non cospectral pairs of equienergetic signed digraphs such that for every pair not both signed digraphs are cycle balanced.

We have the following result.

Theorem 4.6.1. *Let S be a signed digraph of order n having eigenvalues $z_1, z_2, \cdots, z_n$ such that $|\Re z_j| \leq 1$ for every $j = 1, 2, \cdots, n$. Then $E(S \times \overleftrightarrow{K_2}) = 2n$.*

Proof. Let $z_1, z_2, \cdots, z_t$ be eigenvalues with nonnegative real part and $z_{t+1}, \cdots, z_n$ be those with negative real part. Eigenvalues of Cartesian product $S \times \overleftrightarrow{K_2}$ are $z_1 \pm 1, z_2 \pm 1, \cdots, z_t \pm 1, z_{t+1} \pm 1, \cdots, z_n \pm 1$. Therefore

$$E(S \times \overleftrightarrow{K_2}) = \sum_{j=1}^{t}(|\Re z_j + 1| + |\Re z_j - 1|) + \sum_{j=t+1}^{n}(|\Re z_j + 1| + |\Re z_j - 1|).$$

As $|\Re z_j| \leq 1$, for all $i = 1, 2, \cdots, n$, it follows that

$$E(S \times \overleftrightarrow{K_2}) = \sum_{j=1}^{t}(\Re z_j + 1 + 1 - \Re z_j) + \sum_{j=t+1}^{n}(\Re z_j + 1 - \Re z_j + 1) = 2t + 2(n-t) = 2n.$$

□

Now we have the following consequence.

Corollary 4.6.2. *For $n \geq 2$, $E(\mathbf{C}_n \times \overleftrightarrow{K_2}) = E(C_n \times \overleftrightarrow{K_2}) = 2n$. Moreover, $\mathbf{C}_n \times \overleftrightarrow{K_2}$ and $C_n \times \overleftrightarrow{K_2}$ are non cospectral signed digraphs with $2n$ vertices.*

Proof. We know the eigenvalues of $\mathbf{C}_n$ are $e^{\frac{\iota(2j+1)\pi}{n}}$, $j = 0, 1, \cdots, n-1$ and those of C_n are $e^{\frac{2\iota j\pi}{n}}$, $j = 0, 1, \cdots, n-1$. Clearly, eigenvalues of $\mathbf{C}_n$ and C_n meet the requirement of Theorem 4.6.1, so $E(\mathbf{C}_n \times \overleftrightarrow{K_2}) = E(C_n \times \overleftrightarrow{K_2}) = 2n$. Moreover, $2 \notin spec(\mathbf{C}_n \times \overleftrightarrow{K_2})$, but $2 \in spec(C_n \times \overleftrightarrow{K_2})$ implying that $\mathbf{C}_n \times \overleftrightarrow{K_2}$ and $C_n \times \overleftrightarrow{K_2}$ are non cospectral. The number of vertices in both signed digraphs is $2n$ which follows by the definition of Cartesian product. In view of Remark 4.4.7 (ii), $\mathbf{C}_n \times \overleftrightarrow{K_2}$ is non cycle balanced, whereas $C_n \times \overleftrightarrow{K_2}$ is cycle balanced. $\square$

Example 4.6.3. For each odd n, $\mathbf{C}_n$ and C_n is a non cospectral pair of equienergetic signed digraphs, because $spec(\mathbf{C}_n) = -spec(C_n)$ and $1 \notin spec(\mathbf{C}_n)$ but $1 \in spec(C_n)$.

From Corollary 4.6.2 and Example 4.6.3, we see for each positive integer $n \geq 3$, there exits a pair of non cospectral signed digraphs with one signed digraph cycle balanced and another non cycle balanced. Now we construct pairs of non cospectral equienergetic signed digraphs of order $2n$, $n \geq 5$ with both constituents non cycle balanced. Let P_n^l $(n \geq l+1)$ be a signed digraph obtained by identifying one pendant vertex of the path P_{n-l+1} with any vertex of $\mathbf{C}_l$. Sign of non cyclic arcs is immaterial.

Theorem 4.6.4. *For each $n \geq 5$, $P_n^3 \times \overleftrightarrow{K_2}$ and $P_n^4 \times \overleftrightarrow{K_2}$ is a pair of non cospectral equienergetic signed digraphs of order and energy equal to $2n$.*

Proof. Using the fact that $\phi_{P_n^l}(x) = x^{n-l}\phi_{\mathbf{C}_l}(x)$ and Theorem 4.6.1, it follows that $E(P_n^3 \times \overleftrightarrow{K_2}) = E(P_n^4 \times \overleftrightarrow{K_2}) = 2n$. Now 1 is an eigenvalue of $P_n^3 \times \overleftrightarrow{K_2}$ with multiplicity $n-3$ but 1 is an eigenvalue of $P_n^4 \times \overleftrightarrow{K_2}$ with multiplicity $n-4$, therefore these two signed digraphs are non cospectral. The order of both signed digraphs equals to $2n$ follows by the definition of Cartesian product. In view of Remark 4.4.7 (ii), it follows that both $P_n^3 \times \overleftrightarrow{K_2}$ and $P_n^4 \times \overleftrightarrow{K_2}$ are non cycle balanced. $\square$

4.7 Conclusion

We conclude with the following open problems.

