

***THE EIGEN-CHROMATIC RATIO OF CLASSES OF
GRAPHS: MOLECULAR STABILITY, ASYMPTOTES
AND AREA***

by

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Dedication

To my wife Ida Noki Mayala and to my children:
Philippe Mayala, Alpha mayala and Emmanuella Mayala,
I dedicate this work.

Acknowledgments

I thank first of all God who gave me the free breath of life in order to realize this work. May glory and praise come back to him.

I would like to thank Dr. Paul August Winter and Dr. Proscovia Namayanja, respectively my supervisor and co-supervisor for having never ceased to guide me and to advise me during the preparation of this thesis.

I especially thank Dr. Paul August Winter, and that He receive here the expression of my gratitude, for having proposed me the topic of this thesis and also for all the help that He brought me.

Special thanks go also to my lovely wife Dr. Ida Noki Mayala, for her moral and financial support. And to my son Philippe Mayala, and my daughters: Alpha Mayala and Emmanuella Mayala, for their patience and love.

My sincere thanks also go to my parents: Mr. Philippe Mbonga Ngoma and Mrs. Henriette Kasa Mvumbi, to my father-in-law Prof. Philippe Noki Vesituluta (that his soul rests in peace), to my uncle Mr. Emmanuel Mavinga Nzita, and to my brothers and sister, for supporting me spiritually.

Lastly, I would like to thank all those who, far or near, have encouraged me to complete this work.

Preface

The research work described in this dissertation was carried out in the School of Mathematics, Statistics and Computer Science, University of KwaZulu-Natal, Durban, from February 2016 to November 2017, under the supervision of Dr Paul August Winter.

These studies represent original work by the author and have not otherwise been submitted in any form for any degree or diploma to any tertiary institution. Where use has been made of the work of others, it is duly acknowledged in the text.

Declaration

I, Roger Mbonga Mayala, declare that

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Publication

The publications on which the research presented in this dissertation is based, are reproduced in reference [56].

Publication 1. P. A. Winter, R. M. Mayala and P. Namayanja, *The Eigen-chromatic Ratio of classes of Graphs: Asymptotes, Areas and Molecular Stability*, Journal of Progressive Research in Mathematics(JPRM), Volume 12, Issue 2, 1834-1852, July 2017.

Signed:.....

Abstract

This dissertation involves combining the two concepts of *energy* and the *chromatic number* of classes of graphs into a new ratio, the *eigen-chromatic ratio* of a graph G . Associated with this ratio is the importance of its asymptotic convergence in applications, as well as the idea of area involving the Riemann integral of this ratio, when it is a function of the order n of the graph G belonging to a class of graphs.

The energy of a graph G , is the sum of the absolute values of the eigenvalues associated with the adjacency matrix of G , and its importance has found its way into many areas of research in graph theory. The chromatic number of a graph G , is the least number of colours required to colour the vertices of the graph, so that no two adjacent vertices receive the same colour. The importance of ratios in graph theory is evident by the vast amount of research articles: Expanders, The central ratio of a graph, Eigen-pair ratio of classes of graphs, Independence and Hall ratios, Tree-cover ratio of graphs, Eigen-energy formation ratio, The eigen-complete difference ratio, The chromatic-cover ratio and "Graph theory and calculus: ratios of classes of graphs". We combine the two concepts of energy and chromatic number (which involves the order n of the graph G) in a ratio, called the *eigen-chromatic ratio* of a graph. The chromatic number associated with the molecular graph (the atoms are vertices and edges are bonds between the atoms) would involve the partitioning of the atoms into the smallest number of sets of like atoms so that like atoms are not bonded. This ratio would allow for the investigation of the effect of the energy on the atomic partition, when a large number of atoms are involved. The complete graph is associated with the value $\frac{1}{2}$ when the eigen-chromatic ratio is investigated when a large number of atoms are involved; this has allowed for the investigation of molecular stability associated with the idea of hypo/hyper energetic graphs. Attaching the average degree to the Riemann integral of this ratio (as a function of n) would result in an area analogue for investigation.

Once the ratio is defined the objective is to find the eigen-chromatic ratio of various well known classes of graphs such as the complete graph, bipartite graphs, star graphs with rays of length two, wheels, paths, cycles, dual star graphs, lollipop graphs and caterpillar graphs. Once the ratio of each class of graph are determined the asymptote and area of this ratio are determined and conclusions and conjectures inferred.

Key words: Eigenvalue; Energy of graphs; Chromatic number; Ratios; Asymptote; Area.

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Chapter 0

0.1 INTRODUCTION

Many problems in discrete mathematics can be stated and solved using Graph Theory (*Graph Theory* is the study of graphs, which are mathematical structures used to model pairwise relations between objects.), therefore Graph Theory is considered by many to be one of the most important and vibrant fields within discrete mathematics.

Graph theoretical concepts are widely used to study and model various applications, in different areas. They include, study of molecules, construction of bonds in chemistry and the study of atoms. Similarly, graph theory is used in sociology for example to measure actor prestige or to explore diffusion mechanisms. Graph theory is used in biology and conservation efforts where a vertex represents regions where certain species exist and the edges represent migration path or movement between the regions. This information is important when looking at breeding patterns or tracking the spread of disease, parasites and to study the impact of migration that affects other species. Graph theoretical ideas are highly utilized by computer science applications. This dissertation mainly focused on important applications in chemistry with the molecular graph.

Graph theory is everywhere, whenever some system can be visualized as a set of elements that are somehow interconnected. With the advent of computers graph theory has blossomed.

In this dissertation, we present a new ratio associated with classes of graphs, called the eigen-chromatic ratio, by combining the two graph theoretical concepts of energy and chromatic number.

The energy of a graph, the sum of the absolute values of the eigenvalues associated with the adjacency matrix of a graph, arose historically as a result of the energy of the benzene ring being identical to that of the sum of the absolute values of the eigenvalues of the adjacency matrix of the cycle graph on n vertices (see [16]).

The chromatic number of a graph is the smallest number of colour classes that we can partition the vertices of a graph such that each edge of the graph has ends that do not belong to the same colour class, and applications to the real world abound (see [30]). Applying this idea to molecular graph theory, for example, the water molecule would have its two hydrogen atoms coloured with the same colour different to that of the oxygen molecule.

