Energy of digraphs

by

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Abstract

Graph spectra has vast applications in applied chemistry, physics and mathematics. It is also used in modelling virus propagation and error-correcting codes in computer networks. It measures robustness of a network against the spread of viruses. Most work done in graph spectra is related to the energy of graphs or nullity of graphs.

The eigenvalues of a digraph are the eigenvalues of its adjacency matrix. The sum of the absolute values of real part of the eigenvalues is called the energy of the digraph. The extremal energy of bicyclic digraphs with vertex-disjoint directed cycles is known. In this thesis, we consider a class of bicyclic digraphs with exactly two directed cycles of equal length. We find the minimal and maximal energy among the digraphs in this class. We also construct a class of k-cyclic digraphs having exactly k directed cycles of equal length and find extremal energy of this class.

Furthermore, we consider a more general class of tricyclic digraphs and signed digraphs and find the digraphs and signed digraphs with extremal energy.

Acknowledgement

Thanks to Allah Jalla Jalaluhu, Hazrat Muhammad (S.A.W.W) and the Quran Who blessed me the vision which made it possible for me to reach this significant stage, a further step towards the destination.

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No words are enough to elaborate the efforts put in by the parents for the success of there child, neither their is any matching tribute, so I just pray to Almighty Allah to reciprocate them.

Yasir Masood

Preface

Many real life circumstances can be suitably expressed with the help of figures consisting of set of points along with line joining the points. For example points could be people, with lines joining a pair of friends, or the points could be the communication centres with lines representing communication links. Note that in these figures, one is interested in whether the given points are joined by a line or not. A mathematical abstraction of circumstances of this sort give rise to the idea of graph.

The origin of graph theory probably goes back to 1763 when the great Leonhard Euler proposed a famous problem to travel all the seven bridges of the city of Königsberg in a single round trip when every bridge is travelled exactly once. All the graphs satisfying this property are named Eulerian after Leonhard Euler. He modeled this problem in the form of a graph and gave the solution that; "a graph is Eulerian if and only if every vertex has even degree".

Graph theory can be classified into algebraic graph theory, spectral graph theory, association schemes and coherent configurations. In algebraic graph theory graphs are studied by using algebraic properties of the matrix associated with the graphs, while spectral graph theory studies the relationship among the graph properties and the spectrum of the matrices associated with the graphs. The theory of coherent configuration and association scheme studies the algebra generated by the associated matrices.

Spectral graph theory deals with the properties of a graph in relation to its adjacency matrix as well as other associated matrices. The spectral graph theory prompts to make effective use of linear algebra particularly the well established theory of matrices for the purposes of graph theory.

Contents

Chapter 1

Fundamentals of Graph Theory

1.1 Introduction

This chapter gives the necessary characteristics of graphs and some very important definitions. It contains various theoretical terms of graphs and their examples. Idea is to present basic properties of matrices, some common graphs with illustrations that further explain these terms in a brief way.

1.2 What are graphs?

A *graph* $G = (\mathcal{V}, \mathcal{E})$ is composed of two finite sets $\mathcal{V}$ and $\mathcal{E}$. The elements of $\mathcal{V}$ are called *vertices* and the elements of $\mathcal{E}$ are known as *edges*. When two edges have same endpoints, they are called *multiple edges*. If an edge e joins a vertex v with itself, then it is called a *self loop* or simply *loop*. A graph without loops is a *multigraph*. A graph having at least one loop is known as *pseudograph*. A graph is *simple* if it has neither loops nor multiple edges. Two vertices are said to be *adjacent* whenever they are joined by an edge. If two vertices u and v of a graph G are joined by an edge e then we say that e is incident on u and v. Clearly, each edge has two vertices as its endpoints, so usually we denote an edge by its end vertices, that is, e will be denoted as uv.

The *neighbourhood* of a vertex v in G is the set of all vertices of G which are adjacent to v and is denoted as $N_G(v)$ or $N(v)$. The number of vertices and edges in a graph are respectively called the *order* (denoted as $|V(G)|$) and *size* (denoted as $|\mathcal{E}(G)|$) of the graph. When $V(G)$ is empty, the graph is called *null* graph. Similarly a graph is said to be *finite* if its vertex and edge sets are finite.

Consider a graph G_1 in Figure 1.1. The vertex set of the graph is $V(G_1) =$

$\{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and the edge set is $\mathcal{E}(G_1) = \{v_1v_2, v_2v_3, v_1v_3, v_1v_3, v_4v_5, v_6v_6\}$. There is a multiple edge v_1v_3 in G_1 so it is written twice in the edge set. There is a loop joining the vertex v_6 to itself. There is no edge incident on v_7, so it is an isolated vertex. The neighbourhood of v_2 in this graph is $N(v_2) = \{v_1, v_3\}$.

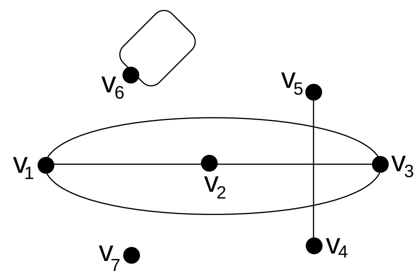

Figure 1.1: G_1

All the edges in Figure 1.1 have certain lengths, different shapes and cross each other at different points. The vertices are at specific positions with respect to each other. But according to the abstract definition of a graph, G_1 is merely a graph with vertex set $\{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and edge set $\{v_1v_2, v_2v_3, v_1v_3, v_1v_3, v_4v_5, v_6v_6\}$. These abstract properties of the graph G_1 in Figure 1.1 are the same as that of another graph G_2 in Figure 1.2. So we say that the graph in Figure 1.1 is the same as that in Figure 1.2 or that G_1 and G_2 are the redrawings of each other.

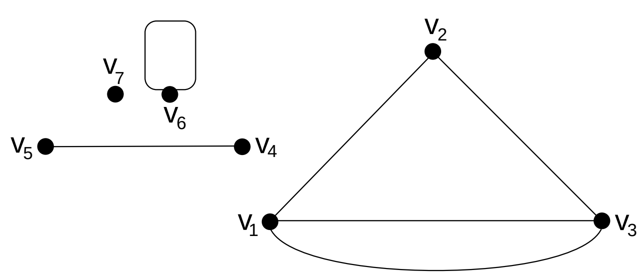

Figure 1.2: G_2

The vertices in a graph can be considered as places and the edges can be considered as links between these vertices. We travel on these edges to reach different vertices. Suppose we travel from a vertex u to a vertex v through an edge e, if we can travel back to the vertex u through the same edge e then the edge e is unordered pair of vertices u and v, that is, $uv = vu = e$, but if we can go through e in only one direction (say from u to v) then the edge e is an ordered pair of vertices, in this case $e = uv \neq vu$. The edges discussed in the second case are called *directed* edges, and the graph all of whose edges are directed is known as *directed graphs* or simply *digraphs*. To avoid ambiguity, the undirected edge or simple edge uv is written as $\{u, v\}$ and directed edge uv is written as (u, v). A graph having both directed and undirected edges is called to be *mixed graph*.

In a graph G, the degree of a vertex v, denoted as $d(v)$ or $d_G(v)$, is the number of edges incident on v. The *maximum degree* of a graph G is the maximum vertex degree in that graph, denoted as $\triangle(G)$, and the *minimum degree* is the minimum vertex degree in the graph, denoted as $\delta(G)$. The *degree sequence* or *graphic sequence* is the non-increasing sequence formed by vertex degrees of the graph. The *degree* of a graph is the sum of degrees of all the vertices. If there is no edge incident on a vertex v, it is called an *isolated vertex*. That is an *isolated vertex* is a vertex of degree 0, and a vertex of degree 1 is called a *leaf* or a *pendent* vertex. A vertex is *even* (odd) if its degree is even (odd). A graph is *even or odd* if all of its vertex degrees are even or odd, respectively. In a simple graph of order p, the maximum degree of a vertex is $p-1$, since any vertex can at most be adjacent to all other $p-1$ vertices. Hence for any vertex v in a graph, $d(v)$ lies between 0 and $p-1$. A graph is called *regular* or *k-regular* if all the vertex degrees are k, that is, $\triangle(G) = \delta(G) = k$. The 3-regular graphs are known as *cubic* graphs. All graphs in Figure 1.3 are cubic.

The *adjacency matrix* of an n-vertex simple graph G, denoted by $A_G = [a_{ij}]_{n\times n}$, is a symmetric matrix ($M^t = M$) of order n whose rows and columns are indexed by the vertices of G, where

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

A loop contributes two to the degree of any vertex. The adjacency matrix of the graph G_1 in Figure 1.1 is given below:

$$A(G_1) = \begin{pmatrix} 0 & 1 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The entries on the principal diagonal represent loops on the respective vertices.

If a_{ii} is 4, it means that there are two loops on vertex v_i.

The *characteristic polynomial* of a graph G is $\Phi_G(x) = det\big(xI - A_G\big)$, where I is the identity matrix of order n. If A is a square matrix of order n, then the scalar λ is called an eigenvalue of A if there is a nonzero $n \times 1$ matrix V, such that $AV = \lambda V$. In this case V is known as an eigenvector of A corresponding to the eigenvalue λ. The *eigenvalues* of a graph are actually the eigenvalues of its adjacency matrix. The eigenvalues of a graph together with their multiplicities form the *spectrum* of a graph.

Now we state the *fundamental theorem of graph theory* also known as the *Euler degree-sum theorem.*

Theorem 1.2.1 ([12])**.** *The sum of degrees of the vertices of a graph G is twice the size of graph, that is,*

$$\sum_{v \in V(G)} d(v) = 2|\mathcal{E}(G)|.$$

Since each edge contributes one to the degree of each of its end-vertex, it contributes two, to the degree of the graph. Alternatively, summing up all the vertex degrees includes every edge twice, so degree of the graph equals twice the number of edges. We can draw some trivial results from this theorem, such as:
1) The degree of a graph is always even.
2) In any graph, the number of vertices of odd degree is even.
3) No graph of odd order is regular with odd degree.

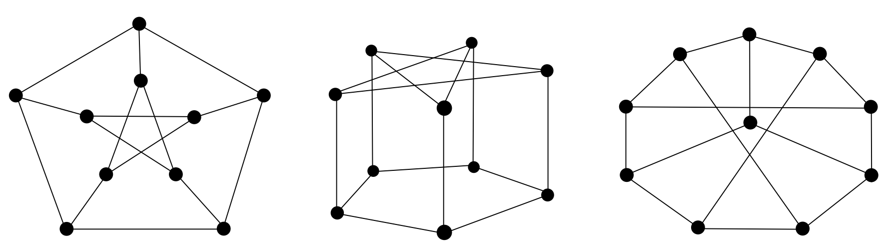

Figure 1.3: Some 3-regular graphs

A graph H is a *subgraph* of a graph G if $V(H)$ and $\mathcal{E}(H)$ are contained in $V(G)$ and $\mathcal{E}(G)$, respectively. The subgraph H of G is said to be *spanning* if $V(H) = V(G)$. If $S \subseteq V(G)$, a subgraph H induced by S, denoted as $H[S]$, is a graph with $V(H) = S$ and all the edges of G which have both ends in S.

Let u and v be two vertices in a graph. A *walk* between u and v in the graph is a finite alternating sequence $u = v_o, e_1, v_1, e_2, v_2, e_3, \ldots, v_{n-1}, e_n, v_n = v$ of vertices and edges of the graph such that each edge e_j in the sequence joins vertex v_{j-1} and vertex v_j. The vertices and edges in a walk are not necessarily distinct. The *length* of the walk is the number of edges in a walk. A walk in which no edge is repeated is called a *trail*. The walk in which all vertices are distinct is called a *path*. From the definition of a path it is obvious that every path is a trail.

A *circuit* is a closed trail, that is, a trail in which first and last vertex are same. Moreover, a circuit with no repeated vertex is called a *cycle*. A cycle of order n is denoted as C_n. A *cycle with a chord* is a cycle in which any two non-adjacent vertices are joined with an edge. The *girth* of a graph is the length of smallest cycle in the graph. If there is no cycle in the graph then girth is undefined. In Figure 1.4, a circuit $\{a, ab, b, bc, b, c, cd, d, de, e, ef, f, fg, g, gh, h, hd, d, di, i, ia, a\}$, a path $\{j, jk, k, kl, l, lm, m\}$ and a cycle $\{n, no, o, op, p, pq, q, qr, r, rn, n\}$ are highlighted. We can observe that a circuit is an edge disjoint union of cycles.

If v and w are vertices in a digraph, a *directed walk* from v to w is a finite sequence $v = v_o, a_1, v_1, a_2, v_2, a_3, ..., a_n, v_n = w$, of vertices and arcs of the digraph such that each arc a_j in the sequence is an edge from v_{j-1} to v_j. A directed walk is called *directed trail* if all arcs are distinct. A *directed path* from v to w in a digraph is a directed walk from v to w in which every vertex occurs only once.

Any graph with $\delta(G) \geq 2$ contains a cycle. This can be proved by a simple algorithm. Suppose there is a maximal path $P = \{v_1, v_2, \ldots, v_n\}$ in the graph. Then the first and the last vertex of P have at least one neighbour which is not on the path, say v_{n+1} is such a vertex. Extend P to $P' = \{v_1, v_2, \ldots, v_n, v_{n+1}\}$, which contradicts the maximality of P. Hence the graph contains a cycle.

An *isomorphism* between simple graphs G and H is a bijection $f : V(G) \rightarrow V(H)$ such that $uv \in \mathcal{E}(G)$ if and only if $f(u)f(v) \in \mathcal{E}(H)$. If such mapping exists we say that G is *isomorphic* to H and write $G \cong H$. In an isomorphism, the adjacency relations of one graph are preserved in the other. While discussing a graph G in this theory we actually are talking about an isomorphism class of graphs containing all the graphs isomorphic to that particular graph G. Our structural comments and conclusions will be true for all the graphs isomorphic to G. For the isomorphic graphs G and H, the image $f(v) \in V(H)$ of a vertex $v \in V(G)$ preserves all the adjacency properties of v in H. For example, the degree of v remains same, if v was adjacent to two vertices of degree r_1 and r_2 in G, then $f(v)$ has the neighbours of same degrees in H, if v was on a cycle of length r in G then its image is on a cycle of length r in H.

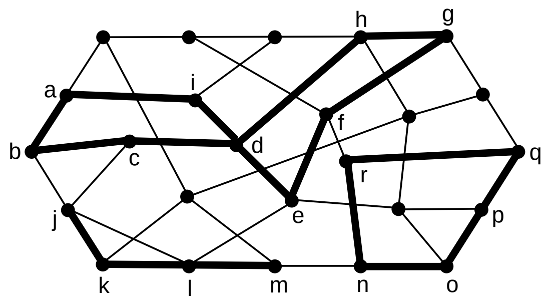

Figure 1.4: Circuit, path and cycle in a graph

Isomorphic graphs satisfy many other properties, for example, both graphs must have the same degree sequence, if the graph G can be drawn in such a way that no two edges cross each other then H can also be drawn in this way. We can use adjacency matrices to check graph isomorphism as well. If we order the vertices of one graph in such a way that its adjacency matrix becomes identical with the adjacency matrix of some other graph then both graphs are isomorphic. All graphs in Figure 1.3 are isomorphic to each other.

A *clique* in a graph G is the set of pairwise adjacent vertices. The maximum cardinality of a clique in G is the *clique number* of G, denoted by $\omega(G)$. An *independent set* is the set of pairwise non-adjacent vertices in the graph, and the maximum number of vertices in such set is called *independence number*, denoted as $\beta(G)$.

The *distance* between two vertices u and v in a graph is the length of shortest path between these vertices, denoted as $d(u, v)$. If no such path exist then $d(u, v) = \infty$. A graph is *connected* if for every pair of vertices, there is at least one path between them, otherwise graph is *disconnected*. The graph in Figure 1.4 is connected but that in Figure 1.1 is disconnected.

An *Eulerian circuit* in a graph G is a circuit (closed trail) which contains all edges of G. A graph is *Eulerian* if it contains an Eulerian circuit. In the following theorem, a characterization of Eulerian graphs is presented.

Theorem 1.2.2 ([12]). *The following statements are equivalent for a connected graph G.*
(1) *G is Eulerian.*
(2) *The degree of every vertex in G is even.*
(3) *$\mathcal{E}(G)$ is the union of edge-disjoint cycles in G.*

If a graph is Eulerian then by definition we have a trail passing from every edge and ending at the point from where we started it. The trail visits a particular vertex through an edge and leaves through some other edge, so every time the trail visits the vertex it uses two from the degree of the vertex. Since the trail used all the edges so it visited all the vertices even number of times, which implies that all vertex degrees are even. When degree of all vertices is even we can partition the edge set in cycles. It can be proved with the help of an algorithm. Consider a maximal path in a graph and extend any of its leaves using the given condition that all vertex degrees are even. It will result in a cycle (or a contradiction). Now, delete the edges of the cycle we obtain and apply the algorithm again on the resultant graph.

A cycle is said to be *Hamiltonian* if it passes through every vertex of the graph. A graph containing a *Hamiltonian cycle* is called a *Hamiltonian graph*. Clearly, a Hamiltonian cycle in a graph is a spanning subgraph of the graph. There is no characterization known for Hamiltonian graph, but we have some results sufficient for a graph to be Hamiltonian. Some of the simplest conditions are stated below.