Problem 4.7.1. Characterize signed digraphs with energy equal to the number of vertices.

Problem 4.7.2. Determine bases other than $\{e_i\}$ for which converse of Theorem 4.4.6 holds.

CHAPTER 5

Spectra and energy of bipartite signed digraphs

In this Chapter, we study spectra and energy in bipartite signed digraphs. We obtain a sufficient condition for the even coefficients of the characteristic polynomial of a bipartite signed digraph to alternate in sign. In this case, we obtain an integral expression and define a quasi-order relation and show it is possible to compare the energy of signed digraphs. Further, it is shown that signed digraph in this case has the property that energy decreases when we delete an arc from a cycle of length 2. We also obtain a sufficient condition for the even coefficients of the characteristic polynomial of a bipartite signed digraph to be non negative. We study integral, real, Gaussian signed digraphs and quasi-cospectral digraphs and show for each positive integer $n \geq 4$, there exists a family of n cospectral, non symmetric, strongly connected, integral, real, Gaussian signed digraphs (non cycle balanced) and quasi-cospectral digraphs of order 4^n.

5.1 Introduction

Esser and Harary [21] showed that a strongly connected digraph is bipartite if and only if its spectrum remains invariant under multiplication by -1. We show that there are non bipartite strongly connected signed digraphs with this property. As in bipartite digraphs, in general the even coefficients of a non cycle balanced bipartite signed digraph do not alternate in sign. For example, the characteristic polynomial of a non cycle balanced bipartite signed digraph S in Fig. 5.3 is $\phi_S(x) = x^4 + x^2$. Clearly, even coefficients do not alternate in sign. Consider the non cycle balanced bipartite signed digraph S_1 shown in Fig. 5.2. The characteristic polynomial is $\phi_{S_1}(x) = x^6 - x^4 + 2x^2$ and in this case even coefficients alternate in sign. Rada, Gutman and Cruz [71] considered bipartite digraphs with characteristic polynomial of the form

$$\phi_D(x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j} x^{n-2j} \tag{5.1}$$

where b_{2j} are nonnegative integers for every $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$ and studied a large family of bipartite digraphs on n vertices Δ_n^* consisting only of cycles of length

$\equiv 2 \pmod 4$ and with characteristic polynomial of the form (5.1). Because of this alternating nature of even coefficients it is possible to compare energies of digraphs in Δ_n^* by means of quasi-order relation. It is natural to consider the same problem for signed digraphs. We show that bipartite signed digraphs on n vertices with each cycle of length $\equiv 0 \pmod 4$ negative (i.e., containing odd number of negative arcs) and each cycle of length $\equiv 2 \pmod 4$ positive (i.e., containing an even number of negative arcs) have characteristic polynomial of the form (5.1). We denote this class of signed digraphs by Δ_n^1. We derive an integral expression for the energy and define a quasi-order relation to compare energies of signed digraphs in this case. We also study another class of bipartite signed digraphs on n vertices with all cycles negative (i.e., each cycle has odd number of negative arcs) and show a signed digraph in this class has characteristic polynomial of the form

$$\phi_S(x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} b_{2j} x^{n-2j} \tag{5.2}$$

where b_{2j} are nonnegative integers for every $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$. We denote this class of signed digraphs by Δ_n^2.

Two signed digraphs of same order are said to be cospectral (or isospectral) if they have same spectrum. Esser and Harrary [20] studied digraphs with integral, real and Gaussian spectra. We study signed digraphs with integral, real and Gaussian spectra and we show for each positive integer $n \geq 4$ there exists a collection of n non cycle balanced, non symmetric, strongly connected, integral, real and Gaussian cospectral signed digraphs of order 4^n. Further, we study quasi-cospectral and strongly quasi-cospectral digraphs.

5.2 Spectra of signed digraphs

Recall a signed digraph S is bipartite if its underlying digraph is bipartite. The following result shows that spectrum of a bipartite signed digraph remains invariant under multiplication by -1.

Theorem 5.2.1. *If S is a bipartite signed digraph of order n, then*

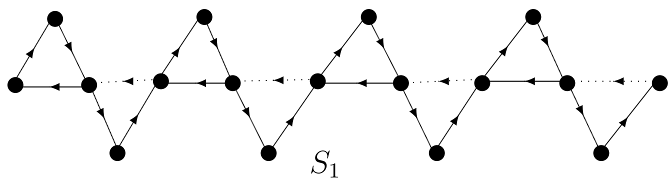
$$\phi_S(x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} a_{2j} x^{n-2j},$$

where a_{2j} are integers for every $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$.