Ratios involving graph theoretical concepts form a large subset of graph theoretical research (see [1], [13], [53]). The eigen-chromatic ratio of a class of graph provides a form of energy distribution among the colour classes determined by the chromatic number of such a class of graphs. The asymptote associated with this eigen-chromatic ratio allows for the behavioural analysis in terms of stability of molecules in molecular graph theory where a large number of atoms are involved. This asymptote can be associated with the concept of graphs being hyper or hypo-energetic (see [53]). The complete graph is associated with the value $\frac{1}{2}$ when the eigen-chromatic ratio is investigated when a large number of atoms are involved; this has allowed for

the investigation of molecular stability associated with the idea of hypo/hyper energetic graphs (see [53]).

This dissertation is organized as follows.

In chapter 1 we present the graph theoretical definitions used in this dissertation, together with the different classes of graphs which will be investigated. All graphs are simple and loopless and on n vertices and m edges.

Chapter 2 involves the different methods for finding eigenvalues of the adjacency matrix of a graph.

In chapter 3 we present the energy of the different classes of graphs discussed in chapter 1.

In chapter 4 we discuss the chromatic number of a graph relevant to our classes of graphs.

Chapter 5 forms the original part of this dissertation (see [56]) where we formally define the eigen-chromatic ratio and asymptote of classes of graph. As is line with previous research involving area of classes of graphs (see [49], [50] and [54]) we attach the average degree of a class of graphs to the Riemann integral of the eigen-chromatic ratio (as a function of the number of vertices n involved) so as to provide a comparative analysis of classes of graphs via their eigen-chromatic ratio.

In chapter 6 we discuss our results and conclude this dissertation with possible further research involving this new ratio.

Chapter 1

GRAPH THEORY DEFINITIONS AND CLASSES OF GRAPHS

In this chapter we provided some basic notions of Graph theory which will be required later in this thesis. We have used the graph theoretical notation of Harris, Hirst, and Mossinghoff (see [25]). We introduced many classes of graphs in this chapter which will be the basis of our research later.

1.1 Graphs, Subgraphs, Complement, and Clique

Definition 1.1. Graphs

A graph $G = (V, E)$ is an ordered pair of finite sets, V and E . Each elements of V is called vertex or node, and elements of $E \subseteq V \times V$ are called edges or arcs. We refer to V as the vertex set of G , with E being the edge set. The vertex set of a graph G is denoted by $V(G)$, and the edge set is denoted by $E(G)$. We may refer to these sets simply as V and E if the context makes the particular graph clear. The cardinality of V denoted $|V|$, is called the *order* of G , and $|E|$ is called the *size* of G .

One can label a graph by attaching labels to its vertices. If $(v_1, v_2) \in E$ is an edge of a graph $G = (V, E)$, we say that v_1 and v_2 are adjacent vertices. For ease of notation, we can write the edges (v_1, v_2) as v_1v_2 . The edge v_1v_2 is also said to be incident with the vertices v_1 and v_2 .

Here is an example of a graph:

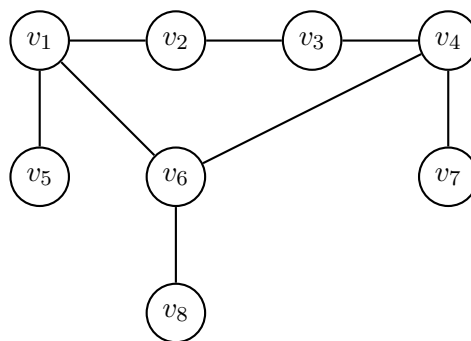


Figure 1.1: An example of a graph

We have:

$V = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8\}$

$E = \{(v_1, v_2), (v_1, v_5), (v_1, v_6), (v_2, v_3), (v_3, v_4), (v_4, v_6), (v_4, v_7), (v_6, v_8)\}$.

Definition 1.2. Neighborhood

The *neighborhood* (or *open neighborhood*) of a

- (i) vertex v , denoted by $N(v)$, is the set of vertices adjacent to v :

$$N(v) = \{x \in V/vx \in E\}.$$

- (ii) set S of vertices, denoted by $N(S)$, is the union of the neighborhoods of the vertices in S .

The *closed neighborhood* of a vertex v , denoted by $N[v]$, is simply the set $\{v\} \cup N(v)$, while the *closed neighborhood* of S , denoted by $N[S]$, is defined to be $S \cup N(S)$.

Definition 1.3. Degree

The *degree* of v , denoted by $deg(v)$, is the number of edges incident with v . In simple graphs, this is the same as the cardinality of the (open) neighborhood of v .

A vertex of degree one is called a ***pendent*** vertex.

The *maximum degree* of a graph G , denoted by $\Delta(G)$, is defined to be

$$\Delta(G) = \max\{deg(v)/v \in V(G)\}.$$

Similarly, the *minimum degree* of a graph G , denoted by $\delta(G)$, is defined to be

$$\delta(G) = \min\{deg(v)/v \in V(G)\}.$$

The *degree sequence* of a graph G of order n is the n -term sequence (usually written in descending order) of the vertex degrees.

Let's use the graph G in the example above, to illustrate some of these concepts: G has order 8 and size 8; vertices v_1 and v_5 are adjacent while vertices v_1 and v_8 are nonadjacent; $N(v_4) = \{v_3, v_6, v_7\}$, $N[v_4] = \{v_3, v_4, v_6, v_7\}$; $\Delta(G) = 3$, $\delta(G) = 1$; and the degree sequence is 3, 3, 3, 2, 2, 1, 1, 1.

Theorem 1.1 (J. Gross and J. Yellen.[23]) In a graph G , the sum of the degrees of the vertices is equal to twice the number of edges. Consequently, the number of vertices with odd degree is even.

Proof. Let $S = \sum_{v \in V} deg(v)$. Notice that in counting S , we count each edge exactly twice. Thus, $S = 2 | E |$ (the sum of the degrees is twice the number of edges). Since S is even, it must be that the number of vertices with odd degrees is even.