Theorem 1.2.3 ([12]). *A simple graph with n vertices (where $n \geq 3$) is Hamiltonian if the degree of every vertex is at least $n/2$.*

Theorem 1.2.4 ([13]). *Let G be a simple n-vertex graph, where ($n > 2$), such that $d(x) + d(y) \geq n$ for each pair of non-adjacent vertices x and y, then G is Hamiltonian.*

A *bipartite* graph is a graph whose vertex set can be partitioned in two sets, called partite sets, in such a way such that the vertices in each partite set are pairwise non-adjacent. The two partite sets are independent of each other and are called *bipartition* of the graph. Similarly, a graph is *s-partite* if its vertex set is the union of s independent sets. A very useful characterization of bipartite graphs is given in the following theorem. A partite graph is called *balanced* if all the partite sets have equal cardinality.

Theorem 1.2.5 ([13]). *A graph G is bipartite if and only if it contains no odd cycle.*

In a bipartite graph with bipartition $[X, Y]$, let us construct a cycle with initial vertex in any partite set, say X. To create a cycle we need to visit both partite sets alternatively, since vertices in one partite set can not be adjacent. So every time we return to the partite set from where we started, we travel even number of edges.

A graph is *complete* if all of its vertices are pairwise adjacent. A complete graph of order n is denoted as K_n. Clearly, a complete graph K_n is a regular graph of degree $n-1$. The complete bipartite graph denoted by $K_{m,n}$ is the graph $(\mathcal{X}, \mathcal{Y}, \mathcal{E})$ with m vertices in $\mathcal{X}$ and n vertices in $\mathcal{Y}$ in which there is an edge between every vertex in $\mathcal{X}$ and every vertex in $\mathcal{Y}$. In Figure 1.5, we present a complete graph K_{10} on 10 vertices and a complete bipartite graph $K_{4,3}$.

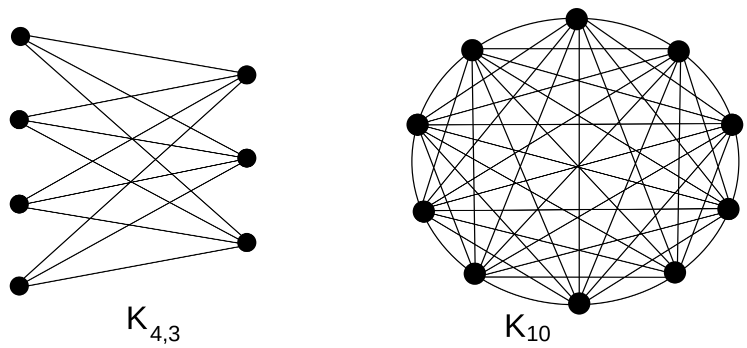

Figure 1.5: Complete graphs

The maximal connected subgraph of a graph G is called a *component* of G. A disconnected graph obviously has atleast two components. The number of components of a graph G is denoted as $c(G)$. The graph in Figure 1.2 has 4 components. A *separating set* (also called *vertex-cut*) of a graph G is a set $S \subseteq V(G)$ such that $G \setminus S$ (the set whose members are the elements belonging to set G which are not the members of set S) is disconnected. Similarly an *edge-cut* is a set $H \subseteq \mathcal{E}(G)$ such that $G \setminus H$ is disconnected. A $\{u, v\}$-separating set in a graph is the set of edges whose deletion disconnect the vertices u and v.

A single vertex whose deletion from a graph increases its number of components, is called a *cut-vertex*. Similarly a single edge whose removal from a connected graph leaves it disconnected, is called a *bridge*. We can observe that a bridge can never be a part of a cycle. It is interesting to know that the deletion of a vertex v from a connected graph G can create many components in $G \setminus \{v\}$, but deletion of one edge can increase the number of components by at most 1.

The *vertex connectivity* $\kappa(G)$ of a connected graph G is the minimum number of vertices whose removal can disconnect the graph G. When $\kappa(G) \geq k$ (where k is the number of vertices in the separating set), graph is called k-connected. In the same way, the *edge connectivity* $\lambda(G)$ of a connected graph is minimum number of edges whose removal can disconnect the graph. The graph G is called *k-edge connected* when $\lambda(G) \geq k$. When a graph is k-edge connected, every two vertices are joined by k internally disjoint paths. The converse of this statement also holds.

The vertex connectivity of a complete graph K_n is not defined since it has no separating set, so we adopt a convention that a graph with one isolated vertex is disconnected, then $\kappa(K_n) = n - 1$. Similarly, the vertex connectivity of a complete bipartite graph $K_{m,n}$ is $min\{m, n\}$, because vertices in one partite set are only adjacent to the vertices of other partite set, so deleting the vertices of one partite set leaves the other partite set isolated. The graph (a) in Figure 1.6 has no cut-vertex, the minimal vertex-cut is $\{x, y\}$ and the minimum $\{u, v\}$-separating set consists of edges $\{e_1, e_2, e_3, e_4\}$. In graph (b) of the same Figure, there is a bridge e, and the end-vertices of e are both cut-vertices. So, the vertex and edge connectivity of the graph (b) is 1.

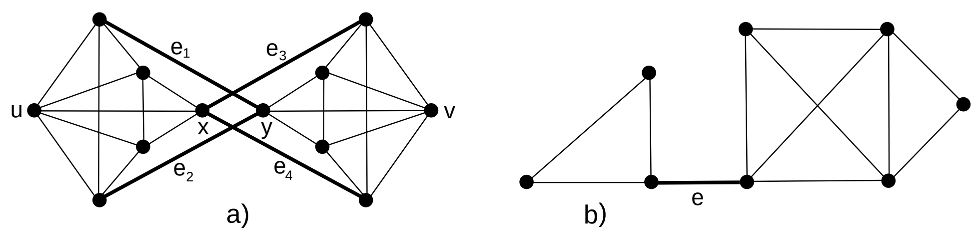

Figure 1.6: vertex/edge-cut in a graph

The connectivity of a graph can also be regarded as the strength of connections between its vertices. After removing some vertices or edges, if the graph is still connected means the connections in the graph are strong. While trying to disconnect a graph by removing edges, it is direct observation that if we remove the edges incident on the vertex with minimum degree in the graph, the connection of all other vertices with that vertex will be destroyed, and the graph becomes disconnected. So, we can say that for a connected graph, $\lambda(G) \leq \delta(G)$. The vertex connectivity and the edge connectivity can be compared with the following theorem.

Theorem 1.2.6 ([13])**.** *If G is a simple graph then vertex connectivity never exceeds edge connectivity, i.e., $\kappa(G) \leq \lambda(G)$.*

For a k-edge connected graph G, there will be an edge cut say S with k edges in G. The edges of S partition $V(G)$ in two sets say V_1 and V_2, each edge of S has on end in V_1 and other end in V_2. If we remove at most k vertices from any of V_1 or V_2, on which the edges in S are incident, we can disconnect the graph G. Hence the edge connectivity exceeds the vertex connectivity.

A graph G is said to be *planar graph* if it can be drawn in a plane in such a way that no two edges cross each other. Such a drawing, if it exist, is called the *planar embedding* of the graph. If a graph is not planar, the minimum number of edges-crossing is called the *crossing number* of the graph. A planar embedding of a graph divides the plane in different regions. Each maximal region which is not partitioned by an edge or path in further subregions is called a *face*. The planar embedding of a finite graph G always has an *unbounded face*. The *boundary* of a face is the set of vertices and edges surrounding the face, and the *length* of the i-th face (denoted as $l(f_i)$) is the length of the closed walk around the face in G. In planar embedding of a graph, a bridge can be included in only one face, and it contributes 2 to the length of that face. We can observe that the sum of lengths of all the faces of a planar graphs equals twice the size of the graph. Since every edge can be at most at the boundary of two neighbouring faces, they are counted twice when adding all face lengths. The edges which lie in a unique face are counted twice because they are the bridges, so we get a degree sum and face relationship $\sum_i l(f_i) = 2|\mathcal{E}(G)|$.

Theorem 1.2.7 ([13])**.** *If a connected planar graph G has exactly n vertices, e edges and f faces, then $n - e + f = 2$.*

The formula in the above theorem is known as *Euler's formula* and it is satisfied by every connected planar graph. For a graph with k components, *Euler's formula* becomes $n - e + f = k + 1$, because we only need to add $k - 1$ edges to make the graph connected. We can find an upper bound for the size of a graph using this theorem. Using the fact that every face should be of length 3 or more, from the degree sum and face relation we get $3f \leq 2|\mathcal{E}(G)|$, where f is the number of faces. Now using this inequality in *Euler's formula* we get $|\mathcal{E}(G)| \leq 3|V(G)| - 6$.

A subdivision of a graph means the subdivision of its edges by replacing the edges with paths internally disjoint from each other. The planar graphs are characterized by the *Kuratowski's theorem* stated below.

Theorem 1.2.8 ([12])**.** *A graph is planar if and only if it does not contain a subdivision of K_5 or $K_{3.3}$.*

The graphs K_5 and $K_{3,3}$ are the smallest graphs which can not be drawn on a plane without edge-crossing. These graphs are known as *Kuratowski's graphs*.

The *eccentricity* of a vertex v in a graph G, denoted as $ecc(v)$, is the distance from v to the farthest vertex in G, that is, $ecc(v) = \max\{d(v, x) | x \in V(G)\}$. The *diameter* of a graph, denoted as $diam(G)$, is the maximum distance between any two vertices of G. So, in terms of eccentricity, $diam(G) = \max\{ecc(v) | v \in V(G)\}$. Similarly, the *radius* of a graph G is the minimum of all the eccentricities of the graph, that is, $rad(G) = \min\{ecc(v)|v \in V(G)\}$. All the vertices having minimum eccentricities are called *central* vertices. The graph (a) in Figure 1.7 has diameter 9 and radius 5, while the graph (b) has constant eccentricity, so $diam(G_1) = rad(G_2) = 5$.

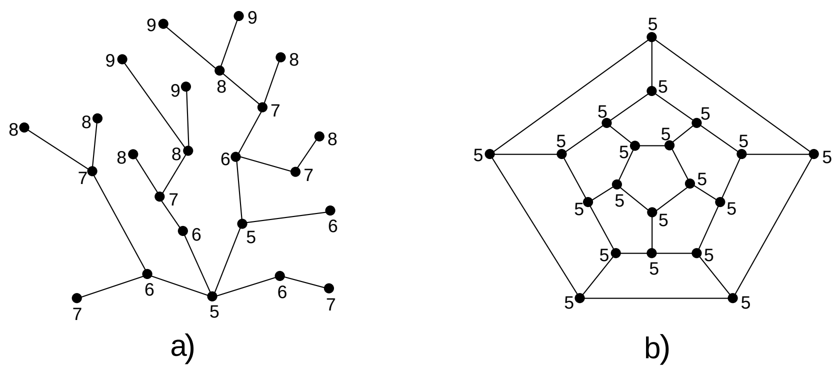

Figure 1.7: Two graphs labeled with vertex eccentricities

1.3 Trees and forests

There are special type of graphs having no cycles, called *acyclic* graphs. An acyclic graph is called a *forest* and a connected forest is called a *tree*. So it is clear that every component of a forest is a tree. This family of graphs is important to the structural understanding of graphs and to the algorithms of the information processing, and they play central role in design of connected networks. Some special tree structures are used in information management to store data in space efficient ways that allow their retrieval and modification to be time efficient [16].

Now we discuss some properties of trees. A very basic property is that every tree of size more than one has at least two leaves. No graph can has one vertex of degree 1, since the number of odd vertices must be even, this can be followed from theorem 1.2.1. So if a tree does not has 2 vertices of degree 1, then its minimum degree is at least two, then there must be a cycle in the graph which is not true because a tree does not contains a cycle. Hence a tree contains at least two leaves. A *spanning* tree of a graph G is a spanning subgraph of G which is a tree.

A tree is a *minimal connected* graph. That is, the deletion of one edge leaves the tree disconnected. A tree of order n has exactly $n - 1$ edges. We can apply induction on the number of vertices to prove this statement. If there is one vertex

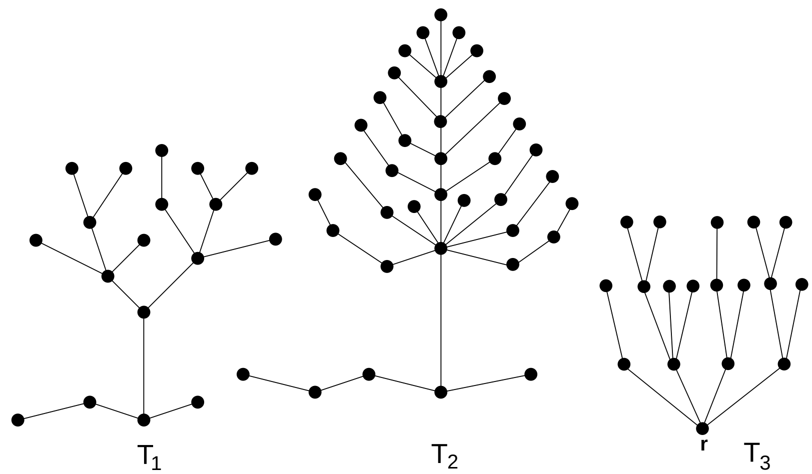

Figure 1.8: Trees in a forest

then the statement is trivial. Let there are k vertices in the tree, then the size of the tree is $k-1$. Now, consider any tree T on $k+1$ vertices. Let x is a leaf in T, then $T-x$ is also acyclic and connected. So, $T-x$ is a tree on k vertices and $k-1$ edges. Since $T-x$ has one vertex less than T, so, T has exactly k edges. Similarly, a tree on n vertices and k components has exactly $n-k$ edges.

Earlier in this chapter a *path* was defined as a trail with no repeated vertex. We can also define a *path* as a tree in which every i-th vertex is adjacent with $(i+1)$-st vertex. A path on n vertices is denoted as P_n. A star is a tree in which a single fixed vertex is adjacent to all other vertices. A star with $n+1$ vertices is denoted as S_n. The forest of stars is known as a *galaxy*.

A *rooted tree* is a tree in which a fixed vertex r (say) is designated as the *root* of the tree. For every vertex v the unique paths from the root r to that vertex v is directed away form the root. In a rooted tree if vertex u and v are adjacent and u lies in the path from the root r to v, then u is called the *parent* of v, and v is called the *child* of u, and all other vertices in the path are called the *ancestors* of v. Every tree can be drawn in the from of a rooted tree. The tree T_3 in Figure 1.8 is a rooted tree. The next theorem provides some useful characterizations of trees.

Theorem 1.3.1 ([12]). *Let T be a connected graph with n vertices. Then the following statements are equivalent.*
(i) T is a tree.
(ii) T contains no cycles and has $n-1$ edges.

(iii) T is connected and has $n-1$ edges.
(iv) T is connected, and every edge is a cut-edge.
(v) Any two vertices of T are connected by exactly one path.
(vi) T has no cycles, and for each new edge e, the graph $T+e$ has exactly one cycle, where $T+e$ is a graph obtained by adding an edge between two pendent vertices of T.

These statements can be derived easily in the light of previously discussed properties of trees. Since a tree is a minimal connected graph, so deletion of any edge leads to disconnection, so every edge is cut-edge. Only a cycle provides alternative paths between vertices of a graph. Since a tree has no cycle so there is a unique path between any two vertices. Now, a tree is connected so there is a path between every pair of vertices say x and y. If we add an edge xy in the tree, it provides an alternative path to travel between x and y, hence produces a cycle.

1.4 Operations on graphs

One very common operation that we perform on graphs is *vertex/edge deletion* from the graph. Once a vertex is deleted from a graph, all the edges incident on that vertex are also removed and when an edge is deleted from a graph, no difference occur other than the size of the graph is reduced by 1. For $e \in \mathcal{E}(G)$, the edge deleted graph G is denoted as $G-e$. Another operation that we perform only on edges of a graph is *contraction* of an edge. An edge uv is contracted by coinciding both of its end-vertices into a single vertex x and joining all edges which were incident on u and v to the new vertex x. The graph we obtain after contracting the edge $e=uv$ is denoted as $G|uv$ or $G|e$. Studying simple graphs, any loops or multiple edges that occur after edge contraction are removed. The deletion and contraction of an edge e in P_5 is Figured in 1.9.

The *disjoint union* of graphs $H_1, H_2, \ldots, H_n$ is the graph $G = H_1 \cup H_2 \cup \cdots \cup H_n$ with vertex set $\bigcup\limits_{i=1}^{n} V(G_i)$ and edge set $\bigcup\limits_{i=1}^{n} \mathcal{E}(G_i)$. The disjoint union of k copies of G is denoted as kG. If G and H are disjoint graphs (two graphs that have no common vertex), then their join $G+H$ or $G \vee H$ is a graph obtained by joining each vertex of G to each vertex of H. That is, $\mathcal{E}(G \vee H) = \mathcal{E}(G) \cup \mathcal{E}(H) \cup \{uv : u \in V(G), v \in V(H)\}$.

The *Cartesian product* of two graphs G and H, denoted as $G \Box H$, is a graph with vertex set $V(G \Box H) = V(G) \times V(H)$ and any two vertices (u, v) and (u', v') are adjacent in $G \Box H$ if and only if either $u = u'$ and v is adjacent to v' or $v = v'$ and u is adjacent to u'. The join and Cartesian product of C_4 and P_5 are shown in Figure 1.10.