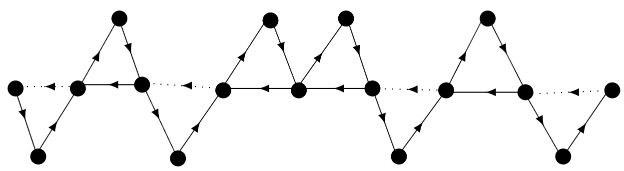
Proof. Let S be a bipartite signed digraph of order n. Then S has no odd cycles and consequently no linear signed subdigraph on odd number of vertices. Therefore, $a_{2j-1} = 0$ for all $j \geq 1$. By Theorem 4.1.1, the characteristic polynomial of S is

$$\begin{aligned}\phi_S(x) &= x^n + a_2 x^{n-2} + a_4 x^{n-4} + \cdots \\ &= x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} a_{2j} x^{n-2j},\end{aligned}$$

where a_{2j} are integers. It is clear from last expression that the spectrum of bipartite signed digraph remains invariant under multiplication by -1. $\square$



S_1



S_2 Fig. 5.1

Remark 5.2.2. Unlike in digraphs, the converse of Theorem 5.2.1 is not true. For example signed digraphs S_1 and S_2 shown in Fig. 5.1 are two strongly connected non bipartite signed digraphs of order 17. It is easy to check that $\phi_{S_1}(x) = \phi_{-S_1}(x) = x^{17} + 3x^{11} + x^5$ and $\phi_{S_2}(x) = \phi_{-S_2}(x) = x^{17} + x^{11} + x^5$. Thus both S_1 and S_2 have the property that spectrum remains invariant under multiplication by -1.

We have the following result.

Theorem 5.2.3. *Let S be a signed digraph of order n. Then the following statements are equivalent.*
(i) Spectrum of S remains invariant under multiplication by -1.
(ii) S and $-S$ are cospectral.
(iii) In S, for each odd j, number of linear signed subdigraphs of order j of type a or type b or both types is equal to number of linear signed subdigraphs of order j of type c or type d or both types.
Proof. $(i) \Longrightarrow (ii)$ This follows from the fact that $spec(-A) = -spec(A)$ for any square matrix A.
$(ii) \Longrightarrow (iii)$ Assume S and $-S$ are cospectral. Then $\phi_S(x) = \phi_{-S}(x) = \pm\phi_S(-x)$. The sign is positive or negative according as the order n of signed digraph is respectively even or odd. This clearly indicates that the coefficient $a_j = 0$ for each odd j and therefore (iii) follows.
$(iii) \Longrightarrow (i)$ Assume (iii) holds. Then $a_j = 0$ for all odd j, therefore $\phi_S(x) = \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} a_{2j}x^{n-2j}$. From this we see that $\phi_S(-x) = \pm\phi_S(x)$, the sign is $+$ or $-$ according as n is even or odd and hence (i) holds. $\square$

Lemma 5.2.4. *If S is a bipartite signed digraph, then for all $j = 1, 2, \cdots$*
(i) *$\pounds_{2j-1} = \emptyset$.*
(ii) *Every element of $\pounds_{4j}$ has an even number of cyclic components of length $\equiv 2 \pmod 4$. The number of components of length $\equiv 0 \pmod 4$ is either even or odd.*
(iii) *Every element of $\pounds_{4j+2}$ has an odd number of cyclic components of length $\equiv 2 \pmod 4$. The number of components of length $\equiv 0 \pmod 4$ is either even or odd.*
Proof. (i). Since S is bipartite, therefore as in Theorem 5.2.1, $\pounds_{2j-1} = \emptyset$, for all $j = 1, 2, \cdots$.
(ii). Assume $L \in \pounds_{4j}$ has p components of length $4l_r + 2$, for $r = 1, 2, \cdots, p$ and q components of length $4m_r$ for $r = 1, 2, \cdots, q$. Then

$$4j = \sum_{r=1}^{p}(4l_r + 2) + \sum_{r=1}^{q}(4m_r),$$

which gives $p = 2j - 2\sum_{r=1}^{p}(l_r) - 2\sum_{r=1}^{q}(m_r)$. This shows that p is even irrespective

of whether q is even or odd.
(iii). Same as in part (ii). $\square$

The following result shows that the characteristic polynomial of a signed digraph in Δ_n^1 is of the form (5.1).

Theorem 5.2.5. *If $S \in \Delta_n^1$, then*

$$\phi_S(x) = x^n + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j} x^{n-2j}, \tag{5.3}$$

where $b_{2j} = |\pounds_{2j}|$ is the cardinality of the set $\pounds_{2j}$.

Proof. Let $\phi_S(x) = x^n + \sum\limits_{j=1}^{n} a_j x^{n-j}$. By Theorem 4.1.1, we have $a_j = \sum\limits_{L \in \pounds_j} (-1)^{p(L)} s(L)$, where $s(L) = \prod\limits_{Z \in c(L)} s(Z)$. By Lemma 5.2.4, for all $j = 1, 2, \cdots$, we have $a_{2j-1} = 0$. Also,

$$\begin{aligned} a_{4j} &= \sum_{L \in \pounds_{4j}} (-1)^{p(L)} s(L) \\ &= \sum_{L \in \pounds_{4j}^1} (-1)^{p(L)} s(L) + \sum_{L \in \pounds_{4j}^2} (-1)^{p(L)} s(L) + \sum_{L \in \pounds_{4j}^3} (-1)^{p(L)} s(L), \end{aligned}$$

where $\sum\limits_{L \in \pounds_{4j}^1}$ denotes the sum over those linear signed subdigraphs $L \in \pounds_{4j}$ whose components are only those cycles whose length $\equiv 0 \pmod 4$, $\sum\limits_{l \in \pounds_{4j}^2}$ denotes the sum over those linear signed subdigraphs $L \in \pounds_{4j}$ whose components are cycles of length $\equiv 2 \pmod 4$ only and $\sum\limits_{l \in \pounds_{4j}^3}$ denotes the sum over those linear signed subdigraphs $L \in \pounds_{4j}$ which have components consisting of both types of cycles.