Definition 1.4. Weighted graphs

Sometimes, we will use edges to denote a connection between a pair of nodes where the connection has a *capacity* or *weight*. For example, we might be interested in the capacity of an Internet fiber between a pair of computers, the resistance of a wire between a pair of terminals, the tension of a spring connecting a pair of devices in a dynamical system, the tension of a bond between a pair of atoms in a molecule, or the distance of a highway between a pair of cities.

In such cases, it is useful to represent the system with a *weighted - edge* graph. A weighted graph is the same as a simple graph except that we associate a real number (that is, the weight) with each edge in the graph.

Mathematically speaking, a weighted graph is a graph for which each edge has an associated weight, usually given by a weight function $w: E \rightarrow \mathbb{R}$.

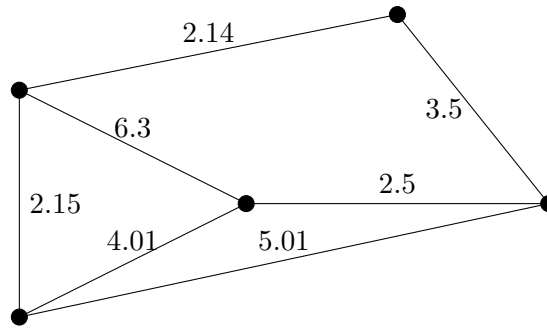


Figure 1.2: A *weighted graph*

Definition 1.5. Directed graphs (Digraphs)

A directed edge is an edge such that one vertex incident with it is designated as the head vertex and the other incident vertex is designated as the tail vertex. A directed edge uv is said to be directed from its tail u to its head v . A directed graph or digraph G is a graph such that each of its edges is directed. The indegree of a vertex $v \in V(G)$ counts the number of edges such that v is the head of those edges. The outdegree of a vertex $v \in V(G)$ is the number of edges such that v is the tail of those edges.

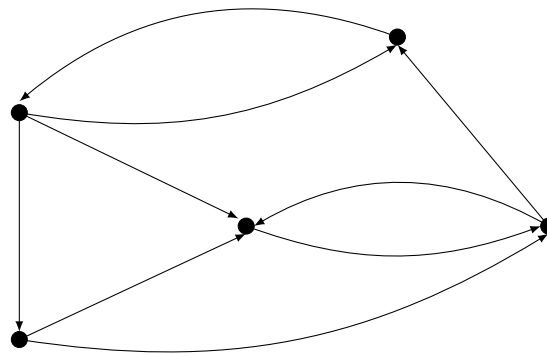


Figure 1.3: A *directed graph*

Definition 1.6. Multigraphs.

A multigraph is a graph in which there are multiple edges between a pair of vertices. A multi-undirected graph is a multigraph that is undirected. Similarly, a multi-digraph is a directed multigraph. Here is an example:

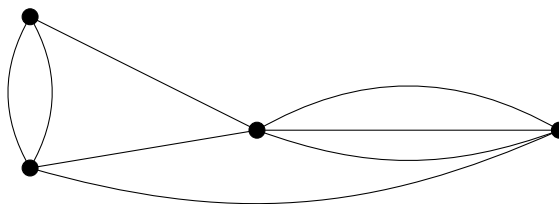


Figure 1.4: A *multigraph*

Definition 1.7. Simple graphs

A simple graph is a graph with no self-loops and no multiple edges.

Definition 1.8. Complete Graph.

A complete graph is a graph $G = (V, E)$ where $|V| = n$, $|E| = n(n - 1)/2$ and every pair of vertices are adjacent. Below a complete graph on 6 vertices,

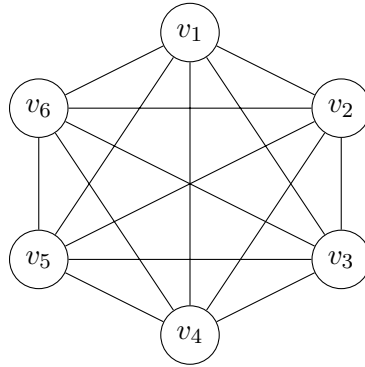


Figure 1.5: Complete Graph with 6 vertices

Theorem 1.2 Euler If $G = (V, E)$ is a graph, then $\sum_{v \in V} \deg(v) = 2|E|$.

Definition 1.9. Isomorphism

Two graphs that look the same might actually be different in a formal sense. For example, two graphs are both simple cycles with 4 vertices, but one graph has vertex set $\{a, b, c, d\}$ while the other has vertex set $\{1, 2, 3, 4\}$. Strictly speaking, these graphs are different mathematical objects, but this is a frustrating distinction since the graphs look the same! Fortunately, we can neatly capture the idea of looks the same through the notion of graph isomorphism.

If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs, then we say that G_1 is *isomorphic* to G_2 iff there exists a bijection $f : V_1 \rightarrow V_2$ such that for every pair of vertices $u, v \in V_1$:

$$\{u, v\} \in E_1 \text{ iff } \{f(u), f(v)\} \in E_2.$$

Then function f is called an *isomorphism* between G_1 and G_2 .

In other words, two graphs are isomorphic if they are the same up to relabeling of their vertices.

Definition 1.10. Subgraphs

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Consider a graph H such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Furthermore, if $uv \in E(H)$ then $u, v \in V(H)$. Then H is called a subgraph of G and G is referred to as a supergraph of H .

Definition 1.11. Induced Subgraphs

Given a graph G and a subset S of the vertex set, the *subgraph of G induced by S* , denoted $G\langle S \rangle$ or $G[S]$, is the subgraph with vertex set S and with edge set $\{uv/u, v \in S \text{ and } uv \in E(G)\}$. So, $G\langle S \rangle$ contains all vertices of S and all edges of G whose end vertices are *both* in S .

Definition 1.12. Complement of a Graph

The *Complement*, \overline{G} , of a graph G is a graph whose vertex set is the same as G and

$$e \in E(\overline{G}) \Leftrightarrow e \notin E(G)$$

Definition 1.13. Independent Set - Independence number

An *independent set* is a set of vertices in a graph, such that no two vertices of the graph $G = (V, E)$ are adjacent. In other words, it is a set $I \subseteq V$ such that for every two vertices in I , there is no edge connecting the two. Equivalently, each edge in the graph has at most one endpoint in I .

A *maximum independent set* is an independent set in a graph G such that, no other independent set in G has larger cardinality. It is called *maximal* if it is contained in on larger independent set.