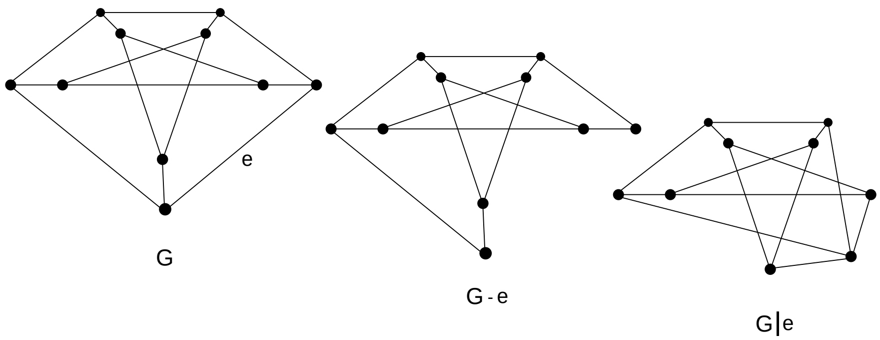

Figure 1.9: Edge contraction in a graph

1.5 Some special classes of graphs

A *wheel* is a graph obtained by joining all the vertices of a cycle to a new vertex. A wheel of order $n+1$ denoted as W_n. If we remove one edge from the outer cycle of a wheel, the resulting graph is called *fan*, denoted by f_n. If we remove the edges from the outer cycle of the wheel alternatively, we get a *friendship* graph, denoted by F_n. The wheel, fan and friendship graphs are elaborated in Figure 1.11.

A fan graph f_n can also be obtained by $P_n \Box K_1$, where K_1 represents complete graph on a single vertex (an isolated vertex). Similarly a wheel graph can be described as $C_n \Box K_1$, and a friendship graph is $(2n)P_2 \Box K_1$, where $(2n)P_2$ represents even number of copies of P_2.

A *circular ladder* is a graph obtained by $C_n \Box P_2$, denoted as D_n. A circular ladder is also called a *prism*. An *antiprism* (denoted as A_n) is a graph formed by combining two n sided polygons by a band of $2n$ triangles. The graph C_4 is known as 2-*hypercube* (Q_2). The graph $C_4 \Box P_2$ is called 3-*hypercube* (Q_3). Similarly, the n-*hypercube* (Q_n) is obtained by $Q_{n-1} \Box P_2$.

The graph $P(n,k)$ denotes the *generalized Petersen graph* and is defined as the graph with vertex sets $\{v_1, v_2, \ldots, v_n\}$ and $\{u_1, u_2, \ldots, u_n\}$ and edges $\{v_j v_{j+1}\}$, $\{v_j u_j\}$ and $\{u_j u_{j+k}\}$, where addition is modulo n. The *Petersen* graph in this notion is $P(5,2)$. The prism D_8, antiprism A_8 and the generalized Petersen graph $P(8,3)$ (also known as Möbius-Cantor graph) are shown in Figure 1.11.

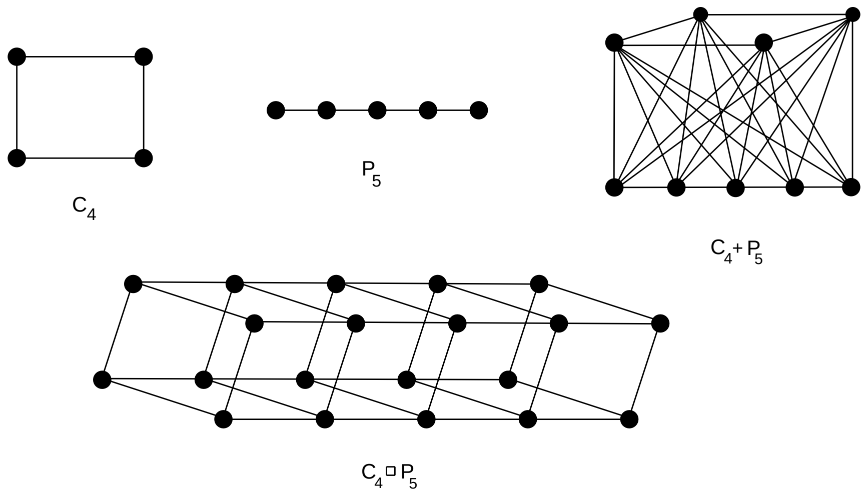

Figure 1.10: Join and cartesian product of C_4 and P_5

1.6 Spectra of a graph

We have already defined adjacency matrix of a graph. In this section, further properties of graph spectrum will be discussed. Let G be a graph without loops. The *incidence* matrix $M = [m_{ij}]$ of G is a $0-1$ matrix whose rows and columns are indexed by vertices and edges of G, respectively, where

$$m_{ij} = \begin{cases} 1; & \text{if vertex } v_i \text{ is endpoint of the edge } e_j \\ 0; & \text{otherwise.} \end{cases}$$

The *Laplace* matrix $L = [l_{ij}]$ of a simple graph G is indexed by the vertices of G, having row sums zero and $l_{ij} = -a_{ij}$ for $i \neq j$, where a_{ij} denotes the elements of the adjacency matrix $A = [a_{ij}]$ of G. Also $L = D - A$, where D is diagonal matrix with elements from vertex set of G such that d_{ii} is the degree of vertex i and A is the adjacency matrix of G. The *signless Laplace matrix* of a graph G is defined by $Q = D + A$.
The incidence, diagonal, adjacency, Laplace and signless Laplace matrix of the graph as shown in Figure 1.12 are respectively as

$$M = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

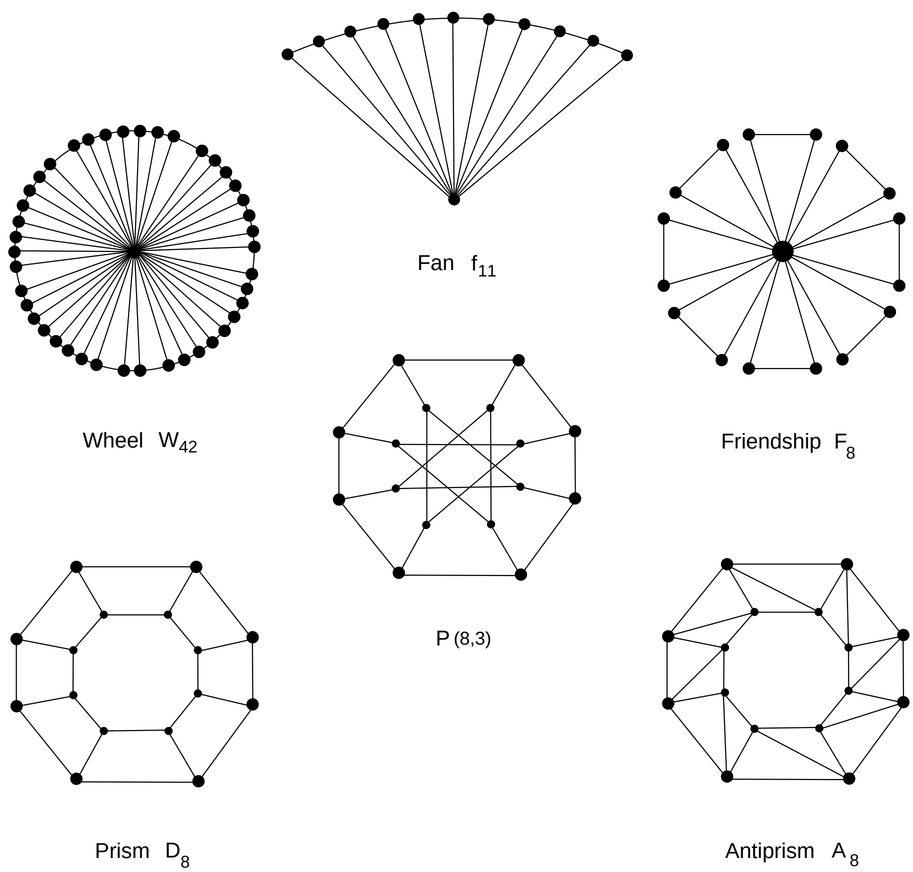

Figure 1.11: Wheel, fan, friendship, prism, antiprism and Petersen graph $P(8,3)$

$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

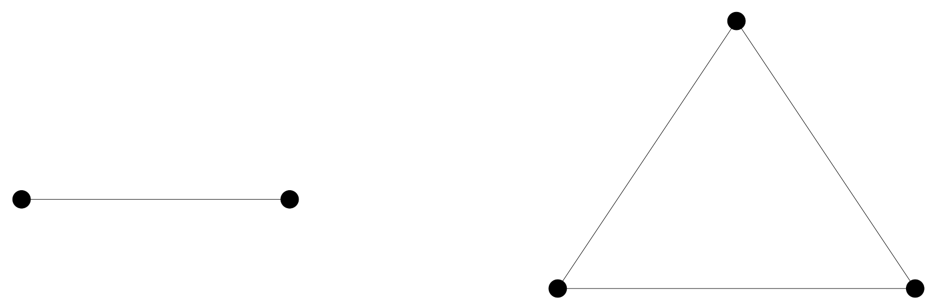

Figure 1.12: A graph G on 5 vertices

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$L = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

and

$$Q = \begin{bmatrix} 2 & 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

Characteristic polynomial of a square matrix B is defined as $\phi_B(x) = |xI - B|$. The values of x that satisfy the characteristic equation $\phi_G(x) = 0$ are called *eigenvalues* of graph G. The *algebraic multiplicity* or simply *multiplicity* of an eigenvalue x_i, is the largest positive integer k such that $(x - x_i)^k$ divides the equation $\phi_G(x) = 0$. The *geometric multiplicity* of an eigenvalue x is the dimension of the eigenspace associated with x, that is, the maximum number of vectors in any linearly independent set of eigenvectors with eigenvalue x. It is clear from the definition of eigenvalue, geometric multiplicity is always greater than or equal to 1.

The *ordinary spectrum* of a graph G is the spectrum of adjacency matrix and is defined as, the set of eigenvalues together with their algebraic multiplicities. The *Laplace spectrum* of a graph G without loops is the spectrum of Laplace matrix L.

Now we define an important term of spectral graph theory, that is, the *energy* of a graph. It was introduced by Ivan Gutman [5] and is defined as the sum of absolute values of eigenvalues of graph. Mathematically if $x_1, x_2, \ldots, x_n$ are eigenvalues of a graph G, then energy of G is given by:

$$E(G) = \sum_{i=1}^{n} |x_i|. \tag{1.1}$$

Since 1940s the sum of absolute values of the eigenvalues of some graphs was considered, it was in 1970s when Gutman used (1.1) as definition. This equation is applicable to every simple graph without any limitations. In 21^{st} century, researchers realized the mathematical value of graph energy and a world wide research of graph energy started. At present, several hundred researchers from all over the world participated or participating in research on graph energy.

In 1930s the German scholar Erich H*ü*ckel presented a method for finding approximate solutions of Schr*ö*dinger equation of a class of organic molecules, known as "unsaturated conjugated hydrocarbons". Its details often referred as H*ü*ckel Molecular Orbital (HMO). Theory can be found in many famous books.

The Schr*ö*dinger equation is a second-order partial differential equation of the form

$$\hat{H}\phi = E\phi, \tag{1.2}$$

where ϕ, $\hat{H}$ and E are wave function, Hamiltonian operator and energy of the system considered. When applied to a particular molecule, the Schrodinger equation enables one to express the behaviour of electrons and to find their energies. Equation (1.2) can be expressed as

$$\mathbf{H}\phi = E\phi,$$

where $\mathbf{H} = [h_{ij}]$ is a matrix of order n and

$$h_{ij} = \begin{cases} \alpha; & \text{if } i = j \\ \beta; & \text{if atom } i \text{ and } j \text{ are chemically bonded} \\ 0; & \text{if there is no chemical bond between atom } i \text{ and } j. \end{cases}$$

It is named as Hamiltonian matrix. Here the parameters α and β are constant, equal for all conjugated molecules.

1.7 Spectra of a digraph

Although many problems can be represented by graph-theoretic formulation, the idea of graph is sometimes not enough. For instance, when dealing with traffic flow problem, it is essential to know that which roads permit the traffic in one way and in which direction traffic flow is allowed. Clearly graph of such network problem cannot provide all the information about the situation.

What we require is a graph in which each edge is given a direction−directed graph. Thus a directed graph D is triplet (V, A, ϕ_D) consisting of set of vertices V, set of directed edges A and and an incidence function ϕ_D that relates each edge an ordered pair of vertices of D. If e is an edge and v_1 and v_2 are vertices such that $e = \phi(v_1, v_2)$, then e joins v_1 and v_2. The vertices v_1 and v_2 are respectively known as tail and head of e. A directed graph or simply a digraph H is called subdigraph of D if both vertex set and edge set of H are contained in vertex set and edge set of D and ϕ_H is a restriction of ϕ_D.

To each digraph D we can associate a graph G both having same vertex set and to an directed edge of D there is an edge of G with same end points as in D, the graph G is known as underlying graph of D. For converse, given any graph G we can obtain a digraph D by orienting each edge of G, the digraph D is called orientation of G.

A directed walk in D is a finite non-null sequence $W = (u_0, e_1, u_2, \ldots, u_{n-1}, e_n, u_n)$ whose terms are alternately vertices and directed edges, such that for $i = 1, 2, \ldots, n$, the edge e_i has tail u_{i-1} and head u_i. A directed trail is a walk that is trail, that is there is no repetition of directed edges in such walks.

The adjacency matrix of an n-vertex digraphs D is a square matrix $A = [a_{ij}]$ of order n, whose elements are indexed by vertices of D, where

$$a_{ij} = \begin{cases} 1 & \text{if there is a directed edge from vertex } v_i \text{ to a vertex } v_j \\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of a digraph D is defined by

$$\phi_D(x) = |xI - A|,$$

where A is the adjacency matrix of D. The values of x that satisfy the equation

$$\phi_D(x) = 0$$

are called eigenvalues of the digraph D. Note that the adjacency matrix of a digraph is not necessarily symmetric, so eigenvalues of digraph can be complex numbers. The energy of an n-vertex digraph D is defined as [1]

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

some important results on energy of digraphs.
where $\Re(x_i)$ denotes the real part of eigenvalues x_i of D, $1\leq i\leq n$. Now we give

Energy of a digraph D can be calculated by a very useful result known as Coulson's integral formula [1], that is

$$E(D)=\frac{1}{\pi}\int_{-\infty}^{\infty}\left(n-\frac{ix\phi'_D(ix)}{\phi_D(ix)}\right)dx,$$

where $\phi_D(x)$ denotes the characteristic polynomial of digraph D, $\phi'_D(x)$ is the first derivative of $\phi_D(x)$ and n is the number of vertices in digraph D.
Let D be a digraph, then the maximal connected subgraph of D is called strong component of D if there is a directed path between each vertex to every other vertex.

Theorem 1.7.1 ([1])**.** *Consider a digraph D and let $H_1,H_2,\ldots,H_k$ be the strong components of D. Then*

$$E(D)=\sum_{i=1}^{k}E(H_i).$$

The next theorem gives the extremal energy of a unicyclic digraph.

Theorem 1.7.2 ([1])**.** *Among all unicyclic digraphs of order n, the minimal energy is obtained in digraphs which contain a cycle of length 2, 3 or 4. The maximal energy is attained in the cycle C_n of length n.*

Now we define skew adjacency matrix of a digraph. The skew adjacency matrix of an n-vertex digraph D is a matrix $S(D)=[s_{ij}]$, where

$$s_{ij}=\begin{cases}+1 & \text{if there is a directed edge from } v_i \text{ to } v_j\\ -1 & \text{if there is a directed edge from } v_j \text{ to } v_i\\ 0 & \text{otherwise.}\end{cases} \tag{1.3}$$

Since $S(D)$ is skew symmetric matrix so its eigenvalues are pure imaginary numbers, and the singular values of $S(D)$ coincides with the absolute values $|\lambda_1|,\ldots,|\lambda_n|$ of its eigenvalues.

Adiga et al. [3] gave the concept of skew energy of a digraph. Let D be an n-vertex digraph and let $S(D)$ be its skew adjacency matrix defined by (1.3). Then the skew energy of D, denoted by $\xi(D)$, and is defined by

$$\xi(D) = \sum_{i=1}^{n} |\lambda_i|.$$

Now we present some important results of skew adjacency matrix of a digraph.

Theorem 1.7.3 ([3])**.** *Let D be an n-vertex digraph and*

$$\phi_D(x) = a_0 x^n + a_1 x^{n-1} + \ldots + a_n$$

be the characteristic polynomial of the skew adjacency matrix $S(D)$ defined by (1.3)*. Then*

1. $a_0 = 1$*,*

2. $a_1 = 0$*,*

3. $a_2 = m$*, where m is the number of arcs of D and*

4. $a_i = 0$*, $\forall$ odd i.*

Theorem 1.7.4 ([3])**.** *Let $x_1, x_2, \ldots, x_n$ be the eigenvalues of $S(D)$. Then*

1. $\sum_{i=1}^{n} x_i^2 = -2m$*,*

2. $\sum_{i=1}^{n} |x_i^2| = 2m$ *and*

3. *For $1 \leq i \leq n$, $|x_i| \leq \triangle$, the maximum degree of the underlying digraph of D.*

Next theorem is used to find upper bound for skew energy of a digraph, similar to McClellands inequality [7] for graph energy.

Theorem 1.7.5 ([3])**.** *Let D be an n-vertex digraph. Then*

$$\sqrt{2m + n(n-1)p^{2/n}} \leq \xi(D) \leq \sqrt{2mn} \leq n\sqrt{\triangle},$$

where $p = det(S(D)) = \prod_{i=1}^{n} \mid x_i \mid$.

The following theorem gives the skew energy of digraph D using the maximum degree of the its underlying digraph.

Theorem 1.7.6 ([3]). *Let D be an n-vertex digraph. Then*

$$\xi(D) = n\sqrt{\triangle} \quad \textit{if and only if} \quad S^T(D)S(D) = \triangle I_n,$$

where I_n is the identity matrix of order n.

Theorem 1.7.7 ([3]). *Let D be a digraph and H be the digraph obtained from D by altering the orientations of all edges incident with a particular vertex of D. Then $\xi(D) = \xi(H)$.*

Following theorems are characterization of skew energy of tree.