Now

$$\sum_{L \in \pounds_{4j}^1} (-1)^{p(L)} s(L) = \sum_{I} (-1)^{p(L)} s(L) + \sum_{II} (-1)^{p(L)} s(L),$$

where $\sum\limits_{I}$ denotes the sum over those $L \in \pounds_{4j}^1$ which have an even number of cycles of length $\equiv 0 \pmod 4$ and $\sum_{II}$ denotes the sum over those $L \in \mathcal{L}_{4j}^1$ which have an odd number of cycles of length $\equiv 0 \pmod 4$.

Therefore, by Lemma 5.2.4, we have

$$\begin{aligned}\sum_{L\in\mathcal{L}_{4j}^1}(-1)^{p(L)}s(L) &= \sum_{I}(-1)^{even}(+1)+\sum_{II}(-1)^{odd}(-1)\\ &= \sum_{I}1+\sum_{II}1 = |\mathcal{L}_{4j}^1|.\end{aligned}$$

Now, by Lemma 5.2.4, we have

$$\begin{aligned}\sum_{L\in\mathcal{L}_{4j}^2}(-1)^{p(L)}s(L) &= \sum_{L\in\mathcal{L}_{4j}^2}(-1)^{even}(+1)\\ &= |\mathcal{L}_{4j}^2|.\end{aligned}$$

Again, by Lemma 5.2.4, we have

$$\sum_{L\in\mathcal{L}_{4j}^3}(-1)^{p(L)}s(L) = \sum_{I}(-1)^{p(L)}s(L)+\sum_{II}(-1)^{p(L)}s(L),$$

where $\sum_{I}$ denotes the sum over those $L \in \mathcal{L}_{4j}^3$ which have an even number of cycles of length $\equiv 0 \pmod 4$ and $\sum_{II}$ denotes the sum over those $L \in \mathcal{L}_{4j}^3$ which have an odd number of cycles of length $\equiv 0 \pmod 4$. Note that the number of cycles of length $\equiv 2 \pmod 4$ is even.

Therefore,

$$\begin{aligned}\sum_{L\in\mathcal{L}_{4j}^3}(-1)^{p(L)}s(L) &= \sum_{I}(-1)^{even}(+1)+\sum_{II}(-1)^{odd}(-1)\\ &= \sum_{I}1+\sum_{II}1 = |\mathcal{L}_{4j}^3|.\end{aligned}$$

Thus $a_{4j} = |\mathcal{L}_{4j}^1| + |\mathcal{L}_{4j}^2| + |\mathcal{L}_{4j}^3| = |\mathcal{L}_{4j}|$.

Also,

$$\begin{aligned}a_{4j+2} &= \sum_{L\in\mathcal{L}_{4j+2}}(-1)^{p(L)}s(L)\\ &= \sum_{l\in\mathcal{L}_{4j+2}^1}(-1)^{p(L)}s(L)+\sum_{L\in\mathcal{L}_{4j+2}^2}(-1)^{p(L)}s(L),\end{aligned}$$

where $\sum\limits_{l\in \pounds^1_{4j+2}}$ denotes the sum over those linear signed subdigraphs $L \in \pounds_{4j+2}$ whose components are only those cycles whose length $\equiv 2 \pmod 4$, and $\sum\limits_{l\in \pounds^2_{4j+2}}$ denotes the sum over those linear signed subdigraphs $L \in \pounds_{4j+2}$ which have components consisting of both types of cycles.

By Lemma 5.2.4, we have

$$\sum_{L\in \pounds^1_{4j+2}} (-1)^{p(L)} s(L) = \sum_{L\in \pounds^1_{4j+2}} (-1)^{odd}(+1) = -|\pounds^1_{4j+2}|.$$

Also,

$$\sum_{L\in \pounds^2_{4j+2}} (-1)^{p(L)} s(L) = \sum_{I} (-1)^{p(L)} s(L) + \sum_{II} (-1)^{p(L)} s(L),$$

where $\sum\limits_{I}$ denotes the sum over those $L \in \pounds^2_{4j+2}$ which have an even number of cycles of length $\equiv 0 \pmod 4$ and $\sum\limits_{II}$ denotes sum over those $L \in \pounds^2_{4j+2}$ which have an odd number of cycles of length $\equiv 0 \pmod 4$.