An *independence number* of a graph G is the number of vertices in a maximum independent set in G , and is denoted $\alpha(G)$.

Definition 1.14. Clique of a Graph

A *clique*, C , in an undirected graph $G = (V, E)$ is a subset of the vertices, $C \subseteq V$, such that every two distinct vertices are adjacent. This is equivalent to the condition that the subgraph of G induced by C is complete. The term clique may also refer to the subgraph directly in some cases.

A *maximal clique* is a clique that cannot be extended by including one more adjacent vertex, that is, a clique which does not exist exclusively within the vertex set of a larger clique.

A *maximum clique* of a graph G , is a clique, such that there is no clique with more vertices.

The *clique number* $\omega(G)$ of a graph G is the number of vertices in a maximum clique in G .

The *intersection number* of G is the smallest number of cliques that together cover all edges of G .

The *clique cover number* of a graph G is the smallest number of cliques of G whose union covers $V(G)$. The opposite of a clique in an independent set, in the sense that every clique corresponds to an independent set in the complement graph. The clique cover problem concerns finding as few cliques as possible that include every vertex in the graph.

1.2 Paths, Cycle, Connectedness, Components, Cut-vertex

Definition 1.15. Paths and walks

- (i) A **walk** in a graph G is a sequence of vertices

$$v_0, v_1, \dots, v_k$$

and edges

$$\{v_0, v_1\}, \{v_1, v_2\}, \dots, \{v_{k-1}, v_k\}$$

such that $\{v_i, v_{i+1}\}$ is an edge of G for all i where $0 \leq i < k$. The walk is said to *start* at v_0 and to *end* at v_k , and the *length* of the walk is defined to be k . An edge, $\{u, v\}$, is traversed n time by the walk if there are n different values of i such that $\{v_i, v_{i+1}\} = \{u, v\}$.

(ii) A **path** is a walk where all the vertices v_i are different, that is, $i \neq j$ implies $v_i \neq v_j$.

A **path** is a simple graph whose vertices can be ordered so that two vertices are adjacent if and only if they are consecutive in the ordering. A path which begins at vertex u and ends at vertex v is called a $u - v$ path. Here is a path with 6 vertices:

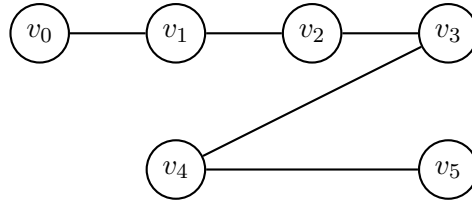


Figure 1.6: A path with 6 vertices

Definition 1.16. Cycle.

A cycle is a simple graph whose vertices can be cyclically ordered so that two vertices are adjacent if and only if they are consecutive in the cyclic ordering. A graph is acyclic if it does not contain any cycles.

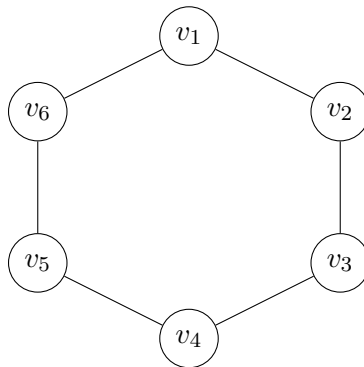


Figure 1.7: A Cycle with 6 vertices

We usually think of paths and cycles as subgraphs within some larger graph.

Definition 1.17. Connectedness

A graph G is connected if for every $u, v \in V(G)$ there exists a u, v -path in G . Otherwise G is called disconnected. In the diagram below, the graph on the left has two pieces, while the graph on the right has just one. So, only the graph on the right is connected.

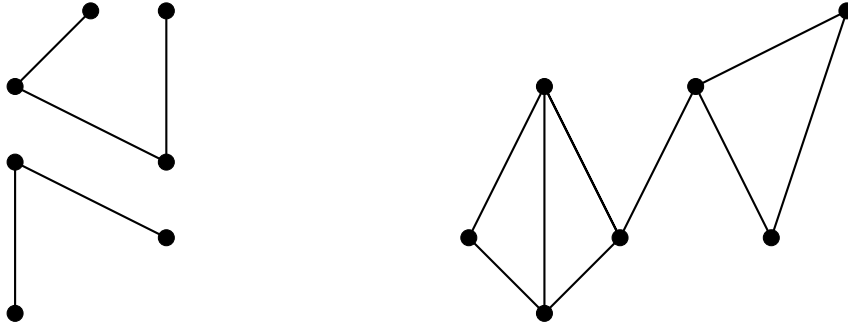


Figure 1.8: *Connectivity*

Definition 1.18. Components

The maximal connected subgraphs of G are called its components.

Theorem 1.3 (J. Gross and J. Yellen.[23])

- (i) If a graph $G = (V, E)$ is acyclic, then $|E| \leq |V| - 1$
- (ii) If a graph $G = (V, E)$ is connected, then $|E| \geq |V| - 1$

Proof

We only prove part(i) of the Theorem; part(ii) can be proven by a similar reasoning. We use induction on $|V|$. Since the theorem trivially holds for $|V| = 2$, we may state our induction-hypothesis that the theorem is true for each graph on $|V| = n - 1$ vertices. we have to show that the theorem then also holds for each graph on n vertices.

Suppose to the contrary that there exists an acyclic graph $G = (V, E)$ on n vertices with $|E| \geq |V| = n$. If G contains a vertex with degree equal to zero or one, then we just remove this vertex and the corresponding edge (in case of degree one) and obtain an acyclic graph on $n - 1$ vertices with at least $n - 1$ edges, which contradicts the induction-hypothesis. Hence, we know that each vertex then must have degree at least equal to two. Since the graph is assumed to be acyclic, we can travel from each vertex to another one that we have not visited before. But after having traversed $n - 1$ edges, we have visited each vertex. We are then in a vertex with degree at least two, so we can leave this vertex through an edge that we have not traversed before and that must be incident to a vertex that we have already visited, which implies that G contains a cycle. this contradiction proves part(i) of Theorem 1.3.

Definition 1.19. A Cut-vertex of a connected graph.