Theorem 1.7.8 ([3]). *The skew energy of a directed tree is independent of its orientations.*

Theorem 1.7.9 ([3]). *The skew energy of a directed tree is same as the energy of its underlying tree.*

Chapter 2

Extremal Energy of Digraphs

In this chapter, we present a new class of digraphs $\mathcal{D}_n$ having number of cycles equal to number of linear subdigraphs. We find digraphs in $\mathcal{D}_n$ with minimal and the maximal energy.

2.1 Preliminaries

First, we give some definitions and terminologies. A directed cycle C_n of length n ($n \geq 2$) is a digraph with vertex set $\{v_i \mid i = 1, \ldots, n\}$ of n elements and arc set $\{v_i v_{i+1} \mid i = 1, \ldots, n-1\} \cup \{v_n v_1\}$ of n elements. A digraph is connected if its underlying graph is connected. A unicyclic digraph is a connected digraph which contains a unique directed cycle. A bicyclic digraph is a connected digraph which contains exactly two directed cycles.

The adjacency matrix $A_G = [a_{ij}]_{n\times n}$ of an n-vertex digraph $D = (\mathcal{V}, \mathcal{A})$ is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in \mathcal{A} \\ 0 & \text{otherwise} \end{cases} \quad (\forall v_i, v_j \in \mathcal{V}).$$

For digraphs, the eigenvalues may be complex numbers since the adjacency matrix of a digraph is not necessarily symmetric. The energy of a digraph is defined as the sum of the absolute values of the real parts of its eigenvalues. That is, if $z_1, z_2, \ldots, z_n$ are eigenvalues of an n-vertex digraph D, then its energy is defined as

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

where $\Re(z_i)$ is the real part of z_i.

Ever since the introduction of energy of graph by Gutman [9], there has been a continuous research on this topic. Moreover, the energy of a graph has close links to chemistry. Chemists prefer to use digraph in place of graph in certain situations. The following theorem gives characteristic polynomial of digraph.

Theorem 2.1.1 ([18] Coefficients theorem for digraphs)**.** *Let D be an n-vertex digraph with characteristic polynomial*

$$\Phi_D(x) = x^n + \sum_{k=1}^{n} b_k x^{n-k}.$$

Then $b_k = \sum\limits_{L \in \mathcal{L}_k} (-1)^{c(L)}$ for each $k = 1, 2, \ldots, n$, where $\mathcal{L}_k$ is the set of all linear subdigraphs of D with exactly k vertices and $c(L)$ denotes the number of components of a linear digraph L.

For $n \geq 3$, we define a set $\mathcal{D}_n$ which consists of n-vertex digraphs with exactly two linear subdigraphs of equal length. Let $D \in \mathcal{D}_n$ be a digraph such that the length of both linear subdigraphs is m, $2 \leq m \leq n-1$. From Theorem 2.1.1, the characteristic polynomial of D is given by

$$\Phi_D(x) = x^{n-m}(x^m - 2).$$

The eigenvalues of D are 0 and $\sqrt[m]{2}\exp(\frac{2k\pi i}{m})$, where $k = 0, 1, \ldots, m-1$ and the multiplicity of eigenvalue 0 is $n - m$. Thus the energy of D is given by

$$E(D) = \sqrt[m]{2} \sum_{k=0}^{m-1} \left| \cos \frac{2k\pi}{m} \right|. \tag{2.1}$$

Example 2.1.2. Consider the digraph $D \in \mathcal{D}_{10}$ shown in Figure 2.1. Using Theorem 2.1.1, the characteristic polynomial of D is given by

$$\Phi_D(x) = x^5\big(x^5 - 2\big).$$

The eigenvalues of D are 0 and $\sqrt[5]{2}\exp\frac{2k\pi i}{5}$, where $k = 0, 1, \ldots, 4$ and the multiplicity of 0 is 5. Thus, the energy of D is

$$\begin{aligned} E(D) &= \sqrt[5]{2} \sum_{k=0}^{4} \left| \cos \frac{2k\pi}{5} \right| \\ &= 3.7172. \end{aligned}$$

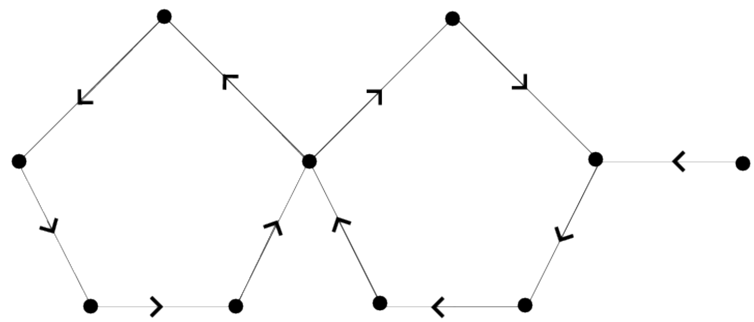

Figure 2.1: A digraph $D \in \mathcal{D}_{10}$.

From (2.1), we compute the energy formulae of D as follows:

$$E(D) = \begin{cases} 2\sqrt[m]{2}\cot\frac{\pi}{m} & \text{if } m \equiv 0(\text{mod}4) \\ 2\sqrt[m]{2}\csc\frac{\pi}{m} & \text{if } m \equiv 2(\text{mod}4) \\ \sqrt[m]{2}\csc\frac{\pi}{2m} & \text{if } m \equiv 1(\text{mod}2). \end{cases} \tag{2.2}$$

The following theorem will be used for calculating minimal and maximal energy of digraphs.

Theorem 2.1.3. [2] *Let x, a, b be real numbers such that $x \geq a > 0$ and $b > 0$. Then we have*

$$\frac{\pi x}{bx^2 - \pi^2} \leq \frac{\pi a}{ba^2 - \pi^2}.$$

For any real number x with $0 < x < \frac{\pi}{2}$, the following inequalities hold:

$$\sin x \leq x, \qquad \sin x \geq x - \frac{x^3}{3!}, \tag{2.3}$$

$$\cot x \leq \frac{1}{x}, \qquad \cot x \geq \frac{1}{x} - \frac{x}{2}, \qquad if \qquad x \neq 0 \tag{2.4}$$

2.2 Extremal energy of a bicyclic digraph

Pena and Rada [1] considered the problem of finding extremal energy among all unicyclic digraphs with fixed number of vertices. Khan et al. [2] considered the same problem for finding extremal energy for bicyclic digraphs with vertex-disjoint directed cycles. In this section, we find the minimal and maximal energy among the digraphs in $\mathcal{D}_n$. The following theorem gives us the lower bound for the energy of a digraph $D \in \mathcal{D}_n$.

Theorem 2.2.1. *Let $D \in \mathcal{D}_n$ such that the length of each linear subdigraph is m, where $2 \le m \le n-1$. Then*

$$E(D) \ge \begin{cases} \sqrt[m]{2}\left(\frac{2m}{\pi} - \frac{\pi}{m}\right) & \text{if } m \equiv 0(\text{mod}4) \\ \sqrt[m]{2}\left(\frac{2m}{\pi}\right) & \text{otherwise.} \end{cases}$$

Proof. Let $m \equiv 0(\text{mod}4)$. Then by (2.2) and (2.4), we get

$$\begin{aligned} E(D) &= 2\sqrt[m]{2}\left(\cot\frac{\pi}{m}\right) \\ &\ge 2\sqrt[m]{2}\left(\frac{m}{\pi} - \frac{\pi}{2m}\right) \\ &= \sqrt[m]{2}\left(\frac{2m}{\pi} - \frac{\pi}{m}\right). \end{aligned}$$

Next, if $m \equiv 2(\text{mod}4)$ then (2.2) and (2.3) yield

$$\begin{aligned} E(D) &= 2\sqrt[m]{2}\left(\csc\frac{\pi}{m}\right) \\ &= 2\sqrt[m]{2}\left(\frac{1}{\sin\frac{\pi}{m}}\right) \\ &\ge \sqrt[m]{2}\left(\frac{2m}{\pi}\right). \end{aligned}$$

Analogously, if $m \equiv 1(\text{mod}2)$ then we can show that

$$E(D) \ge \sqrt[m]{2}\left(\frac{2m}{\pi}\right).$$

The proof is complete. □

Example 2.2.2. Let $D \in \mathcal{D}_{15}$ be a digraph in which each linear subdigraph has length 13 as shown in Figure 2.2. Then from equation (2.2), we get

$$\begin{aligned} E(D) &= \sqrt[13]{2}\csc\frac{\pi}{26} \\ &= 8.7506. \end{aligned} \tag{2.5}$$

Also

$$\sqrt[m]{2}\left(\frac{2m}{\pi}\right) = \sqrt[13]{2}\left(\frac{26}{\pi}\right) \tag{2.6}$$

$$= 8.7293 \tag{2.7}$$

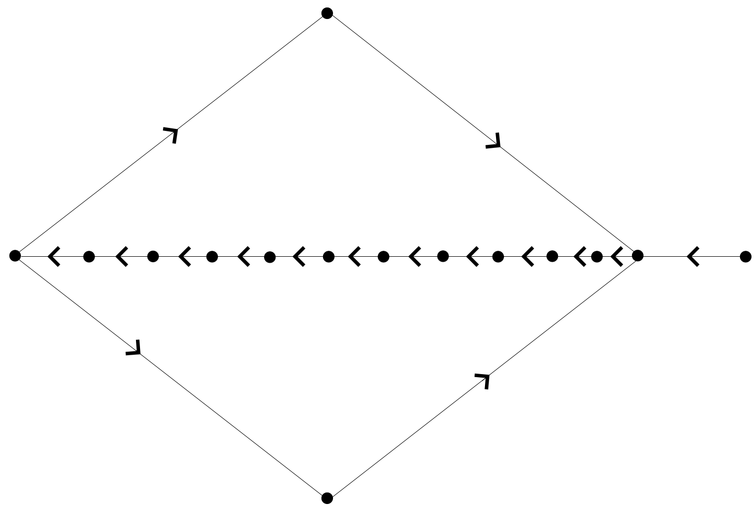

Figure 2.2: A digraph $D \in \mathcal{D}_{15}$.

From (2.5) and (2.6), we get

$$E(D) > \sqrt[m]{2}\left(\frac{2m}{\pi}\right),$$

which is a lower bound for $E(D)$.

The following theorem gives the upper bound for the energy of a digraph $D \in \mathcal{D}_n$.

Theorem 2.2.3. *Let $D \in \mathcal{D}_n$ such that the length of each linear subdigraph is m, where $2 \leq m \leq n-1$. Then*

$$E(D) \leq \begin{cases} \sqrt[m]{2}(\frac{2m}{\pi}) & \text{if } m \equiv 0(\text{mod}4) \\ \sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{6m^2-\pi^2}) & \text{if } m \equiv 2(\text{mod}4) \\ \sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{24m^2-\pi^2}) & \text{if } m \equiv 1(\text{mod}2). \end{cases}$$

Proof. First, let $m \equiv 0(\text{mod}4)$. By (2.2) and (2.4), we get

$$\begin{aligned} E(D) &= 2\sqrt[m]{2}\cot\frac{\pi}{m} \\ &\leq 2\sqrt[m]{2}(\frac{m}{\pi}) \\ &= \sqrt[m]{2}(\frac{2m}{\pi}). \end{aligned}$$

Next, we take $m \equiv 2(\text{mod}4)$. By (2.2) and (2.3), we get

$$\begin{aligned} E(D) &= 2\sqrt[m]{2}\csc\frac{\pi}{m} \\ &\leq 2\sqrt[m]{2}\left(\frac{1}{\frac{\pi}{m}(1-\frac{\pi^2}{6m^2})}\right) \\ &= 2\sqrt[m]{2}\left(\frac{m}{\pi}(\frac{6m^2}{6m^2-\pi^2})\right) \\ &= 2\sqrt[m]{2}\left(\frac{m}{\pi}(1+\frac{\pi^2}{6m^2-\pi^2})\right) \\ &= \sqrt[m]{2}\left(\frac{2m}{\pi}+\frac{2m\pi}{6m^2-\pi^2}\right). \end{aligned}$$

Finally, if $m \equiv 1(\text{mod}2)$ then one can analogously show that

$$E(D) \leq \sqrt[m]{2}\left(\frac{2m}{\pi}+\frac{2m\pi}{24m^2-\pi^2}\right).$$

This completes the proof. □

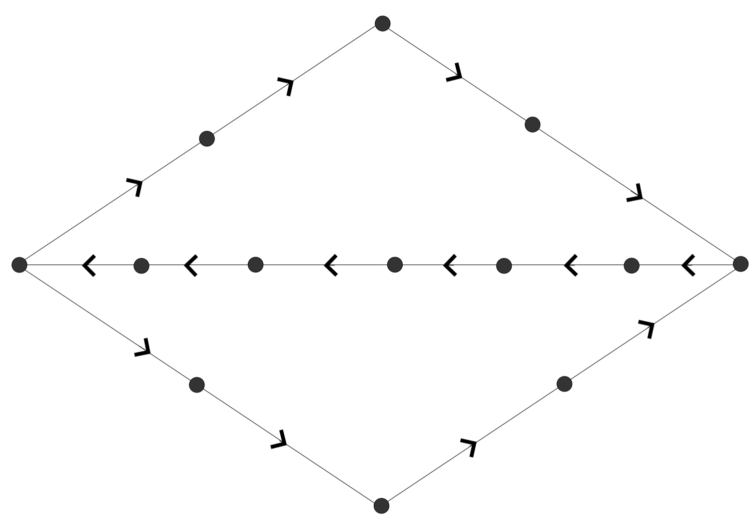

Figure 2.3: A digraph $D \in \mathcal{D}_{13}$.

Example 2.2.4. Let $D \in \mathcal{D}_{13}$ be a digraph in which each linear subdigraph has length 10 as shown in Figure 2.3, then from (2.2)

$$\begin{aligned} E(D) &= 2\sqrt[10]{2}\csc\frac{\pi}{10} \\ &= 6.9367. \end{aligned} \tag{2.8}$$

Now from Theorem 2.2.3

$$\sqrt[m]{2}\left(\frac{2m}{\pi}+\frac{2m\pi}{6m^2-\pi^2}\right) = \sqrt[10]{2}\left(\frac{20}{\pi}+\frac{20\pi}{6(10)^2-\pi^2}\right) \\ = 6.9372. \tag{2.9}$$

From (2.8) and (2.9), we obtain

$$E(D) < \sqrt[m]{2}\left(\frac{2m}{\pi}+\frac{2m\pi}{6m^2-\pi^2}\right),$$

which is a upper bound for $E(D)$.

Next theorem shows that the energy of digraphs in $\mathcal{D}_n$ increases monotonically with the increase in length of their linear subdigraphs.

Theorem 2.2.5. *Let $n \geq 6$ and $5 \leq m \leq n-1$. Take $D \in \mathcal{D}_n$ with length of each linear subdigraph $m+1$ and $H \in \mathcal{D}_n$ with length of each linear subdigraph m. Then*

$$E(D) \geq E(H).$$

Proof. Let $m \equiv 0(\text{mod}4)$. In this case, $m \geq 8$ and $m+1 \equiv 1(\text{mod}2)$ and Theorem 2.2.1 implies

$$E(D) \geq \sqrt[m+1]{2}\left(\frac{2m}{\pi}+\frac{2}{\pi}\right). \tag{2.10}$$

On the other hand, Theorem 2.2.3 gives

$$E(H) \leq \sqrt[m]{2}(\frac{2m}{\pi}). \tag{2.11}$$

One can easily see that the following inequality holds:

$$\sqrt[m+1]{2}\left(\frac{2m}{\pi}+\frac{2}{\pi}\right) \geq \sqrt[m]{2}(\frac{2m}{\pi}). \tag{2.12}$$

Combining $(2.10)-(2.12)$, we get

$$E(D) \geq E(H).$$

Next, let $m \equiv 2(\text{mod}4)$. In this case $m \geq 6$ and $m+1 \equiv 1(\text{mod}2)$. From Theorem 2.2.1, we get

$$E(D) \geq \sqrt[m+1]{2}(\frac{2m}{\pi}+\frac{2}{\pi}). \tag{2.13}$$

From Theorem 2.2.3, we get

$$E(H) \leq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{6m^2 - \pi^2}). \tag{2.14}$$

Furthermore, Theorem 2.1.3 implies that

$$\sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{6m^2 - \pi^2}) \leq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{12\pi}{6^3 - \pi^2}). \tag{2.15}$$

One can easily see that the following inequality holds:

$$\sqrt[m+1]{2}(\frac{2m}{\pi} + \frac{2}{\pi}) \geq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{12\pi}{6^3 - \pi^2}). \tag{2.16}$$

Combining $(2.13) - (2.16)$, we get

$$E(D) \geq E(H).$$

Finally, let $m \equiv 1(\text{mod}2)$. In this case $m \geq 7$, $m+1 \equiv 2(\text{mod}4)$ or $m+1 \equiv 0(\text{mod}4)$.
If $m+1 \equiv 2(\text{mod}4)$ then Theorem 2.2.1 implies

$$E(D) \geq \sqrt[m+1]{2}(\frac{2m}{\pi} + \frac{2}{\pi}). \tag{2.17}$$

On the other hand, Theorem 2.2.3 gives

$$E(H) \leq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}). \tag{2.18}$$

Theorem 2.1.3 implies that

$$\sqrt[m]{2}(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}) \leq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{14\pi}{24.7^2 - \pi^2}). \tag{2.19}$$

The following inequality is easily seen:

$$\sqrt[m+1]{2}(\frac{2m}{\pi} + \frac{2}{\pi}) \geq \sqrt[m]{2}(\frac{2m}{\pi} + \frac{14\pi}{24.7^2 - \pi^2}). \tag{2.20}$$

Combining $(2.17) - (2.20)$, we get

$$E(D) \geq E(H).$$

If $m+1 \equiv 0(\text{mod}4)$, one can analogously show that

$$E(D) \geq E(H).$$

This completes the proof. □

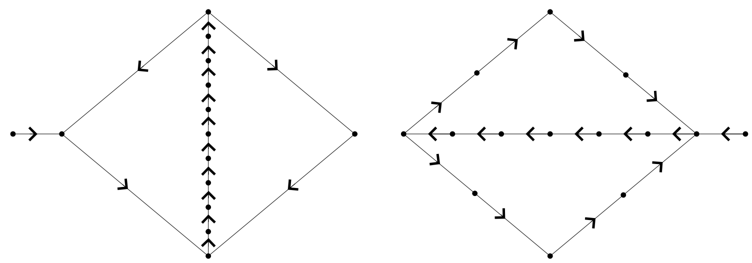

Figure 2.4: Digraphs $D, H \in \mathcal{D}_{14}$, D on left and H on right.