Again, by Lemma 5.2.4, we have

$$\begin{aligned}\sum_{L\in \pounds^2_{4j+2}} (-1)^{p(L)} s(L) &= \sum_{I} (-1)^{odd}(+1) + \sum_{II} (-1)^{even}(-1)\\ &= \sum_{I}(-1) + \sum_{II}(-1) = -|\pounds^2_{4j+2}|.\end{aligned}$$

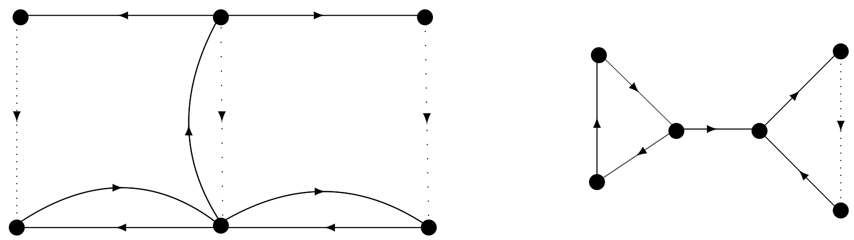
Therefore, $a_{4j+2} = -|\pounds^1_{4j+2}| - |\pounds^2_{4j+2}| = -|\pounds_{4j+2}|$.

Thus we conclude that

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

where $b_{2j} = |\pounds_{2j}|$ is the cardinality of the set $\pounds_{2j}$. □

Remark 5.2.6. Here we note that there exist bipartite and non bipartite non cycle balanced signed digraphs not in Δ^1_n which have characteristic polynomial with alternating coefficients. Signed digraphs S_1 and S_2 shown in Fig. 5.2 clearly do not belong to Δ_n^1. By Theorem 4.1.1, $\phi_{S_1}(x) = x^6 - x^4 + 2x^2$ and $\phi_{S_2}(x) = x^6 - 1$.



S_1 S_2

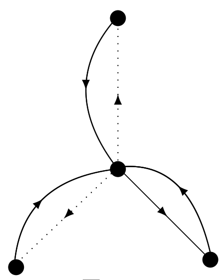
Fig. 5.2

The following result shows that the characteristic polynomial of a signed digraph in Δ_n^2 is of the form (5.2). Proof is same as the proof of Theorem 5.2.5.

Theorem 5.2.7. *If $S \in \Delta_n^2$, then characteristic polynomial is given by*

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

where $b_{2j} = |\pounds_{2j}|$ is the cardinality of the set $\pounds_{2j}$.



S Fig. 5.3

Remark 5.2.8. We note that there exist bipartite and non bipartite non cycle balanced signed digraphs not in Δ_n^2 which have characteristic polynomial of the form (5.2). Signed digraphs S_1 and S_2 shown in Fig. 5.1 and signed digraph S shown in Fig. 5.3 do not belong to Δ_n^2, because former are non bipartite and latter has a positive cycle of length 2. By Theorem 4.1.1, $\phi_{S_1}(x) = x^{17} + 3x^{11} + x^5$,

$\phi_{S_2}(x) = x^{17} + x^{11} + x^5$ and $\phi_S(x) = x^4 + x^2$.

Recall the definition of Cartesian product of two signed digraphs. Let $S_1 = (V_1, \mathscr{A}_1, \sigma_1)$ and $S_2 = (V_2, \mathscr{A}_2, \sigma_2)$ be two signed digraphs, their Cartesian product (or sum) denoted by $S_1 \times S_2$ is the signed digraph $(V_1 \times V_2, \mathscr{A}, \sigma)$, where the arc set is that of the Cartesian product of underlying unsigned digraphs and the sign function is defined by

$$\sigma((u_i, v_j), (u_k, v_l)) = \begin{cases} \sigma_1(u_i, u_k), & \text{if } j = l, \\ \sigma_2(v_j, v_l), & \text{if } i = k. \end{cases}$$

Unlike Kronecker product [56], Cartesian product of two strongly connected signed digraphs is always strongly connected as can be seen in the following result.

Lemma 5.2.9. *If S_1 and S_2 be two strongly connected signed digraphs, then $S_1 \times S_2$ is strongly connected.*

Proof. Let $(u_i, v_j), (u_p, v_q) \in V(S_1 \times S_2)$, where we assume $p \leq q$ (case $p > q$ can be dealt similarly). Since S_1 is strongly connected, there exists a directed path $(u_i, u_{i+1})(u_{i+1}, u_{i+2}) \cdots (u_{p-1}, u_p)$. Also, strong connectedness of S_2 implies there exists a directed path $(v_j, v_{j+1})(v_{j+1}, v_{j+2}) \cdots (v_{q-1}, v_q)$. By definition of Cartesian product, Fig. 5.4 illustrates that there exists a directed path from (u_i, v_j) to (u_p, v_q). Signs do not play any role in connectedness, so we take all arcs in Fig. 5.4 positive. Similarly, one can prove the existence of a directed path from (u_p, v_q) to (u_i, v_j). $\square$