A *cut-vertex* is a vertex, whose removal from a connected graph, would disconnect the graph. In others words, a *cut-vertex* of a connected graph $G = (V, E)$ is a vertex whose removal from V , increases the number of components in G .

And a *vertex separator* is a collection of vertices, whose removal from a connected graph, would disconnect the graph.

1.3 Strong cliques, Co-cliques and Colouring

Definition 1.20. Strong cliques

A *strong clique* is a subgraph of G which is a maximal clique and has at least one cut-vertex.

Definition 1.21. Co-cliques

A set of vertices of a graph G which are non-adjacent in G is a *co-clique* of G . The order of the largest *co-clique* of G is called the *co-clique number* of G .

Definition 1.22. Colouring and Chromatic number

A *proper colouring* of the vertices of a graph G is an assignment of colours to the vertices so that no two adjacent vertices receive the same colour. The least number of colours required to form a proper colouring of a graph is called the *chromatic number* of G and is denoted by $\chi(G)$.

1.4 Distance in graph and Adjacency matrix

Definition 1.23. Distance in graph

Let $G = (V, E)$ be a connected graph. We define the distance of two vertices $v_1, v_2 \in V(G)$, denoted by $d_G(v_1, v_2)$, as the length of a shortest path from v_1 to v_2 in G .

Hence d_G is a function, $d_G: V \times V \rightarrow \mathbb{R}$, and it is called the distance function or the metric of the graph G . The metric of G has the following properties:

1. $d_G(v_1, v_2) \geq 0$, and $d_G(v_1, v_2) = 0$ if and only if $v_1 = v_2$,
2. $d_G(v_1, v_2) = d_G(v_2, v_1)$ for any pair of vertices v_1, v_2 ;
3. $d_G(v_1, v_3) \leq d_G(v_1, v_2) + d_G(v_2, v_3)$ for any three vertices $v_1, v_2, v_3 \in V(G)$. The validity of these statements can be readily checked from the definition of the distance function $d_G(v_1, v_2)$. Each mapping $d: V \times V \rightarrow \mathbb{R}$ with properties 1-3 is called a *metric* on the set V , and the set V together with such a mapping d is called a *metric space*. The distance function d_G of a graph has, moreover, the following special properties:
4. $d_G(v_1, v_2)$ is a nonnegative integer for any two vertices v_1, v_2 ;
5. if $d_G(v_1, v_3) > 1$ then there exists a vertex v_2 , $v_1 \neq v_2 \neq v_3$, such that $d_G(v_1, v_2) + d_G(v_2, v_3) = d_G(v_1, v_3)$.

Conditions 1-5 already characterize functions arising as distance functions of graphs with vertex set V .

Graph representations

We have seen representations of graphs by drawings, and also by out a list of vertices and edges. Graphs can also be represented in many others ways. Some of them become particularly important if we want to store and manipulate graphs in a computer. A very basic and very common representation is by an adjacency matrix:

Definition 1.24. Adjacency matrix

Let $G = (V, E)$ be a graph with n vertices. Denote the vertices by v_1, v_2, \dots, v_n (in some arbitrary order). The adjacency matrix of G , with respect to the chosen vertex numbering, in an $n \times n$ matrix $A(G) = (a_{ij})_{i,j=1}^n$ defined by the following rule:

$$a_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

The adjacency matrix of a graph is always a symmetric square matrix with entries 0 and 1, with 0s on the main diagonal. Conversely, each matrix with these properties is the adjacency matrix of some graph.

Example. The graph G given in section 1.1. has the adjacency matrix

$$A(G) = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

Proposition 1.1 Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and let $A = A(G)$ be its adjacency matrix. Let A^k denote the k -th power of the adjacency matrix (the matrices are multiplied as is usual in linear algebra). Let $a_{ij}^{(k)}$ denote the element of the matrix A^k at position (i, j) . Then $a_{ij}^{(k)}$ is the number of walks of length exactly k from the vertex v_i to the vertex v_j in the graph G .

Corollary 1.1 The distance of any two vertices v_i, v_j satisfies

$$d_G(v_i, v_j) = \min\{k \geq 1 : a_{ij}^{(k)} \neq 0\}.$$

1.5 Laplace and signless Laplace matrix

Given a graph G with n vertices, the *degree matrix* $D(G)$ is a $n \times n$ diagonal matrix defined as

$$d_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

The *Laplace matrix* of G is defined as the $n \times n$ matrix $L(G)$, where

$$L(G) = D(G) - A(G),$$

i.e., it is the difference between the degree matrix $D(G)$ and the adjacency matrix $A(G)$ of the graph. From the definitions it follows that $L(G)$ is defined as

$$l_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j, \text{ and } v_i \text{ adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

where $\text{deg}(v_i)$ is degree of the vertex v_i .

The matrix $A(G) + D(G)$ is called the *signless Laplace matrix* of G .

1.6 Trees and Forests

Recall, a path in a graph $G = (V, E)$ whose start and end vertices are the same is called a cycle. We say G is acyclic, or a forest, if it has no cycles. A vertex of a forest of degree one is called an endpoint or a leaf. A connected forest is a tree.

Definition 1.25. Trees.

A tree $T = (V, E)$ is a connected acyclic graph. It contains a unique path between each pair of vertices. Here is an example of a tree:

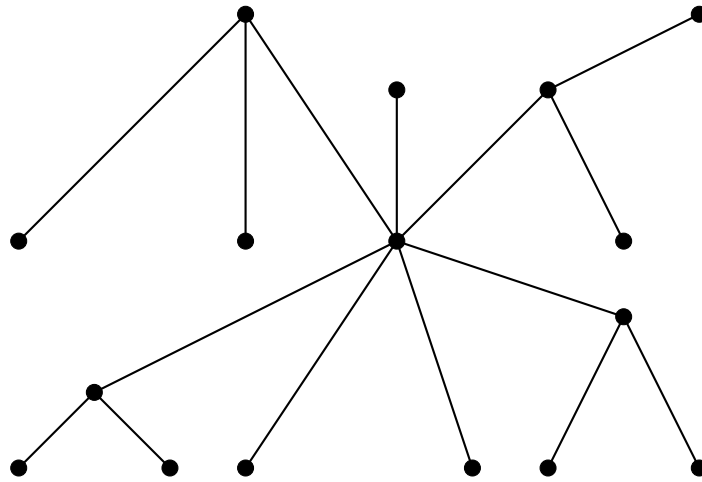


Figure 1.9: A Tree

The graph shown above would no longer be a tree if any edge were removed, because it would no longer be connected. The graph would also not remain a tree if any edge were added between two of its vertices, because then it would contain a cycle.