The following theorem is an easy consequence of Theorem 2.2.5.

Theorem 2.2.6. *Let $n \geq 6$ and $2 \leq m_2 \leq m_1 \leq n-1$. Take $D \in \mathcal{D}_n$ with length of each linear subdigraph m_1 and $H \in \mathcal{D}_n$ with length of each linear subdigraph m_2. Then*

$$E(D) \geq E(H).$$

Example 2.2.7. Let $D, H \in \mathcal{D}_{14}$ be digraphs each having two linear subdigraphs of equal length 12 and 10 respectively, as shown in Figure 2.4 then $E(D) \geq E(H)$. From (2.2) energy of D and H are given by

$$\begin{aligned} E(D) &= 2\sqrt[12]{2}\cot\frac{\pi}{12} \\ &= 7.9079. \end{aligned} \tag{2.21}$$

Similarly

$$\begin{aligned} E(H) &= 2\sqrt[10]{2}\csc\frac{\pi}{10} \\ &= 6.9367. \end{aligned} \tag{2.22}$$

From (2.21) and (2.22), it follows that

$$E(D) \geq E(H).$$

Using Theorem 2.2.6, we finally prove the main theorem.

Theorem 2.2.8. *Let $n \geq 6$ and $D \in \mathcal{D}_n$ be a digraph with length of each linear subdigraph m, where $2 \leq m \leq n-1$. Then D has minimal energy when $m = 4$ and maximal energy when $m = n-1$ among all digraphs of $\mathcal{D}_n$.*

Proof. Let $D \in \mathcal{D}_n$ be a digraph with linear subdigraphs of equal length m, where $2 \leq m \leq n-1$. Then it can easily be seen from (2.2) that

$$E(D) = \begin{cases} 2\sqrt[2]{2} & \text{if } m = 2 \\ 2\sqrt[3]{2} & \text{if } m = 3 \\ 2\sqrt[4]{2} & \text{if } m = 4. \end{cases} \tag{2.23}$$

However, if $m \geq 5$, then from Theorem 2.2.6, we get

$$2\sqrt[2]{2} \leq E(D) \leq E(H), \tag{2.24}$$

where H is a digraph having linear subdigraphs of equal length r, $r \geq m$. It is clear from (2.23) and (2.24) that $E(D)$ is minimal when $m = 4$. Furthermore, $\mathcal{D}_n$ contains a digraph with maximum length of each linear subdigraph $n-1$. Therefore, from (2.24) it is evident that $E(D)$ is maximal when $m = n - 1$. □

2.3 Comparison of extremal energies

Let $\mathcal{B}_n$ $(n \geq 4)$ be a set consisting of n-vertex bicyclic digraphs such that directed cycles in a digraph are vertex-disjoint. Khan et al. in [2], studied the problem of finding minimal and maximal energy among the digraphs in $\mathcal{B}_n$. For a digraph $G \in \mathcal{B}_n$ with vertex-disjoint directed cycles C_{n-2} and C_2, the following theorem gives a lower bound on the energy of G.

Theorem 2.3.1 ([2]). *Let $n \geq 4$ and $G \in \mathcal{B}_n$ with vertex-disjoint directed cycles C_{n-2} and C_2. Then we have the following inequalities:*

$$E(G) = E(C_{n-2}) + E(C_2) \geq \begin{cases} \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{3(n-2)^2} + 2 & \text{if } n \equiv 0(\text{mod}4) \\ \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi}{n-2} + 2 & \text{if } n \equiv 2(\text{mod}4) \\ \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{12(n-2)^2} + 2 & \text{if } n \equiv 1(\text{mod}2). \end{cases}$$

Theorem 2.3.2 ([2]). *Let $G \in \mathcal{D}_n$ with directed cycles C_{r_1} and C_{r_2}, where $2 \leq r_1, r_2 \leq n-2$. Then G has minimal energy if $2 \leq r_1, r_2 \leq 4$ and maximal energy if $r_1 = n-2$ and $r_2 = 2$ or the vice versa.*

In the following theorem, we compare the maximal energy among the digraph in $\mathcal{B}_n$ and $\mathcal{D}_n$.

Theorem 2.3.3. *Let $n \geq 6$. Then the maximal energy among the digraphs in $\mathcal{B}_n$ is always greater than the maximal energy among the digraphs in $\mathcal{D}_n$.*

Proof. Let $G \in \mathcal{B}_n$ with vertex-disjoint directed cycles C_{n-2} and C_2. Also take $D \in \mathcal{D}_n$ with linear subdigraphs of equal length $n-1$.

Let $n \equiv 0(\text{mod}4)$. In this case we have $n - 2 \geq 6$ and from Theorem 2.3.1 we have

$$\begin{aligned} E(G) = E(C_{n-2}) + E(C_2) &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{3(n-2)^2} + 2 \\ &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{108} + 2. \end{aligned} \tag{2.25}$$

On the other hand, from Theorem 2.2.3 we have

$$E(D) \leq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{2(n-1)\pi}{24(n-1)^2 - \pi^2}\right). \tag{2.26}$$

By using Theorem 2.1.3 we have

$$\sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{2(n-1)\pi}{24(n-1)^2 - \pi^2}\right) \leq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{14\pi}{24(7)^2 - \pi^2}\right). \tag{2.27}$$

One can easily see that the following inequality holds:

$$\frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{108} + 2 \geq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{14\pi}{24(7)^2 - \pi^2}\right). \tag{2.28}$$

Inequalities (2.25) – (2.28) imply

$$E(G) \geq E(D).$$

Next, let $n \equiv 2(\text{mod}4)$. In this case we have $n - 2 \geq 4$ and from Theorem 2.3.1 we have

$$\begin{aligned} E(G) = E(C_{n-2}) + E(C_2) &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi}{n-2} + 2 \\ &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi}{4} + 2. \end{aligned} \tag{2.29}$$

On the other hand, we have from Theorem 2.2.3 that

$$E(D) \leq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{2(n-1)\pi}{24(n-1)^2 - \pi^2}\right). \tag{2.30}$$

By using Theorem 2.1.3 we have

$$\sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{2(n-1)\pi}{24(n-1)^2 - \pi^2}\right) \leq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{14\pi}{24(7)^2 - \pi^2}\right).$$

The following inequality holds true:

$$\frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi}{4} + 2 \geq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{2}{\pi} + \frac{14\pi}{24(7)^2 - \pi^2}\right).$$

Inequalities (2.29) – (2.30) imply

$$E(G) \geq E(D).$$

Finally, let $n \equiv 1(\text{mod}2)$. In this case we have $n-2 \geq 5$ and from Theorem 2.3.1 we have

$$\begin{aligned} E(G) = E(C_{n-2}) + E(C_2) &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{12(n-2)^2} + 2 \\ &\geq \frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{12(5)^2} + 2. \end{aligned} \tag{2.31}$$

On the other hand, we have from Theorem 2.2.3 that

$$E(D) \leq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{4}{\pi}\right). \tag{2.32}$$

The following inequality is easily seen:

$$\frac{2n}{\pi} - \frac{4}{\pi} - \frac{\pi^2}{12(5)^2} + 2 \geq \sqrt[n-1]{2}\left(\frac{2n}{\pi} - \frac{4}{\pi}\right).$$

From inequalities (2.31) − (2.32), we get

$$E(G) \geq E(D).$$

Thus, from Theorem 2.2.8 and Theorem 2.3.3, the assertion is true. □

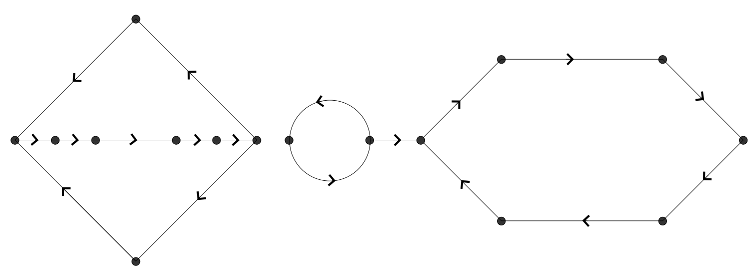

Figure 2.5: Digraphs D_8 (on left) and B_8 (on right).

Example 2.3.4. Let $D \in \mathcal{D}_8$ and $G \in \mathcal{B}_8$ be two digraphs, as shown in Figure 2.5. Then

$$\begin{aligned} E(G) &= E(C_6) + E(C_2) \\ &= 2\csc\frac{\pi}{6} + 2 \\ &= 6. \end{aligned} \tag{2.33}$$

Also $E(D)$ of is given by

$$E(D) = \sqrt[7]{2}\csc\frac{\pi}{14} \tag{2.34}$$
$$= 4.9617$$

Equations (2.34) and (2.34) imply that

$$E(D) < E(G).$$

2.4 Energy of a digraph with k linear subdigraphs

In this section, we extend the idea of energy of bicyclic digraphs to digraphs with $k \geq 2$ linear subdigraphs. We also find the minimal and maximal energy of these digraphs.

For $n \geq 3$, we define a set $\mathcal{K}_n$ which consists of n-vertex digraphs with exactly $k \geq 2$ linear subdigraphs of equal length. Let $G \in \mathcal{K}_n$ be a digraph such that the length of each linear subdigraphs is m, $2 \leq m \leq n+1-k$. From Theorem 2.1.1, the characteristic polynomial of G is given by

$$\Phi_G(x) = x^{n-m}(x^m - k).$$

The eigenvalues of G are 0 and $\sqrt[m]{k}\exp\frac{2j\pi i}{m}$, where $j = 0, 1, \ldots, m-1$ and the multiplicity of eigenvalue 0 is $n-m$. Thus the energy of G is given by

$$E(G) = \sqrt[m]{k}\sum_{j=0}^{m-1}\left|\cos\frac{2\pi j}{m}\right|. \tag{2.35}$$

Example 2.4.1. Consider the digraph $G \in \mathcal{K}_{12}$ and $k = 4$ shown in Figure 2.6. Using Theorem 2.1.1, the characteristic polynomial of G is given by

$$\Phi_G(x) = x^3\big(x^9 - 4\big).$$

The eigenvalues of G are 0 and $\sqrt[9]{4}\exp\frac{2j\pi i}{9}$, where $j = 0, 1, \ldots, 8$ and the multiplicity of eugenvalue 0 is 3. Thus, the energy of G is

$$\begin{aligned} E(G) &= \sqrt[9]{4}\sum_{j=0}^{8}\left|\cos\frac{2\pi j}{9}\right| \\ &= 6.7172. \end{aligned}$$

From (2.35), we compute the energy formulae of G as follows:

$$E(G) = \begin{cases} 2\sqrt[m]{k}\cot\frac{\pi}{m} & \text{if } m \equiv 0(\text{mod}4) \\ 2\sqrt[m]{k}\csc\frac{\pi}{m} & \text{if } m \equiv 2(\text{mod}4) \\ \sqrt[m]{k}\csc\frac{\pi}{2m} & \text{if } m \equiv 1(\text{mod}2). \end{cases} \tag{2.36}$$

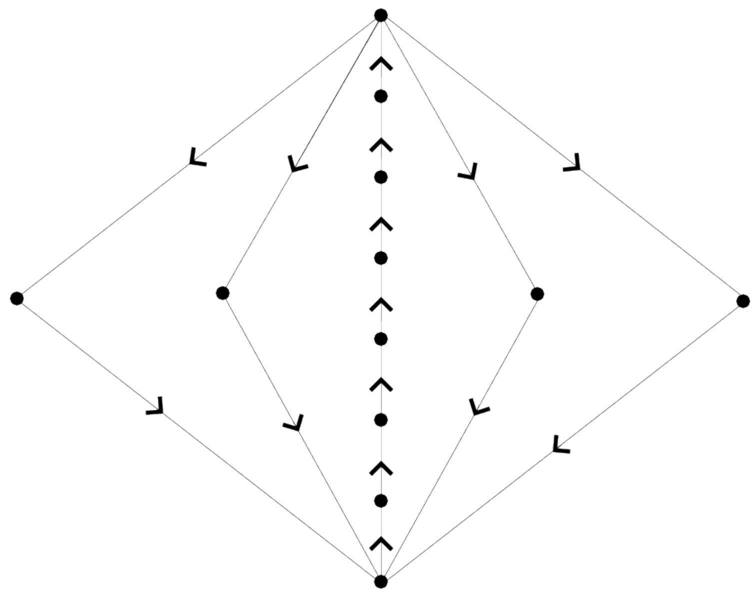

Figure 2.6: Digraph $G \in \mathcal{K}_{12}$.

2.5 Extremal energy of digraphs in $\mathcal{K}_n$

In this section, we find the digraphs with minimal and maximal energy among the digraphs in $\mathcal{K}_n$. The following theorem gives lower bound for the energy of a digraph in $\mathcal{K}_n$.

Theorem 2.5.1. *Let $G \in \mathcal{K}_n$ such that the length of each linear subdigraph is m, where $2 \leq m \leq n+1-k$. Then*

$$E(G) \geq \begin{cases} \sqrt[m]{k}\left(\frac{2m}{\pi} - \frac{\pi}{m}\right) & \text{if } m \equiv 0(\text{mod}4) \\ \sqrt[m]{k}\left(\frac{2m}{\pi}\right) & \text{otherwise.} \end{cases}$$

Proof. Let $m \equiv 0(\text{mod}4)$. Then by (2.4) and (2.36), we get

$$\begin{aligned} E(G) &= 2\sqrt[m]{k}\left(\cot\frac{\pi}{m}\right) \\ &\geq 2\sqrt[m]{k}\left(\frac{m}{\pi} - \frac{\pi}{2m}\right) \\ &= \sqrt[m]{k}\left(\frac{2m}{\pi} - \frac{\pi}{m}\right). \end{aligned}$$

Next, if $m \equiv 2(\text{mod}4)$ then (2.3) and (2.36) yield

$$\begin{aligned} E(G) &= 2\sqrt[m]{k}\left(\csc\frac{\pi}{m}\right) \\ &= 2\sqrt[m]{k}\left(\frac{1}{\sin\frac{\pi}{m}}\right) \\ &\geq \sqrt[m]{k}\left(\frac{2m}{\pi}\right). \end{aligned}$$

Analogously, if $m \equiv 1(\text{mod}2)$ then we can show that

$$E(G) \geq \sqrt[m]{k}\left(\frac{2m}{\pi}\right).$$

The proof is complete. □

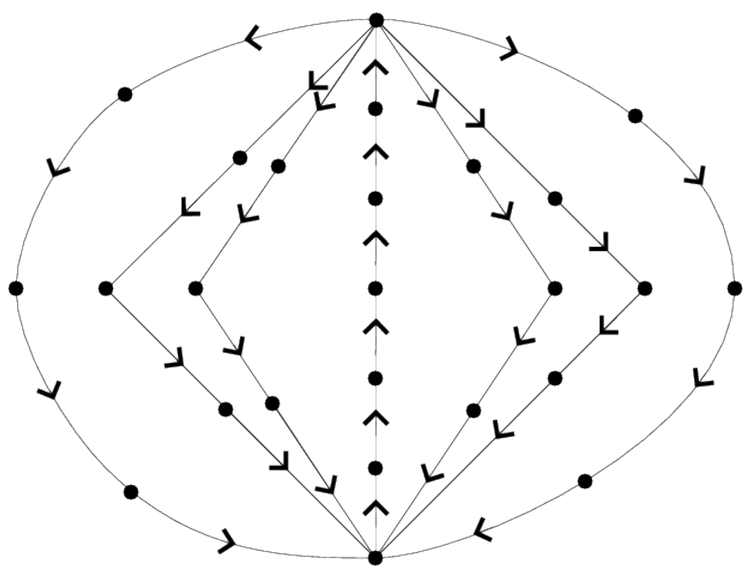

Figure 2.7: Digraph $G \in \mathcal{K}_{25}$.

Example 2.5.2. Let $G \in \mathcal{K}_{25}$ be a digraph having six linear subdigraphs of equal length 10, as shown in Figure 2.7. Then

$$\begin{aligned} E(G) &= 2\sqrt[10]{6}\csc\frac{\pi}{10} \\ &= 7.7422. \end{aligned} \tag{2.37}$$

Also

$$\sqrt[m]{k}\left(\frac{2m}{\pi}\right) = \sqrt[10]{6}\left(\frac{20}{\pi}\right) = 7.6154. \tag{2.38}$$

Equations (2.37) and (2.38) give,

$$E(G) \geq \sqrt[m]{k}\frac{2\pi}{m},$$

which is lower bound of $E(G)$.

The following theorem gives the upper bound for the energy of a digraph $G \in \mathcal{K}_n$.