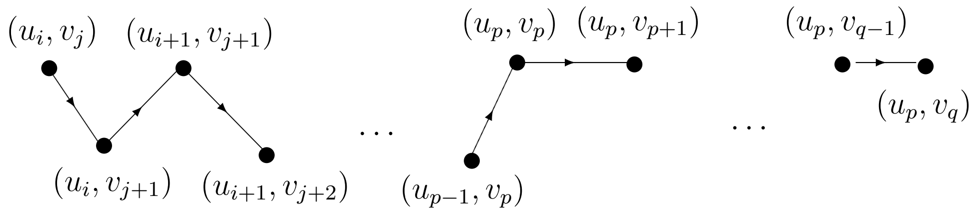
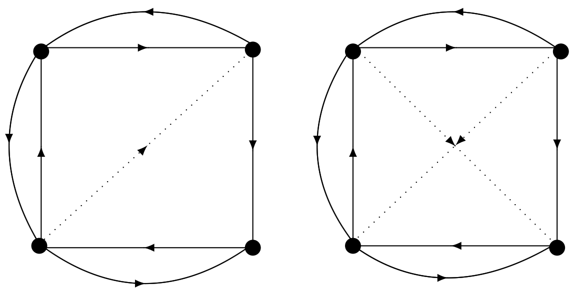


Fig. 5.4

Definition 5.2.10. A signed digraph is said to integral (real or Gaussian) according as spectrum of S is integral (real or Gaussian) respectively.

The following three results show the existence of non cycle balanced integral, real and Gaussian signed digraphs.



S_1 Fig. 5.5 S_2

Theorem 5.2.11. *For each positive integer $n \geq 4$, there exists a family of n integral cospectral, strongly connected, non symmetric and non cycle balanced signed digraphs of order 4^n.*

Proof. Consider signed digraphs S_1 and S_2 shown in Fig. 5.5. Clearly S_1 and S_2 are non cycle balanced and strongly connected. By Theorem 4.1.1,

$$\phi_{S_1}(x) = \phi_{S_2}(x) = x^4 - 3x^2 + 2x.$$

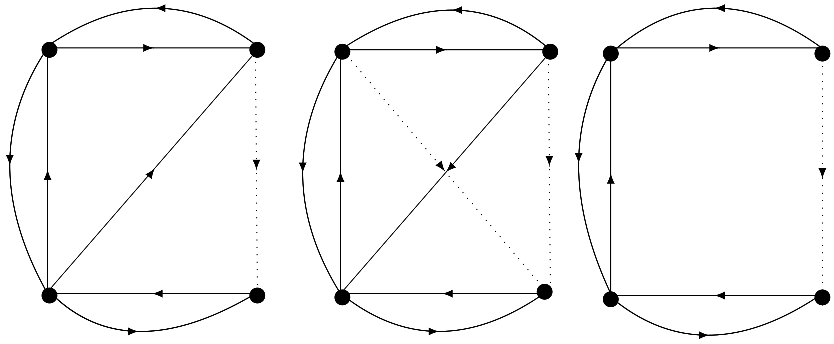
Therefore, $spec(S_1) = spec(S_2) = \{-2, 0, 1^{(2)}\}$. That is, S_1 and S_2 are integral cospectral.

Let

$$S^{(k)} = S_1 \times S_1 \times \cdots \times S_1 \times S_2 \times S_2 \times \cdots \times S_2,$$

where we take k copies of S_1 and $n-k$ copies of S_2. Clearly, for each n, we have n cospectral signed digraphs $S^{(k)}$, $k = 1, 2, \cdots, n$ of order 4^n. Now, S_1 and S_2 are non symmetric implies $S^{(k)}$ is non symmetric. By repeated application of Lemma 5.2.9 and using the fact that Cartesian product of signed digraphs is cycle balanced if and only if the constituent signed digraphs are cycle balanced, the result follows. $\square$

Integral signed digraphs are obviously real. There exists non integral real signed digraphs as can be see in the following result.



S_1 S_2 S_3

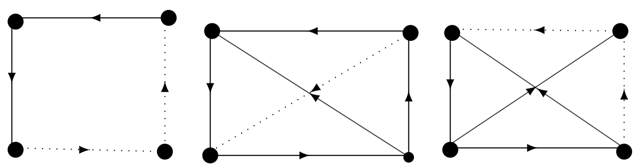
Fig. 5.6

Theorem 5.2.12. *For each positive integer $n \geq 4$, there exists a family of n real cospectral, strongly connected, non symmetric and non cycle balanced signed digraphs of order 4^n.*

Proof. Consider signed digraphs S_1, S_2 and S_3 shown in Fig. 5.6. Clearly, all three signed digraphs are non cycle balanced and strongly connected. By Theorem 4.1.1,

$$\phi_{S_1}(x) = \phi_{S_2}(x) = \phi_{S_3}(x) = x^4 - 3x^2 + 2.$$

Therefore, $spec(S_1) = spec(S_2) = spec(S_3) = \{-\sqrt{2}, -1, 1, \sqrt{2}\}$. Take any two signed digraphs among S_1, S_2 and S_3 and apply the procedure of Theorem 5.2.11, the result follows. $\square$



S_1 S_2 S_3

Fig. 5.7

Every integral signed digraph is obviously Gaussian. The next result shows that there exists non integral Gaussian signed digraphs i.e., signed digraphs with eigenvalues of the form $a + \iota b$, where a and b are integers with $b \neq 0$ for some b.