Theorem 1.4 The following conditions are all equivalent for a graph $G = (V, E)$:

- (i) G is a tree.
- (ii) For every two vertices $x, y \in V$, there exists exactly one path from x to y .
- (iii) The graph G is connected, and deleting any of its edges gives rise to a disconnected graph.
- (iv) The graph G contains no cycle, and any graph arising from G by adding an edge already contains a cycle.
- (v) G is connected and $|V| = |E| + 1$

Note that this theorem not only describe various properties of trees, such as: any tree on n vertices has $n - 1$ edges, but also lists properties equivalent to definition 1.25., so for instance it says: A graph on n vertices is a tree if and only if it is connected and has $n - 1$ edges.

Definition 1.26 Spanning Tree

Let G be a connected graph on n vertices. Then a *spanning tree* in G is a subgraph, S_G , of G that includes every vertex and is also a tree on n vertices. Below, we have, at the left the graph G , and at the right a spanning tree of G

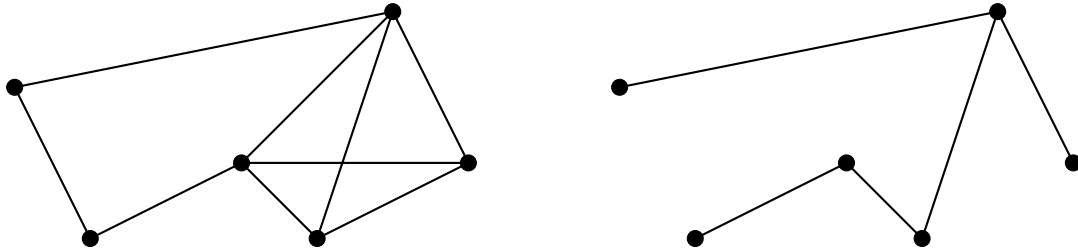


Figure 1.10: A *spanning tree*

Theorem 1.5 Every connected graph $G = (V, E)$ contains a spanning tree.

Proof Let $T = (V, E')$ be a connected subgraph of G with the smallest number of edges. We show that T is acyclic by contradiction. So suppose that T has a cycle with the following edges:

$$v_0 - v_2, v_1 - v_2, \dots, v_n - v_0$$

Suppose that we remove the last edge, $v_n - v_0$. If a pair of vertices x and y was joined by a path not containing $v_n - v_0$, then they remain joined by that path. On the other hand, if x and y were joined by a path containing $v_n - v_0$, then they remain joined by a path containing the remainder of the cycle. This is a contradiction, since T was defined to be a connected subgraph of G with the smallest number of edges. Therefore, T is acyclic.

Definition 1.27. The Forest

If every connected component of a graph G is a tree, then G is a forest. So a forest is a set of trees.

Definition 1.28. The Leaf

One of the first things we will notice about trees is that they tend to have a lot of nodes with degree one. Such nodes are called leaves. So the leaf is a node with degree 1 in a tree (or forest). For example, the tree in Figure 1.9. contains 11 leaves.

1.7 Union of graphs, Subdivision graph and Join of graphs

Let G and H be two graphs with vertex sets $V(G)$, $V(H)$ and edge sets $E(G)$, $E(H)$ respectively.

Definition 1.29. The *Union* of G and H , denoted by $G \cup H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

Definition 1.30. The *subdivision graph* of a graph G , denoted by $S(G)$, is the graph obtained by inserting a new vertex into every edges of G .

Definition 1.31. The *join* of G and H , denoted by $G \oplus H$, is formed when every vertex in G is joined to every vertex in H .

Definition 1.32. The *SG - vertex join* of G and H , denoted by $G \diamond H$, is the graph obtained from $S(G) \cup G$ and H by joining every vertex of $V(G)$ to every vertex of $V(H)$.

1.8 Classes of Graphs

In this section We define and show some different types of graphs.

1.8.1 Complete graph K_n

A complete graph K_n is a connected graph on n vertices where all vertices are of degree $n - 1$, i.e. there is an edge between a vertex and every other vertex. A complete graph has $\frac{n(n - 1)}{2}$ edges. Below a complete graph K_8 ,

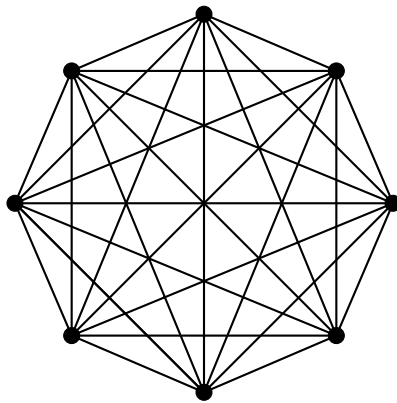


Figure 1.11: A complete graph K_8

1.8.2 Empty graphs E_n

The empty graph on n vertices denoted by E_n , is the graph of order n and of size 0. So an empty graph has no edges. See below an example of an empty graph on 8 vertices,

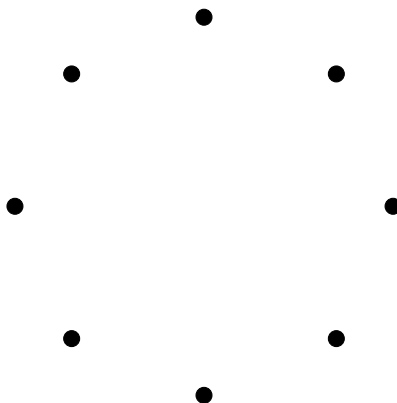


Figure 1.12: Empty graph E_8

1.8.3 Complete bi-partite graph $K_{m,n}$

A bipartite graph is a graph on $(m + n)$ vertices where the vertices are partitioned into two independent sets, V_1 (containing m disconnected vertices) and V_2 (containing n disconnected vertices), such that there are no edges between vertices in the same set. A complete bipartite graph $K_{m,n}$ is a bipartite graph in which there is an edge between every vertex in V_1 and every vertex in V_2 . Below a complete bi-partite graph $K_{3,4}$