Theorem 2.5.3. *Let $G \in \mathcal{K}_n$ such that the length of each linear subdigraph is m where $2 \leq m \leq n+1-k$. Then*

$$E(G) \leq \begin{cases} \sqrt[m]{k}(\frac{2m}{\pi}) & \text{if } m \equiv 0(\text{mod}4) \\ \sqrt[m]{k}(\frac{2m}{\pi} + \frac{2m\pi}{6m^2-\pi^2}) & \text{if } m \equiv 2(\text{mod}4) \\ \sqrt[m]{k}(\frac{2m}{\pi} + \frac{2m\pi}{24m^2-\pi^2}) & \text{if } m \equiv 1(\text{mod}2). \end{cases}$$

Proof. First, let $m \equiv 0(\text{mod}4)$. By (2.4) and (2.36), we get

$$\begin{aligned} E(G) &= 2\sqrt[m]{k}\cot\frac{\pi}{m} \\ &\leq 2\sqrt[m]{k}(\frac{m}{\pi}) \\ &= \sqrt[m]{k}(\frac{2m}{\pi}). \end{aligned}$$

Next, we take $m \equiv 2(\text{mod}4)$. By (2.3) and (2.36), we get

$$\begin{aligned} E(G) &= 2\sqrt[m]{k}\csc\frac{\pi}{m} \\ &\leq 2\sqrt[m]{k}\left(\frac{1}{\frac{\pi}{m}(1-\frac{\pi^2}{6m^2})}\right) \\ &= 2\sqrt[m]{k}\left(\frac{m}{\pi}(\frac{6m^2}{6m^2-\pi^2})\right) \\ &= 2\sqrt[m]{k}\left(\frac{m}{\pi}(1+\frac{\pi^2}{6m^2-\pi^2})\right) \\ &= \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{6m^2-\pi^2}\right). \end{aligned}$$

Finally, if $m \equiv 1(\text{mod}2)$ then one can analogously show that

$$E(G) \leq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}\right).$$

This completes the proof. □

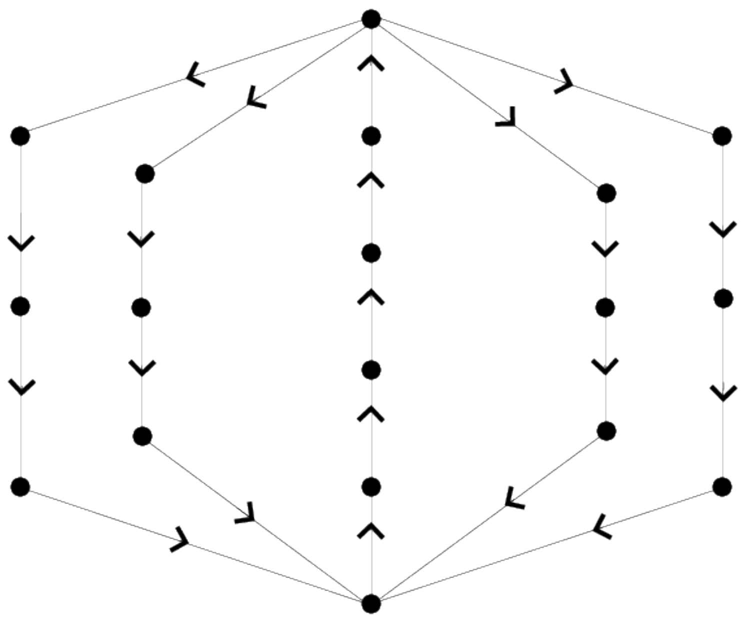

Figure 2.8: Digraph $G \in \mathcal{K}_{18}$.

Example 2.5.4. Let $G \in \mathcal{K}_{18}$ be a digraph having four linear subdigraphs of equal length 9 as shown in Figure 2.8.
First we calculate energy by using $E(G) = \sqrt[9]{4}\csc\frac{\pi}{18}$, here $k = 4$ and $m = 9$. This gives

$$\begin{aligned} E(G) &= \sqrt[9]{4}\csc\frac{\pi}{18} \\ &= 6.7173. \end{aligned} \tag{2.39}$$

Also

$$\sqrt[9]{4}\left(\frac{18}{\pi} + \frac{18\pi}{24(9)^2 - \pi^2}\right) = 6.9213. \tag{2.40}$$

From equations (2.39) and (2.40), we get

$$E(G) \leq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}\right),$$

which is a upper bond of $E(G)$.

Next theorem shows that the energy of digraphs in $\mathcal{K}_n$ increases monotonically with the increase in length of their linear subdigraphs.

Theorem 2.5.5. *Let $n \geq 6$ and $5 \leq m \leq n+1-k$. Take $G \in \mathcal{K}_n$ with length of each linear subdigraph $m+1$ and $H \in \mathcal{K}_n$ with length of each linear subdigraph m. Then*

$$E(G) \geq E(H).$$

Proof. Let $m \equiv 0(\mathrm{mod}4)$. In this case, $m \geq 8$ and $m+1 \equiv 1(\mathrm{mod}2)$. Theorem 2.5.1 implies

$$E(G) \geq \sqrt[m+1]{2}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right). \tag{2.41}$$

On the other hand, Theorem 2.5.3 gives

$$E(H) \leq \sqrt[m]{2}\left(\frac{2m}{\pi}\right). \tag{2.42}$$

One can easily see that the following inequality holds:

$$\sqrt[m+1]{2}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right) \geq \sqrt[m]{2}\left(\frac{2m}{\pi}\right). \tag{2.43}$$

Combining $(2.41) - (2.43)$, we get

$$E(G) \geq E(H).$$

Next, let $m \equiv 2(\mathrm{mod}4)$. In this case $m \geq 6$ and $m+1 \equiv 1(\mathrm{mod}2)$. Theorem 2.5.1 implies that

$$E(G) \geq \sqrt[m+1]{k}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right). \tag{2.44}$$

On the other hand, Theorem 2.5.3 gives

$$E(H) \leq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{6m^2 - \pi^2}\right). \tag{2.45}$$

Furthermore, Theorem 2.1.3 implies that

$$\sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{6m^2 - \pi^2}\right) \leq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{12\pi}{6^3 - \pi^2}\right). \tag{2.46}$$

One can easily see that the following inequality holds:

$$\sqrt[m+1]{k}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right) \geq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{12\pi}{6^3 - \pi^2}\right). \tag{2.47}$$

Combining (2.44) − (2.47), we get

$$E(G) \geq E(H).$$

Finally, let $m \equiv 1(\text{mod}2)$. In this case $m \geq 7$, $m+1 \equiv 2(\text{mod}4)$ or $m+1 \equiv 0(\text{mod}4)$. If $m+1 \equiv 2(\text{mod}4)$ then Theorem 2.5.1 implies

$$E(G) \geq \sqrt[m+1]{k}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right). \tag{2.48}$$

On the other hand, Theorem 2.5.3 gives

$$E(H) \leq \sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}\right). \tag{2.49}$$

Theorem 2.1.3 implies that

$$\sqrt[m]{k}\left(\frac{2m}{\pi} + \frac{2m\pi}{24m^2 - \pi^2}\right) \leq \sqrt[m]{2}\left(\frac{2m}{\pi} + \frac{14\pi}{24.7^2 - \pi^2}\right). \tag{2.50}$$

The following inequality is easily seen:

$$\sqrt[m+1]{k}\left(\frac{2m}{\pi} + \frac{2}{\pi}\right) \geq \sqrt[m]{2}\left(\frac{2m}{\pi} + \frac{14\pi}{24.7^2 - \pi^2}\right). \tag{2.51}$$

Combining (2.48) − (2.51), we get

$$E(G) \geq E(H).$$

If $m+1 \equiv 0(\text{mod}4)$, then one can analogously show that

$$E(G) \geq E(H).$$

This completes the proof. □

The following result is an easy consequence of Theorem 2.5.5.

Theorem 2.5.6. *Let $n \geq 6$ and $2 \leq m_2 \leq m_1 \leq n-1$. Take $G \in \mathcal{K}_n$ with length of each linear subdigraph m_1 and $H \in \mathcal{K}_n$ with length of each linear subdigraph m_2. Then*

$$E(G) \geq E(H).$$

Example 2.5.7. Let $G, H \in \mathcal{K}_{16}$ be two digraphs having four linear subdigrphs of equal lengths 7 and 12 respectively as shown in Figures 2.9 and 2.10.

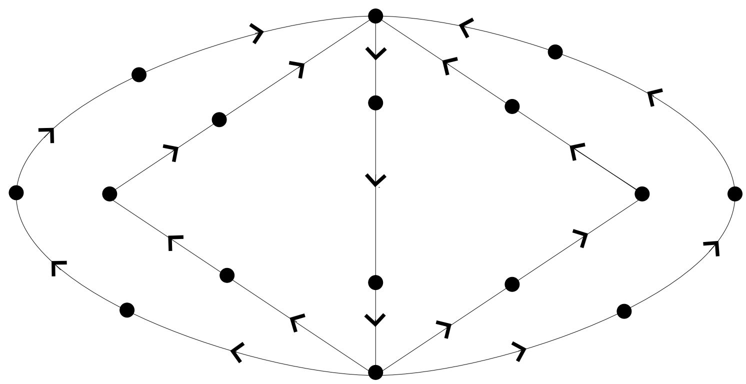

Figure 2.9: Digraph $G \in \mathcal{K}_{16}$.

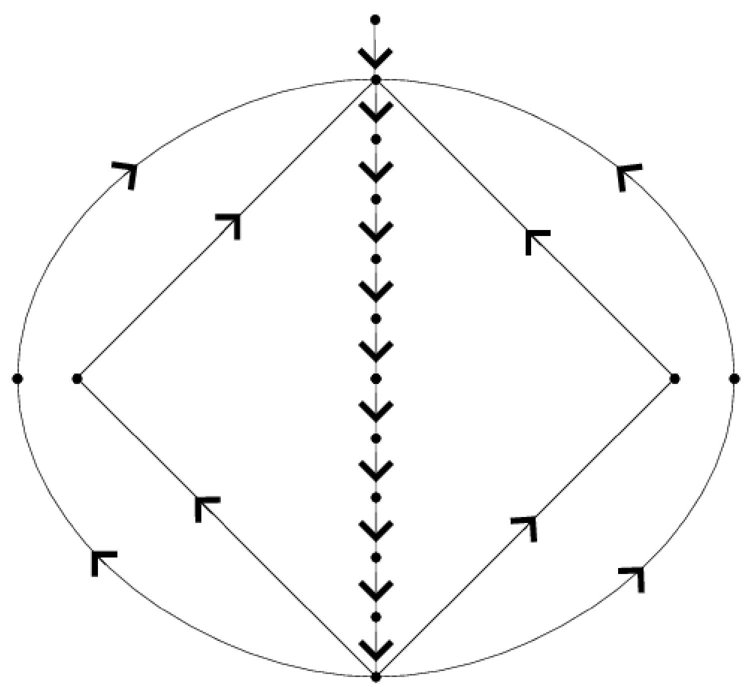

Figure 2.10: Digraph $H \in \mathcal{K}_{16}$.

Firstly, we will find energy of G:

$$\begin{aligned} E(G) &= \sqrt[7]{4}\csc\frac{\pi}{14} \\ &= 5.4782. \end{aligned} \tag{2.52}$$

Secondly, we find energy of H:

$$E(H) = 2\sqrt[12]{4}\cot\frac{\pi}{12} \\ = 7.9079. \tag{2.53}$$

It is clear from equations (2.52) and (2.53) that,

$$E(H) \geq E(G).$$

Using Theorem 2.5.6, we finally prove the main result of this section.

Theorem 2.5.8. *Let $n \geq 6$ and $G \in \mathcal{K}_n$ be a digraph with length of each linear subdigraph m, where $2 \leq m \leq n+1-k$. Then G has minimal energy when $m = 4$ and maximal energy when $m = n+1-k$ among all digraphs of $\mathcal{K}_n$.*

Proof. Let $G \in \mathcal{K}_n$ be a digraph with linear subdigraphs of equal length m where $2 \leq m \leq n+1-k$. Then it can easily be seen from (2.36) that

$$E(G) = \begin{cases} 2\sqrt[2]{k} & \text{if } m = 2 \\ 2\sqrt[3]{k} & \text{if } m = 3 \\ 2\sqrt[4]{k} & \text{if } m = 4. \end{cases} \tag{2.54}$$

However, if $m \geq 5$, then from Theorem 2.5.6, we get

$$2\sqrt[2]{k} \leq E(G) \leq E(H), \tag{2.55}$$

where $H \in \mathcal{K}_n$ is a digraph with linear subdigraphs of equal length r, $r \geq m$. It is clear from (2.54) and (2.55) that $E(G)$ is minimal when $m = 4$. Moreover, $\mathcal{K}_n$ contains a digraph with maximum length of each linear subdigraph $n+1-k$. Therefore, from (2.55) it is obvious that $E(G)$ is maximal when $m = n+1-k$. ☐

2.6 Conclusion

In this chapter, we firstly introduced a new class $\mathcal{D}_n$ of digraph having two linear subdigraphs of equal length. We found the digraphs in $\mathcal{D}_n$ which has extremal energy. We prove that a digraph in $\mathcal{D}_n$ has minimal energy if the length of each linear digraph is 4 and it has maximal energy if the length of each linear subdigraph is $n-1$.

Moreover, we extend this concept by introducing a class $\mathcal{K}_n$ which contains all those n-vertex digraphs which contains exactly k linear subdigraphs of equal length, where $k \geq 2$. We proved that a digraph $G \in \mathcal{K}_n$ has minimal energy if length of each linear subdigraph is 4 and it has maximal energy if length of each linear subdigraph is $n-1+k$.

Open problem: It will be interesting to consider a class of n-vertex digraphs having linear subdigraphs whose lengths are not necessarily equal. Find the minimal and maximal energy of digraphs among this class will be worthwhile.

Chapter 3

Energy of a Tricyclic Digraph and Sidigraph

Khan et al. in [2], studied the extremal energy of bicyclic digraphs with vertex-disjoint directed cycles. In Khan and Farooq [On the energy of bicyclic signed digraphs, Submitted] the authors studied the problem of finding extremal energy of bicyclic signed digraphs. In this chapter, we consider a class of tricyclic digraphs with exactly five linear subdigraphs and find minimal and maximal energy of these digraphs. Later on, in this chapter we consider a class of tricyclic signed digraphs with exactly five linear signed subdigraphs and calculate the extremal energy of tricyclic signed digraphs.

3.1 Preliminaries

For $n \geq 5$, we define a set $\mathcal{D}_n$ which consists of n-vertex tricyclic digraphs, each cycle of equal length, and having exactly five linear subdigraphs. Then it is clear form the definition of $\mathcal{D}_n$ that a digraph $D \in \mathcal{D}_n$ has exactly two cycles which shares atleast one vertex. Obviously one cycle of D is vertex disjoint from the other two cycles. Let $D \in \mathcal{D}_n$ be a digraph such that the length of each cycle is m, $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$. For fixed n, we can draw tricyclic digraph in which length of each cycle cannot exceeds $\lfloor \frac{n}{2} \rfloor$. From Theorem 2.1.1, the characteristic polynomial of D is given by

$$\Phi_D(x) = x^{n-2m}(x^m - 2)(x^m - 1). \tag{3.1}$$

The eigenvalues of D are 0, $\sqrt[m]{2} \exp \frac{2k\pi i}{m}$ and $\exp \frac{2k\pi i}{m}$, where $k = 0, 1, \ldots, m-1$ and the multiplicity of eigenvalue 0 is $n - 2m$. Thus the energy of D is given by

$$E(D) = (1 + \sqrt[m]{2}) \sum_{k=0}^{m-1} \left| \cos \frac{2k\pi}{m} \right|. \tag{3.2}$$

Moreover, if m is odd we can write (3.2) as follows:

$$E(D) = (1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m} - 2\sum_{j=\lfloor \frac{m}{4} \rfloor+1}^{\lfloor \frac{m}{2} \rfloor} \cos\frac{2\pi j}{m}\big). \tag{3.3}$$

If m is even then (3.2) can be written as:

$$E(D) = (1 + \sqrt[m]{2})\big(2\sum_{j=0}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m} - 2\sum_{j=\lfloor \frac{m}{4} \rfloor+1}^{\lfloor \frac{m}{2} \rfloor} \cos\frac{2\pi j}{m}\big). \tag{3.4}$$

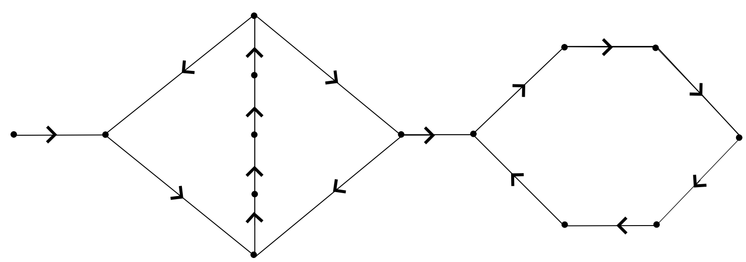

Figure 3.1: A digraph $D \in \mathcal{D}_{14}$.

Example 3.1.1. Consider a digraph $D \in \mathcal{D}_{14}$ shown in Fig. 3.1, where the length of each cycle is 6. Using equation (3.1), the characteristic polynomial of D is given by

$$\Phi_D(x) = x^2\big(x^6 - 2\big)\big(x^6 - 1\big).$$

The eigenvalues of D are 0, $\sqrt[6]{2}\exp\frac{2k\pi i}{6}$ and $\exp\frac{2k\pi i}{6}$, $k = 0, 1, \ldots, 5$ and the multiplicity of 0 is 2. Thus, the energy of D is

$$\begin{aligned} E(D) &= (1 + \sqrt[6]{2})\sum_{k=0}^{5} \big|\cos\frac{2k\pi}{6}\big| \\ &= 8.4898. \end{aligned}$$

3.2 Extremal energy of tricyclic digraphs

Pena and Rada [1] considered the problem of finding extremal energy among all unicyclic digraphs with fixed number of vertices. Khan et al. [2] considered the same problem for finding extremal energy for bicyclic digraphs with vertex-disjoint directed cycles. In this section, we find the minimal and maximal energy among the digraphs in $\mathcal{D}_n$. The following lemma gives us the lower bound for the energy of a digraph $D \in \mathcal{D}_n$.