Theorem 5.2.13. *For each positive integer $n \geq 4$, there exists a collection of n Gaussian cospectral, strongly connected, non symmetric and non cycle balanced signed digraphs of order 4^n.*

Proof. Consider signed digraphs S_1, S_2 and S_3 shown in Fig. 5.7. It is clear that S_1 is cycle balanced, whereas S_2 and S_3 are non cycle balanced. Moreover all three signed digraphs are strongly connected. By Theorem 4.1.1,

$$\phi_{S_1}(x) = \phi_{S_2}(x) = \phi_{S_3}(x) = x^4 - 1.$$

Therefore, $spec(S_1) = spec(S_2) = spec(S_3) = \{-1, 1, -\iota, \iota\}$. Hence S_1, S_2 and S_3 are Gaussian cospectral. Take any two signed digraphs among S_1, S_2 and S_3 and proceed in a similar way as in Theorem 5.2.11, the result follows. $\square$

Two digraphs D_1 and D_2 are said to be quasi-cospectral if there exist signed digraphs S_1 and S_2 respectively on D_1 and D_2 such that $\phi_{S_1}(x) = \phi_{S_2}(x)$. That is, S_1 and S_2 are cospectral. Two cospectral digraphs are quasi-cospectral by Theorem 4.1.2, for we can take any two cycle balanced signed digraphs one on each digraph. Two digraphs are said to be strictly quasi-cospectral if they are quasi-cospectral but not cospectral. Two digraphs D_1 and D_2 are said to be strongly quasi-cospectral if both D_1 and D_2 are cospectral and there exists non cycle balanced signed digraphs respectively S_1 and S_2 on them such that $\phi_{S_1}(x) = \phi_{S_2}(x)$. Clearly, if D_1 and D_2 are strongly quasi-cospectral digraphs, then both should have at least on cycle.

Definition 5.2.14. We say two digraphs D_1 and D_2 are integral, real and Gaussian strongly quasi-cospectral if both D_1 and D_2 are respectively integral, real and Gaussian cospectral and there exists non cycle balanced signed digraphs S_1 and S_2 on them which are respectively integral, real and Gaussian cospectral.

The following result shows the existence of integral strongly quasi-cospectral digraphs.

Theorem 5.2.15. *For each positive integer $n \geq 4$, there exists a family of n integral, strongly connected, non symmetric and strongly quasi-cospectral digraphs of order 4^n.*

Proof. Let D_1 and D_2 respectively be the underlying digraphs of integral signed digraphs S_1 and S_2 shown in Fig. 5.5. Then D_1 and D_2 are all-positive signed digraphs. By Theorem 4.1.1, we have

$$\phi_{D_1}(x) = \phi_{D_2}(x) = x^4 - 3x^2 - 2x.$$

Therefore, $spec(D_1) = spec(D_2) = \{-1^{(2)}, 0, 2\}$.

Put $D^{(k)} = D_1 \times D_1 \times \cdots \times D_1 \times D_2 \times D_2 \times \cdots \times D_2$, where we take k copies of D_1 and $n-k$ copies of D_2. In this way, for each $n \geq 4$ we get n cospectral, non symmetric and strongly connected integral digraphs. Thus for any two of these integral cospectral digraphs $D^{(k_1)}$ and $D^{(k_2)}$ there exist corresponding non cycle balanced signed digraphs $S^{(k_1)}$ and $S^{(k_2)}$ on them which are integral cospectral. □

The following result shows the existence of real strongly quasi-cospectral digraphs.

Theorem 5.2.16. *For each positive integer $n \geq 4$, there exists a collection of n real, strongly connected, non symmetric and strongly quasi-cospectral digraphs of order 4^n.*

Proof. Let D_1 and D_2 be the underlying digraphs of signed digraphs S_1 and S_2 as shown in Fig. 5.6. It is easy to see that $\phi_{D_1}(x) = \phi_{D_2}(x) = x^4 - 3x^2 - 2x$ and $spec(D_1) = spec(D_2) = \{-1^{(2)}, 0, 2\}$. Also $spec(S_1) = spec(S_2) = \{-\sqrt{2}, -1, 1, \sqrt{2}\}$.

Thus D_1 and D_2 are real strongly quasi-cospectral. Applying the same technique as in Theorem 5.2.15, the result follows. □

5.3 Energy of bipartite signed digraphs

Rada, Gutman and Cruz [71] compared the energies of digraphs in Δ_n^*. We now derive integral expressions for signed digraphs in Δ_n^1 and Δ_n^2 and compare energies of signed digraphs in Δ_n^1 by means of quasi-order relation.
Given signed digraphs S_1 and S_2 in Δ_n^1, by Theorem 5.2.5, for $i = 1, 2$, we have

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

where $b_{2j}(S_i)$ are non negative integers for all $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$. If $b_{2j}(S_1) \leq b_{2j}(S_2)$ for all $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, then we define $S_1 \preceq S_2$. If in addition $b_{2j}(S_1) < b_{2j}(S_2)$ for some $j = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, then we write $S_1 \prec S_2$. The following result shows that energy increases with respect to this quasi-order relation.

Theorem 5.3.1. *If $S \in \Delta_n^1$, then*

$$E(S) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log[1 + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(S) x^{2j}] dx.$$

In particular, if $S_1, S_2 \in \Delta_n^1$ and $S_1 \prec S_2$ then $E(S_1) < E(S_2)$.