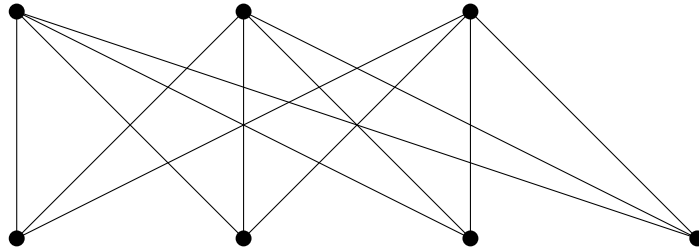


Figure 1.13: A complete bi-partite graph $K_{3,4}$

1.8.4 The Complete Split-bipartite Graph $K_{\frac{n}{2}, \frac{n}{2}}$

A *split graph* is a graph in which the vertices can be partitioned into a clique and an independent set.

The *double split graphs* is a family of graphs derived from split graphs by doubling every vertex.

The *complete split-bipartite graph* is when we split the vertex-set of the complete bipartite graph into identical parts of size $\frac{n}{2}$.

1.8.5 Path graph P_n

A path graph P_n is a connected graph of n vertices where 2 vertices are pendant and the other $n-2$ vertices are of degree 2. A path has $n-2$ edges. The following graph is a Path on 7 vertices,

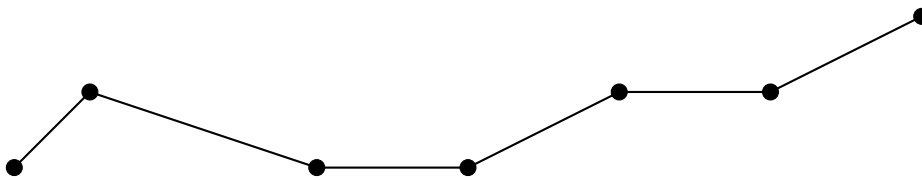


Figure 1.14: A Path P_7

1.8.6 Cycle graph C_n

A cycle graph C_n is a connected graph on n vertices where all vertices are of degree 2. A cycle graph can be created from a path graph by connecting the two pendant vertices in the path by an edge. A cycle has an equal number of vertices and edges. Below a C_8 ,

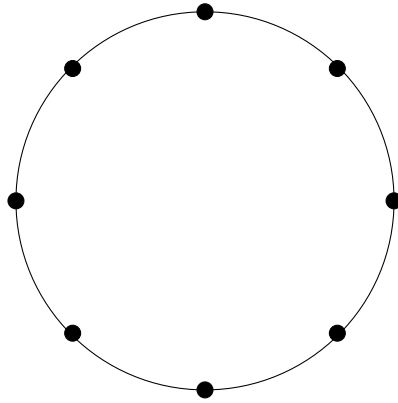


Figure 1.15: A Cycle C_8

1.8.7 Wheel graph W_n

A wheel graph W_n is a connected graph on n vertices, constructed by taking a cycle on $n - 1$ vertices, together with a single centre vertex, and joining each vertex in the cycle with the centre vertex. In other words, the wheel graph W_n is the join of K_1 and C_n . The wheel graph W_n has $(2n - 2)$ edges.

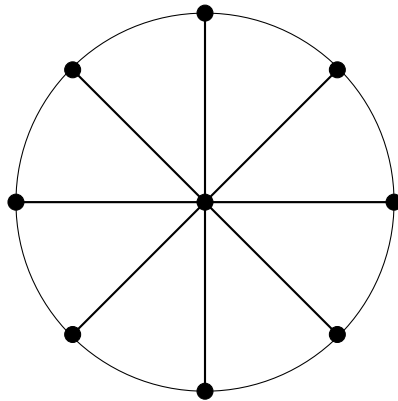


Figure 1.16: A wheel W_9

1.8.8 Lollipop graph LP_n

A lollipop graph LP_n is a connected graph on n vertices, comprising of the complete graph K_{n-1} on $n - 1$ vertices, joined to a single end vertex x_2 by an edge x_1x_2 , with $x_1 \in K_{n-1}$ and $n \geq 3$. A lollipop graph LP_n has $(n - 1)(n - 2) + 1$ edges.

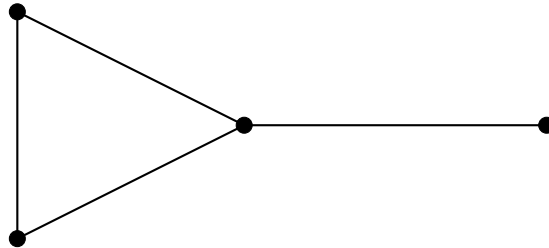


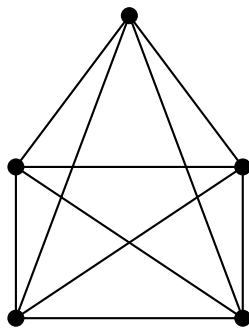
Figure 1.17: A Lollipop LP_4

1.8.9 Regular graph

A graph G is *regular* of degree (or valency) k , if every vertex has the same degree. So, G is said to be *regular* of degree k (or k -regular) if $\deg(v) = k$, for all $v \in G$, i.e. all its vertices have degree exactly k .

Empty graphs are regular of degree 0, and the complete graphs on n vertices are regular of degree $n - 1$. See in figure below examples of regular graphs,

4- regular graph



3- regular graph

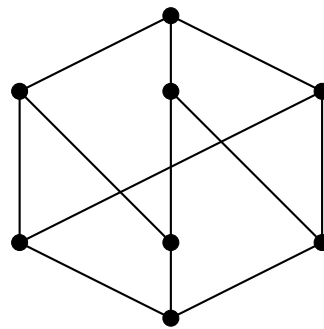


Figure 1.18: Examples of regular graphs.

1.8.10 Star graph $S_{n-1,1}$ with $n - 1$ rays of length 1

A star graph $S_{n-1,1}$ is a connected graph on n vertices where one vertex has degree $n - 1$ and the other $n - 1$ vertices have degree 1. A star graph is a special case of a complete bipartite graph in which one set has 1 vertex and the other set has $n - 1$ vertices. A star graph has $n - 1$ edges.