Lemma 3.2.1. *Let $D \in \mathcal{D}_n$ be a digraph with each directed cycle of length m and $H \in \mathcal{D}_n$ be a digraph with each directed cycle of length l, where $5 \leq m \leq l \leq \lfloor \frac{n}{2} \rfloor$. Then*

$$E(D) \leq E(H).$$

Proof. Consider $D \in D_n$ be a digraph with each directed cycles of length m and $H \in \mathcal{D}_n$ be a digraph with each directed cycle of length $m+1$. Then

$$\frac{2\pi j}{m+1} < \frac{2\pi j}{m},$$

where $\frac{2\pi j}{m+1}, \frac{2\pi j}{m} \in \left(0, \frac{\pi}{2}\right)$ for each $j = 1, \ldots, \lfloor \frac{m}{4} \rfloor$. Thus

$$\cos \frac{2\pi j}{m} < \cos \frac{2\pi j}{m+1}. \tag{3.5}$$

If m is odd, then

$$1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos \frac{2\pi j}{m} = -2 \sum_{j=\lfloor \frac{m}{4} \rfloor + 1}^{\lfloor \frac{m}{2} \rfloor} \cos \frac{2\pi j}{m}. \tag{3.6}$$

If m is even, then

$$1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos \frac{2\pi j}{m} = -1 - 2 \sum_{j=\lfloor \frac{m}{4} \rfloor + 1}^{\frac{m}{2}} \cos \frac{2\pi j}{m}. \tag{3.7}$$

Suppose that m is odd. Then from equation (3.3),

$$E(D) = (1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos \frac{2\pi j}{m} - 2 \sum_{j=\lfloor \frac{m}{4} \rfloor + 1}^{\lfloor \frac{m}{2} \rfloor} \cos \frac{2\pi j}{m}\big).$$

Using equation (3.6) in above equation, we get

$$E(D) = 2(1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos \frac{2\pi j}{m}\big). \tag{3.8}$$

Since $m+1$ is even, therefore from equation (3.4),

$$\begin{aligned} E(H) &= (1 + \sqrt[m+1]{2})\big(2 \sum_{j=0}^{\lfloor \frac{m+1}{4} \rfloor} \cos \frac{2\pi j}{m+1} - 2 \sum_{j=\lfloor \frac{m+1}{4} \rfloor + 1}^{\frac{m+1}{2}} \cos \frac{2\pi j}{m+1}\big) \\ &= (1 + \sqrt[m+1]{2})\big(1 + 2 \sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos \frac{2\pi j}{m+1} - 1 - 2 \sum_{j=\lfloor \frac{m+1}{4} \rfloor + 1}^{\frac{m+1}{2}} \cos \frac{2\pi j}{m+1}\big). \end{aligned}$$

Using equation (3.7) in above equation, we obtain

$$E(H) = 2(1 + \sqrt[m+1]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos\frac{2\pi j}{m+1}\big). \tag{3.9}$$

Using (3.5), one can easily see that

$$2(1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m}\big) \le 2(1 + \sqrt[m+1]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos\frac{2\pi j}{m+1}\big).$$

Therefore from (3.8) and (3.9), we get

$$E(D) \le E(H). \tag{3.10}$$

Now suppose that m is even, so from equation (3.4),

$$\begin{aligned} E(D) &= (1 + \sqrt[m]{2})\big(2\sum_{j=0}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m} - 2\sum_{j=\lfloor \frac{m}{4} \rfloor + 1}^{\lfloor \frac{m}{2} \rfloor} \cos\frac{2\pi j}{m}\big) \\ &= (1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m} - 1 - 2\sum_{j=\lfloor \frac{m}{4} \rfloor + 1}^{\lfloor \frac{m}{2} \rfloor} \cos\frac{2\pi j}{m}\big). \end{aligned}$$

Equation (3.7) and above equation imply

$$E(D) = 2(1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m}\big). \tag{3.11}$$

Since $m+1$ is odd, so from equation (3.3)

$$E(D) = (1 + \sqrt[m+1]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos\frac{2\pi j}{m+1} - 2\sum_{j=\lfloor \frac{m+1}{4} \rfloor + 1}^{\lfloor \frac{m+1}{2} \rfloor} \cos\frac{2\pi j}{m+1}\big).$$

From above equation and (3.6) we get,

$$E(D) = 2(1 + \sqrt[m+1]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos\frac{2\pi j}{m+1}\big). \tag{3.12}$$

Following inequality holds from (3.5),

$$2(1 + \sqrt[m]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m}{4} \rfloor} \cos\frac{2\pi j}{m}\big) \le 2(1 + \sqrt[m+1]{2})\big(1 + 2\sum_{j=1}^{\lfloor \frac{m+1}{4} \rfloor} \cos\frac{2\pi j}{m+1}\big).$$

Using equations (3.11) and (3.12) in above inequality, we get

$$E(D) \leq E(H). \tag{3.13}$$

From (3.10) and (3.13), we conclude that the energy of digraphs $D \in \mathcal{D}_n$ increases with respect to length of cycle when this length is greater than 4. □

Theorem 3.2.1. *Let $D \in \mathcal{D}_n$ such that the length of each cycle is m, where $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$. Then D has minimal energy if length of each cycle is 4 and maximal energy if length of each cycle is $\lfloor \frac{n}{2} \rfloor$.*

Proof. Consider $D \in \mathcal{D}_n$ be a digraph such that the length of each cycle is m, where $2 \leq m \leq n-3$. Then

$$E(D) = (1 + \sqrt[m]{2}) \sum_{j=0}^{m-1} \big| \cos \frac{2\pi j}{m} \big|.$$

One can easily see that

$$(1 + \sqrt[4]{2}) \sum_{j=0}^{3} \big| \cos \frac{2\pi j}{4} \big| < (1 + \sqrt[3]{2}) \sum_{j=0}^{2} \big| \cos \frac{2\pi j}{3} \big| < (1 + \sqrt{2}) \sum_{j=0}^{1} \big| \cos \pi j \big|. \tag{3.14}$$

Let $m \geq 5$. We show that

$$E(D) > (1 + \sqrt{2}) \sum_{j=0}^{1} \big| \cos \pi j \big|.$$

As $m \geq 5$, it is readily seen that

$$1 + \cos \frac{2\pi}{m} < \sum_{j=2}^{m-1} \big| \cos \frac{2\pi j}{m} \big|. \tag{3.15}$$

Equation (3.2) together with inequalities (3.14) and (3.15) implies

$$\begin{aligned} E(D) &= (1 + \sqrt[m]{2})\big(1 + \cos \frac{2\pi}{m}\big) + (1 + \sqrt[m]{2}) \sum_{j=2}^{m-1} \big| \cos \frac{2\pi j}{m} \big| \\ &> 2(1 + \sqrt[m]{2})\big(1 + \cos \frac{2\pi}{m}\big) \\ &> (1 + \sqrt{2}) \sum_{j=0}^{1} \big| \cos \pi j \big|. \end{aligned}$$

This shows that D has minimal energy if $m = 4$.
From Lemma 3.2.1 energy of digraph $D \in \mathcal{D}_n$ increases with increase in length of cycle and the maximum length of each cycle in $D \in \mathcal{D}_n$ can be $\lfloor \frac{n}{2} \rfloor$. Hence D has maximal energy if length of each cycle is $\lfloor \frac{n}{2} \rfloor$. □

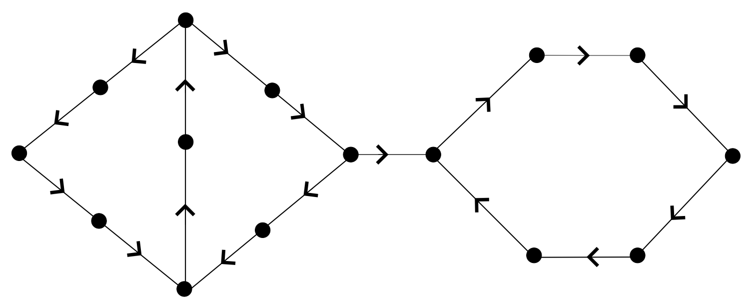

Figure 3.2: $D \in \mathcal{D}_{15}$

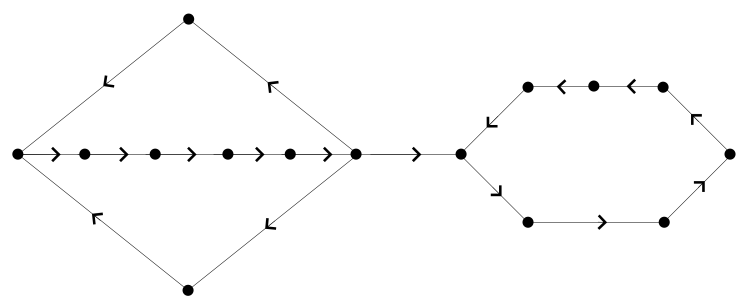

Figure 3.3: $H \in \mathcal{D}_{15}$

Example 3.2.2. Let $D \in \mathcal{D}_{15}$ be digraphs each cycle of length 6 and $H \in \mathcal{D}_{15}$ with length of each cycle 7, as shown in Figures 3.2 and 3.3. Then from equation (3.2), energy of D is:

$$E(D) = (1 + \sqrt[6]{2}) \sum_{j=1}^{5} |\cos \frac{2\pi j}{6}| = 8.4898.$$

The energy of $H \in \mathcal{D}_{15}$, can be calculated similarly and it is $E(H) = 9.4557$, which shows that energy of H is exceeds the energy of D.

3.3 Energy of tricyclic sidigraphs

In this section, we extend the concept of energy to signed digraphs. A signed digraph (or briefly sidigraph) is defined to be a pair $S = (D, \sigma)$, where $D = (\mathcal{V}, \mathcal{A})$ is the underlying digraph and $\sigma : A \to \{-1, 1\}$ is the signing function and $A = A^+ \cup A^-$. Here A^+ and A^- denotes the sets of positive and negative arcs of S respectively.
A sidigraph is homogeneous if all of its arcs have either positive sign or negative sign, otherwise heterogeneous. Two vertices are adjacent if they are connected by a signed arc. A path of length $n-1$ ($n \geq 2$), denoted by P_n, is a sidigraph on n vertices $v_1, v_2, \ldots, v_n$ with $n-1$ signed arcs (v_i, v_{i+1}), $i = 1, 2, \ldots, n-1$. A cycle of length n is a sidigraph having vertices $v_1, v_2, \ldots, v_n$ and signed arcs (v_i, v_{i+1}) where $i = 1, 2, \ldots, n-1$ and (v_n, v_1). A sidigraph is linear if each vertex v has both indegree (number of signed arcs with head v) and outdegree (number of signed arcs with tail v) equal to one.

The sign of a sidigraph is defined as the product of signs of its arcs. A sidigraph is said to be positive (negative) if its sign is positive (negative) that is, it contains an even (odd) number of negative arcs. A sidigraph is said to be all-positive (respectively, all negative) if all its arcs are positive (negative). A signed digraph is said to be cycle balanced if each of its cycle is positive, otherwise non cycle balanced. Here 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 number of vertices.

The adjacency matrix of a sidigraph S whose vertices are $v_1, v_2, \ldots, v_n$ is the square matrix $A_S = [a_{ij}]_{n \times n}$, 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 $|xI - A|$ of the adjacency matrix A of the sidigraph S is called the characteristics polynomial of sidigraph S and is denoted by $\phi_S(x)$. The eigenvalues of $A(S)$ are called the eigenvalues of S. The energy of sidigraph is defined as

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

where $\Re(z_i)$ denotes the real part of eigenvalues $z_1, z_2, \ldots, z_n$. The next theorem is the coefficients theorem for sidigraphs.

Theorem 3.3.1 ([11]). *Let S be a sidigraph of order n and*

$$\Phi_S(x) = x^n + d_1 x^{n-1} + \ldots, + d_{n-1} x + d_n$$

be the characteristic polynomial S. Then

$$d_i = \sum_{L \in L_i} (-1)^{comp(L)} \prod_{Z \in C(L)} s(Z)$$

for all $i = 1, 2, \ldots, n$, L_i is the set of all linear subdigraphs of S with exactly i vertices, comp(L) is the number of components of L (maximal connected subgraph of graph L) and $s(Z)$ is the sign of cycle Z.

For $n \geq 5$, we define a set $\mathcal{S}_n$ which consists of n-vertex tricyclic signed digraphs, each cycle of length r and having exactly 5 linear subdigraphs, where $2 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Let $S \in \mathcal{S}_n$ be a sidigraph such that the length of each cycle is r, $2 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Then it is clear from the definition of $\mathcal{S}_n$ that S has exactly two directed signed cycles which share atleast one vertex. It is obvious that one cycle of S is vertex disjoint from the other two cycles.

Remarks 3.3.2.

Let $S \in \mathcal{S}_n$ be an n-vertex sidigraph.

1. If all three cycles in S are positive, then characteristic polynomial of S is given by

$$\phi_S(x) = x^{n-2m}(x^m - 2)(x^m - 1).$$

The eigenvalues of S are 0, $\sqrt[m]{2} \exp \frac{2\pi j i}{m}$ and $\exp \frac{2\pi j i}{m}$, where $j = 0, 1, \ldots, m-1$. Therefore energy of S is given by

$$E(S) = (1 + \sqrt[r]{2}) \sum_{j=0}^{r-1} \left| \cos \frac{2\pi j}{r} \right|.$$

2. If all the three cycles in S are negative, then the characteristic polynomial of S is given by

$$\phi_S(x) = x^{n-2m}(x^m + 2)(x^m + 1).$$

The eigenvalues of S are 0, $\sqrt[m]{2} \exp \frac{(2j+1)\pi i}{m}$ and $\exp \frac{(2j+1)\pi i}{m}$, where $j = 0, 1, \ldots, m-1$. Hence energy of S is given by

$$E(S) = (1 + \sqrt[r]{2}) \sum_{j=0}^{r-1} \left| \cos \frac{(2j+1)\pi}{r} \right|.$$

3. If vertex-disjoint cycle is positive and other two cycles are negative, then

$$\phi_S(x) = x^{n-2m}(x^m + 2)(x^m - 1).$$

In this case eigenvalues of S are 0, $\sqrt[m]{2}\exp\frac{(2j+1)\pi i}{m}$ and $\exp\frac{2\pi j i}{m}$, where $j = 0, 1, \dots, m-1$. Therefore

$$E(S) = \sqrt[r]{2}\sum_{j=0}^{r-1}\big|\cos\frac{(2j+1)\pi}{r}\big| + \sum_{j=0}^{r-1}\big|\cos\frac{2\pi j}{r}\big|.$$

4. If vertex-disjoint cycle is negative and other two cycles are positive, then characteristic polynomial of S is given by

$$\phi_S(x) = x^{n-2m}(x^m - 2)(x^m + 1).$$

The eigenvalues of S are 0, $\sqrt[m]{2}\exp\frac{2\pi j i}{m}$ and $\exp\frac{(2j+1)\pi i}{m}$. Hence the energy of S is given by

$$E(S) = \sqrt[r]{2}\sum_{j=0}^{r-1}\big|\cos\frac{2\pi j}{r}\big| + \sum_{j=0}^{r-1}\big|\cos\frac{(2j+1)\pi}{r}\big|.$$

5. If one of the cycle other than vertex-disjoint cycle is negative, and the vertex-disjoint cycle is positive then the characteristic polynomial of S is given by

$$\phi_S(x) = x^{n-2m}(x^m - 1 + 1)(x^m - 1).$$

The eigenvalues of S are 0 and $\exp\frac{2\pi j i}{m}$. Therefore energy of S is

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

6. If one of the cycle other than vertex-disjoint cycle is negative, and the vertex-disjoint cycle is negative then the characteristic polynomial of S is given by

$$\phi_S(x) = x^{n-2m}(x^m - 1 + 1)(x^m + 1).$$

The eigenvalues of S are 0 and $\exp\frac{(2j+1)\pi i}{m}$. The energy of S is

$$E(S) = \sum_{j=0}^{r-1}\big|\cos\frac{(2j+1)\pi}{r}\big|.$$

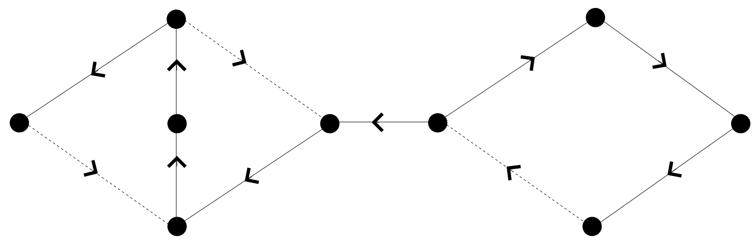

Figure 3.4: The sidigraph $S \in \mathcal{S}_9$.