Proof. We know that the energy of a signed digraph S satisfies the integral expression

$$E(S) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log |x^n \phi_S(\frac{\iota}{x})| dx.$$

Assume $S \in \Delta_n^1$, then $\phi_{S(x)} = x^n + \sum\limits_{j=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^j b_{2j}(S) x^{n-2j}$,
so that

$$E(S) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \log |x^n \frac{\iota^n}{x^n} (1 + \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(S) x^{2j})| dx$$

$$=\frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{1}{x^2}\log|\iota^n(1+\sum_{j=1}^{\lfloor\frac{n}{2}\rfloor}b_{2j}(S)x^{2j})|dx$$

$$=\frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{1}{x^2}\log[1+\sum_{j=1}^{\lfloor\frac{n}{2}\rfloor}b_{2j}(S)x^{2j}]dx.$$

If $S_1 \prec S_2$, then from the last integral expression it is clear that $E(S_1) < E(S_2)$. That is, energy increases with respect to quasi-order relation defined above. $\square$

The following integral expression whose proof is same as that of Theorem 5.3.1, holds good for a signed digraph in Δ_n^2.

Theorem 5.3.2. *If $S \in \Delta_n^2$, then*

$$E(S) = \frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{1}{x^2}\log|1+\sum_{j=1}^{\lfloor\frac{n}{2}\rfloor}(-1)^j b_{2j}(S)x^{2j}|dx.$$

Remark 5.3.3. We note that the same integral expression holds for all non bipartite signed digraphs which have characteristic polynomial of the form (5.2). It remains a question to define a quasi-order relation (if possible) for signed digraphs in Δ_n^2 for comparison of energy.

Rada et al. [71] proved that the energy of a digraph in Δ_n^* decreases when we delete an arc from a cycle of length 2. As in digraphs, in general it is not possible to predict the change in the energy of a non cycle balanced signed digraph by deleting an arc from a cycle of length 2. It can decrease, increase or remain same by deleting an arc of a cycle of length 2 as can be seen in the following example.

Example 5.3.4. Consider the signed digraphs S_1, S_2 and S_3 as shown in Fig. 5.8. It is easy to see that $\phi_{S_1}(x) = x^6 + 2x^4 + 1$ and $\phi_{S_1^{(v_1,v_2)}}(x) = x^6 + x^4 + 1$, where $S_1^{(v_1,v_2)}$ denotes the signed digraph obtained by deleting the arc (v_1, v_2). Note $E(S_1) \approx 2.4916$ and $E(S_1^{(v_1,v_2)}) \approx 2.9104$. So the energy increases in this case. Also, $\phi_{S_2}(x) = x^6 + x^4 - x^2 - 1$ and $spec(S_2) = \{-1, 1, -\iota^{(2)}, \iota^{(2)}\}$ so that $E(S_2) = 2$. If we delete arc (v_1, v_2), the resulting signed digraph has eigenvalues

$\{-1, 0^{(2)}, 1, -\iota, \iota\}$ so the energy of the resulting signed digraph is again 2. That is, energy remains same in this case. It is not difficult to check that $E(S_3) = 2+2\sqrt{2}$ and $E(S_3^{(v_1,v_2)}) = 2\sqrt{2}$. So the energy decreases in this case.

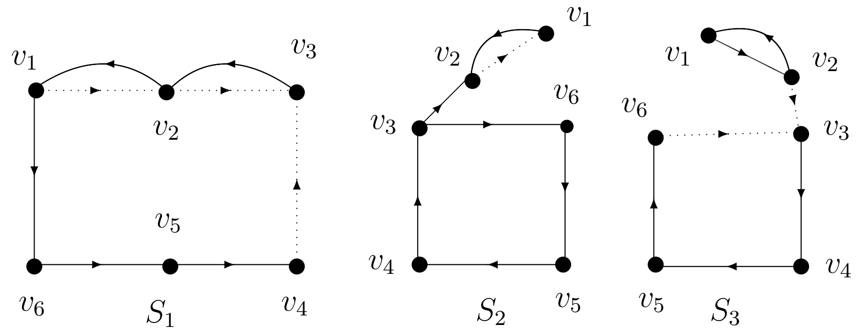


Fig. 5.8

The following result shows that the energy of a signed digraph in Δ_n^1 decreases when we delete an arc from a cycle of length 2.

Theorem 5.3.5. *Let S be a signed digraph in Δ_n^1 with a pair of symmetric arcs and let S' be the signed digraph obtained by deleting one of these arcs. Then $E(S') < E(S)$.*

Proof. Let $S \in \Delta_n^1$. If we delete an arc of S from a cycle of length two, then the resulting signed digraph S'(say) also belongs to Δ_n^1. By Theorem 5.2.5, the characteristic polynomial of S is given by

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

where $b_{2j}(S) = |\mathcal{L}_{2j}|$ is the cardinality of the set $\mathcal{L}_{2j}$.

It is clear that $S' \preceq S$ and $b_2(S') < b_2(S)$. So, $S' \prec S$. By Theorem 5.3.1 $E(S') < E(S)$. $\square$

5.4 Conclusion

We conclude with the following open problem.

Problem 5.4.1. *Characterize signed digraphs with characteristic polynomial of the form* (5.1) *or* (5.2).

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