Example 3.3.3. Consider $S \in \mathcal{S}_9$ be a sidigraph in which each cycle is negative as shown in Figure 3.4. In this chapter we denotes the negative arcs by dotted lines and positive arcs by bold lines. The characteristic polynomial of S is:

$$\phi_S(x) = x(x^4 + 2)(x^4 + 1).$$

The eigenvalues of S are 0, $\sqrt[4]{2}\exp\frac{(2j+1)\pi i}{4}$ and $\exp\frac{(2j+1)\pi i}{4}$, where $j = 0, 1, 2, 3$. Thus energy of S is

$$\begin{aligned} E(S) &= (1+\sqrt[4]{2})\sum_{j=0}^{3}\left|\cos\frac{(2j+1)\pi}{4}\right| \\ &= (1+\sqrt[4]{2})(2\sqrt{2}) \\ &= 6.1920. \end{aligned}$$

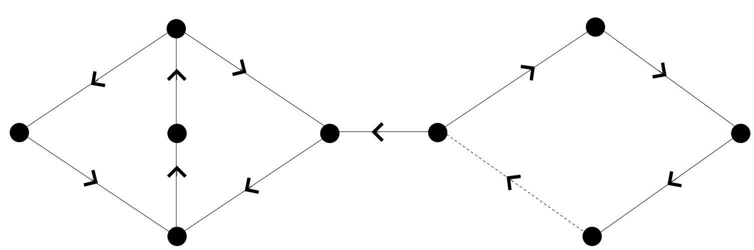

Figure 3.5: The sidigraph $S \in \mathcal{S}_9$.

Example 3.3.4. Let $S \in \mathcal{S}_9$ be a sidigraph in which only vertex-disjoint cycle is negative. Obviously the other two cycles are positive. It is shown in Figure 3.5. The characteristic polynomial of S is:

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

The eigenvalues of S are $0, \sqrt[4]{2}\exp\frac{2\pi ji}{4}$ and $\exp\frac{(2j+1)\pi i}{4}$, where $j = 0, 1, 2, 3$. Thus energy of S is The energy of S is given by

$$\begin{aligned} E(S) &= \sum_{j=0}^{3} \Big| \cos\frac{(2j+1)\pi}{4} \Big| + \sqrt[4]{2}\sum_{j=0}^{3} \Big| \cos\frac{2j\pi}{4} \Big| \\ &= 2(\sqrt{2} + \sqrt[4]{2}) \\ &= 5.2068. \end{aligned}$$

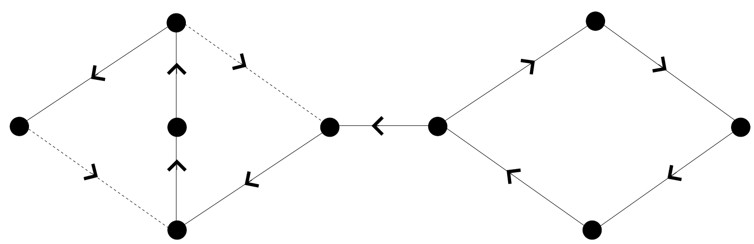

Figure 3.6: The sidigraph $S \in \mathcal{S}_9$.

Example 3.3.5. Let $S \in \mathcal{S}_9$ be a sidigraph in which only vertex-disjoint cycle is positive. The other two cycles are negative. It is shown in Figure 3.6. Then the characteristic polynomial of S is:

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

The eigenvalues of S are 0, $\sqrt[4]{2}\exp\frac{(2j+1)\pi i}{4}$ and $\exp\frac{2\pi ji}{4}$, where $j = 0, 1, 2, 3$. Therefore energy of S is

$$\begin{aligned} E(S) &= \sum_{j=0}^{3} \Big| \cos\frac{2j\pi}{4} \Big| + \sqrt[4]{2}\sum_{j=0}^{3} \Big| \cos\frac{(2j+1)\pi}{4} \Big| \\ &= 2(1 + \sqrt{2}\sqrt[4]{2}) \\ &= 5.3630. \end{aligned}$$

Example 3.3.6. Let $S \in \mathcal{S}_9$ be a sidigraph in which non vertex-disjoint cycles have opposite signs and vertex-disjoint cycle is positive as shown in Figure 3.7. Then its characteristic polynomial is

$$\phi_S(x) = (x^5 + x - x)(x^4 - 1).$$

The eigenvalues of S are 0 and $\exp\frac{2\pi ji}{4}$. Therefore energy of S is given by

$$\begin{aligned} E(S) &= \sum_{j=0}^{3} \Big| \cos\frac{2j\pi}{4} \Big| \\ &= 2 \end{aligned}$$

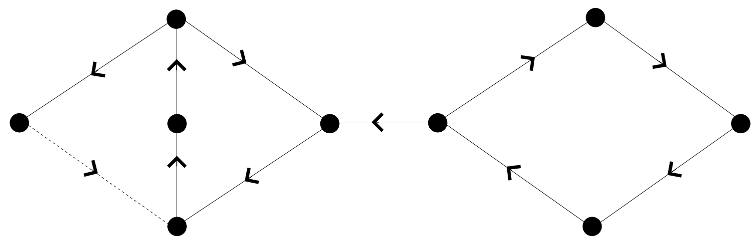

Figure 3.7: The sidigraph $S \in \mathcal{S}_9$.

Lemma 3.3.1. *Let $S \in \mathcal{S}_n$ be a sidigraph with cycles of equal length r and $H \in \mathcal{S}_n$ be a sidigraph with cycles of equal length l such that $5 \leq r \leq l \leq \lfloor \frac{n}{2} \rfloor$. Then*

$$E(S) \leq E(H).$$

Proof. We consider five cases.

1. If each cycle in S is positive, then the result follows from Lemma 3.2.1.

2. If each cycle of S is negative, then

$$E(S) = (1 + \sqrt[r]{2}) \sum_{j=0}^{r-1} \Big| \cos \frac{(2j+1)\pi}{r} \Big|.$$

Let $H \in \mathcal{S}_n$ be a sidigraph having exactly three negative cycles each of length $r+1$, where $r + 1 \leq \lfloor \frac{n}{2} \rfloor$. Thus

$$\frac{(2j+1)\pi}{r+1} < \frac{(2j+1)\pi}{r},$$

where $\frac{(2j+1)\pi}{r+1}, \frac{(2j+1)\pi}{r} \in (0, \frac{\pi}{2})$. Also for $j = 1, 2, \ldots, \lfloor \frac{r}{4} \rfloor$, we have

$$\cos \frac{(2j+1)\pi}{r} < \cos \frac{(2j+1)\pi}{r+1}. \tag{3.16}$$

If r is odd then we know that

$$2 \sum_{+} \cos \frac{(2j+1)\pi}{r} = 1 - 2 \sum_{-} \cos \frac{(2j+1)\pi}{r}. \tag{3.17}$$

Here $\sum_{+}$ and $\sum_{-}$ denotes the sum over all eigenvalues with positive and negative real parts respectively.

If r is even then we can write

$$2 \sum_{+} \cos \frac{(2j+1)\pi}{r} = -2 \sum_{-} \cos \frac{(2j+1)\pi}{r}. \tag{3.18}$$

Suppose that r is odd, then

$$\begin{aligned} E(S) &= (1+\sqrt[r]{2})\sum_{j=0}^{r-1}\Big|\cos\frac{(2j+1)\pi}{r}\Big| \\ &= (1+\sqrt[r]{2})\Bigg(1+2\sum_{+}\cos\frac{(2j+1)\pi}{r}-2\sum_{-}\cos\frac{(2j+1)\pi}{r}\Bigg). \end{aligned}$$

Using equation (3.17) in above expression, we get

$$E(S) = 4(1+\sqrt[r]{2})\sum_{+}\cos\frac{(2j+1)\pi}{r}. \tag{3.19}$$

Since r is odd, so $r+1$ is even, then

$$E(H) = (1+\sqrt[r+1]{2})\Bigg(2\sum_{+}\cos\frac{(2j+1)\pi}{r+1}-2\sum_{-}\cos\frac{(2j+1)\pi}{r+1}\Bigg).$$

Using equation (3.18) in above equation, we get

$$E(H) = 4(1+\sqrt[r+1]{2})\sum_{+}\cos\frac{(2j+1)\pi}{r+1}. \tag{3.20}$$

Using (3.16), one can see that

$$4(1+\sqrt[r]{2})\sum_{+}\cos\frac{(2j+1)\pi}{r} \leq 4(1+\sqrt[r+1]{2})\sum_{+}\cos\frac{(2j+1)\pi}{r+1}. \tag{3.21}$$

Using equations (3.19) and (3.20) in above inequality, we get

$$E(S) \leq E(H). \tag{3.22}$$

If r is even, then we can write.

$$E(S) = (1+\sqrt[r]{2})\Bigg(2\sum_{+}\cos\frac{(2j+1)\pi}{r}-2\sum_{-}\cos\frac{(2j+1)\pi}{r}\Bigg).$$

Equation (3.18) along with above equation gives

$$E(S) = 4(1+\sqrt[r]{2})\sum_{+}\cos\frac{(2j+1)\pi}{r}. \tag{3.23}$$

As r is even, then $r+1$ is odd, therefore

$$E(H) = (1+\sqrt[r+1]{2})\Bigg(1+2\sum_{+}\cos\frac{(2j+1)\pi}{r+1}-2\sum_{-}\cos\frac{(2j+1)\pi}{r+1}\Bigg).$$

Using equation (3.17) in above equation we get

$$E(H) = 4(1 + \sqrt[r+1]{2}) \sum_{+} \cos\frac{(2j+1)\pi}{r+1}. \tag{3.24}$$

Using (3.16), we can write

$$4(1 + \sqrt[r]{2}) \sum_{+} \cos\frac{(2j+1)\pi}{r} \leq 4(1 + \sqrt[r+1]{2}) \sum_{+} \cos\frac{(2j+1)\pi}{r+1}.$$

From equations (3.23), (3.24) and above inequality, we get

$$E(S) \leq E(H). \tag{3.25}$$

From (3.22) and (3.25), we prove that energy of sidigraph S having all negative cycles increases with increase in length of cycle when this length is greater than 4.

3. If only vertex-disjoint cycle in S is positive then

$$E(S) = \sum_{j=0}^{r-1} \sqrt[r]{2} |\cos\frac{(2j+1)\pi}{r}| + \sum_{j=0}^{r-1} |\cos\frac{2\pi j}{r}|.$$

Suppose r is odd, then

$$\begin{aligned} E(S) &= \sqrt[r]{2}\big(1 + 2\sum_{+} \cos\frac{(2j+1)\pi}{r} - 2\sum_{-} \cos\frac{(2j+1)\pi}{r}\big) \\ &+ 1 + 2\sum_{j=1}^{\lfloor \frac{r}{4} \rfloor} \cos\frac{2\pi j}{r} - 2\sum_{j=\lfloor \frac{r}{4} \rfloor+1}^{\lfloor \frac{r}{2} \rfloor} \cos\frac{2\pi j}{r} \\ &= 4\sum_{+} \cos\frac{(2j+1)\pi}{r} + 2\big(1 + 2\sum_{j=1}^{\lfloor \frac{r}{4} \rfloor} \cos\frac{2\pi j}{r}\big). \end{aligned}$$

Since $r+1$ is even, so

$$\begin{aligned} E(H) &= \sqrt[r+1]{2}\big(2\sum_{+} \cos\frac{(2j+1)\pi}{r+1} - 2\sum_{-} \cos\frac{(2j+1)\pi}{r+1}\big) \\ &+ 2\sum_{j=0}^{\lfloor \frac{r+1}{4} \rfloor} \cos\frac{2\pi j}{r+1} - 2\sum_{j=\lfloor \frac{r+1}{4} \rfloor+1}^{\frac{r+1}{2}} \cos\frac{2\pi j}{r+1} \\ &= 4\sqrt[r+1]{2}\sum_{+} \cos\frac{(2j+1)\pi}{r+1} + 2\big(1 + 2\sum_{j=1}^{\lfloor \frac{r+1}{4} \rfloor} \cos\frac{2\pi j}{r+1}\big). \end{aligned}$$

Using (3.5) and (3.16), we can write

$$4\sqrt[r]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r}+2\big(1+2\sum_{j=1}^{\lfloor\frac{r}{4}\rfloor}\cos\frac{2\pi j}{r}\big) \;\leq\; 4\sqrt[r+1]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r+1} + 2\big(1+2\sum_{j=1}^{\lfloor\frac{r+1}{4}\rfloor}\cos\frac{2\pi j}{r+1}\big).$$

That is

$$E(S)\leq E(H).$$

Now suppose that r is even, then

$$\begin{aligned}E(S) &= \sqrt[r]{2}\big(2\sum_{+}\cos\frac{(2j+1)\pi}{r}-2\sum_{-}\cos\frac{(2j+1)\pi}{r}\big)\\ &+ 2\sum_{j=0}^{\lfloor\frac{r}{4}\rfloor}\cos\frac{2\pi j}{r}-2\sum_{j=\lfloor\frac{r}{4}\rfloor+1}^{\frac{r}{2}}\cos\frac{2\pi j}{r}\\ &= 4\sqrt[r]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r}+2\big(1+2\sum_{j=1}^{\lfloor\frac{r}{4}\rfloor}\cos\frac{2\pi j}{r}\big).\end{aligned}$$

Since $r+1$ is odd, so

$$\begin{aligned}E(H) &= \sqrt[r+1]{2}\big(1+2\sum_{+}\cos\frac{(2j+1)\pi}{r+1}-2\sum_{-}\cos\frac{(2j+1)\pi}{r+1}\big)\\ &+ 1+2\sum_{j=0}^{\lfloor\frac{r+1}{4}\rfloor}\cos\frac{2\pi j}{r+1}-2\sum_{j=\lfloor\frac{r+1}{4}\rfloor+1}^{\frac{r+1}{2}}\cos\frac{2\pi j}{r+1}\\ &= 4\sqrt[r+1]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r+1}+2\big(1+2\sum_{j=1}^{\lfloor\frac{r+1}{4}\rfloor}\cos\frac{2\pi j}{r+1}\big).\end{aligned}$$

Using (3.5) and (3.16), we can write

$$4\sqrt[r]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r}+2\big(1+2\sum_{j=1}^{\lfloor\frac{r}{4}\rfloor}\cos\frac{2\pi j}{r}\big) \;\leq\; 4\sqrt[r+1]{2}\sum_{+}\cos\frac{(2j+1)\pi}{r+1} + 2\big(1+2\sum_{j=1}^{\lfloor\frac{r+1}{4}\rfloor}\cos\frac{2\pi j}{r+1}\big).$$

Hence

$$E(S)\leq E(H).$$

4. When only vertex-disjoint cycle is negative, then

$$E(S) = \sum_{j=0}^{r-1} \left(\sqrt[r]{2} |\cos \frac{2j\pi}{r}| + |\cos \frac{(2j+1)}{r}| \right).$$

Similarly $E(S) \leq E(H)$.

5. When one of the cycle other than vertex disjoint cycle is negative, then

$$\phi_S(x) = (x^{r+1} - x + x)(\phi_{c_r}(x)).$$

Then

$$E(S) = E(C_r).$$

From [1] we know that

$$E(C_r) \leq E(C_l), \tag{3.26}$$

for $r \leq l$. Hence from all the above possibilities we conclude that energy of sidigraphs in $\mathcal{S}_n$ increases with increase in length of cycle.

□

The next theorem is a consequence of Lemma 3.3.1.

Theorem 3.3.7. *Let $S \in \mathcal{S}_n$ be a sidigraph having cycles of equal length r. Then S has minimal energy if length of each cycle is 3 and maximal energy if length of each cycle is $\lfloor \frac{n}{2} \rfloor$.*

If each cycle of S is negative, then

$$E(S) = (1 + \sqrt[r]{2}) \sum_{j=0}^{r-1} |\cos \frac{(2j+1)\pi}{r}|. \tag{3.27}$$

For $r \geq 5$, we show that

$$E(S) > (1 + \sqrt[3]{2}) \sum_{j=0}^{2} |\cos \frac{(2j+1)\pi}{3}|.$$

The following inequality holds:

$$\frac{1}{2}(1 + \sqrt[3]{2}) \sum_{j=0}^{2} |\cos \frac{(2j+1)\pi}{3}| < (1 + \sqrt[r]{2}) \sum_{j=3}^{r-1} |\cos \frac{(2j+1)\pi}{r}|. \tag{3.28}$$

Then from equation (3.27),

$$E(S) = (1+\sqrt[3]{2})\sum_{j=0}^{2}\left|\cos\frac{(2j+1)\pi}{3}\right| + (1+\sqrt[r]{2})\sum_{j=3}^{r-1}\left|\cos\frac{(2j+1)\pi}{r}\right|.$$

Inequality (3.28) and above equation give

$$E(S) > (1+\sqrt{2})\sum_{0}^{1}\left|\cos\frac{(2j+1)\pi}{2}\right|.$$

This shows that S has minimal energy if $r = 3$.

Now from Lemma 3.3.1, energy of $S \in \mathcal{S}_n$ increases with increase in length of cycle. For fixed n, the maximum length of each cycle in S can be $\lfloor \frac{n}{2} \rfloor$. Thus we conclude that S has maximal energy if length of each cycle is $\lfloor \frac{n}{2} \rfloor$.

3.4 Conclusion

In this chapter, we introduced a new class $\mathcal{D}_n$ of tricyclic digraphs. Each $D \in \mathcal{D}_n$ has exactly five linear subdigraphs. For $n \geq 6$, we showed that $D \in \mathcal{D}_n$ has maximal energy among the digraphs of $\mathcal{D}_n$ if the length of each cycle is $\lfloor \frac{n}{2} \rfloor$. Also D has minimal energy if length of each cycle is 4.

Further, we extend this concept by introducing a class $\mathcal{S}_n$ which contains all those n-vertex tricyclic signed digraphs which has exactly five linear subdigraphs. We proved that a signed digraph $S \in \mathcal{S}_n$ has minimal energy if length of its each cycle is 3 and maximal energy if length of each cycle is $\lfloor \frac{n}{2} \rfloor$.

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