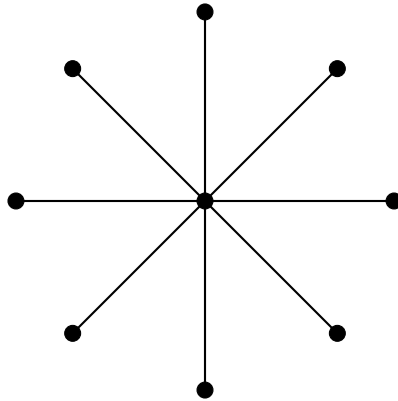


Figure 1.19: *Star graph $S_{8,1}$*

1.8.11 Star graph $S_{\frac{n-1}{2},2}$ with $\frac{n-1}{2}$ rays of length 2

A star graph $S_{\frac{n-1}{2},2}$ is a connected graph on n vertices, n odd and $n \geq 7$, where one vertex has degree $\frac{n-1}{2}$, $\frac{n-1}{2}$ vertices have degree 2, and $\frac{n-1}{2}$ vertices have degree 1. A star graph with $\frac{n-1}{2}$ rays of length 2, has $n - 1$ edges.

A star graph on n vertices with $k = \frac{n-1}{2}$ rays of length 2, denoted by $S_{k,2}$ or $S_{n,k(2)}$, is obtained from the star graph with rays of length 1 by inserting a vertex in each edge i.e. by subdividing each edge with a vertex.

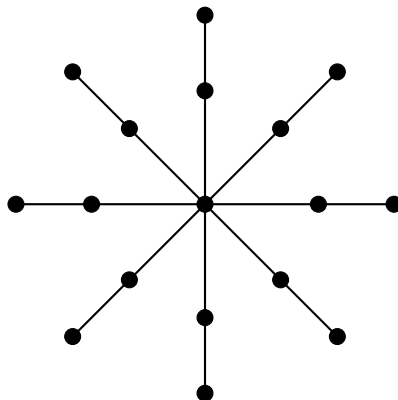


Figure 1.20: *Star graph $S_{8,2}$*

1.8.12 Dual star graph DuS_n

A dual star graph DuS_n is a connected graph on n vertices, comprising of two star graphs with m rays of length 1 (each on $\frac{n}{2}$ vertices) joined by an edge (its center edge) connecting the centers of the two star graphs.

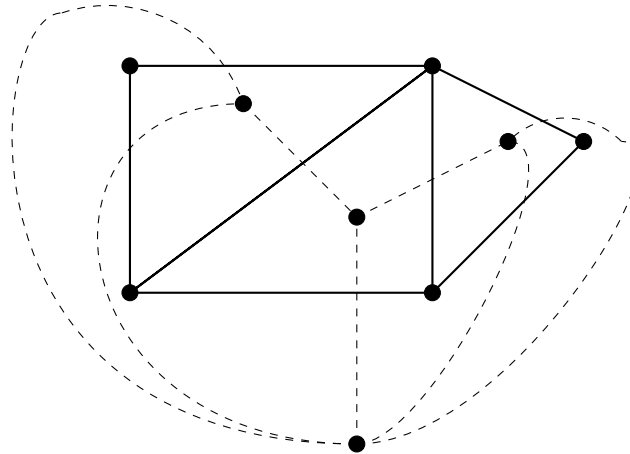


Figure 1.21: *Dual star graph*

1.8.13 Generalized Sun graph $SG(h,p)$

The generalized sun graph $SG(h,p)$ is a graph which consists of the base graph G on p vertices, with h end vertices appended to each of the p vertices in the graph G .

For a simple undirected graph G with n vertices and m edges, the **sun graph** of order $2n$ is a cycle C_n with an edge terminating in a pendent vertex attached to each vertex, and it is denoted by SG_n . Here is an example of SG_n :

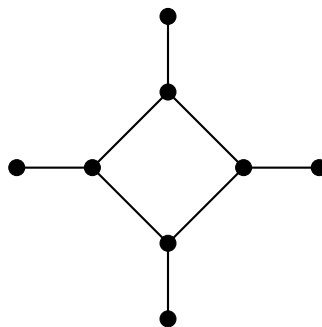


Figure 1.22: *Sun graph SG_4*

The **Complete sun graph** is a complete graph on $\frac{n}{2}$ vertices with end appended to each vertex.

The double Comb graph

The *double comb graph* is a complete-split bipartite graph on $\frac{n}{2}$ vertices with end vertex appended to each of its vertices. The double comb graph is a generalized sun graph with base graph the complete split bipartite graph.

l - regular caterpillar graph $CT(k, l)$

A *caterpillar graph* is a tree with the property that the removal of its end points leaves a path. The caterpillar graph is a generalized sun graph with base graph a path.

A l -regular *caterpillar graph* is obtained by attaching l pendant edges to each vertex of the path P_k . It is denoted by $CT(k, l)$ where k and l denote the number of vertices on the path and the number of pendant edges respectively. This graph will have $n = k(l + 1)$ vertices and $k(l + 1) - 1$ edges.

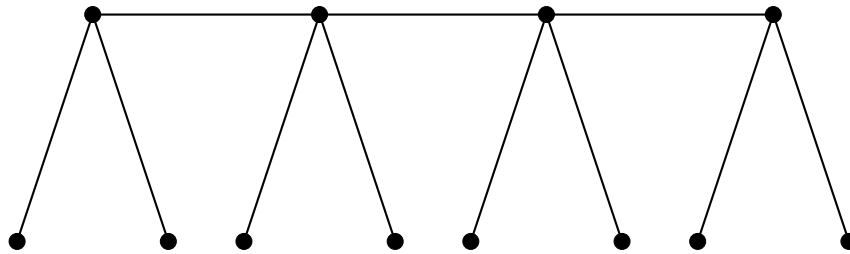


Figure 1.23: l - regular caterpillar graph $CT(4,2)$

1.8.14 Friendship graph $F_{\frac{n-1}{2}}$

A *friendship graph* $F_{\frac{n-1}{2}}$ (also called the $\frac{n-1}{2}$ -fan) is a graph with n vertices and $\frac{3n-3}{2}$ edges, constructed by joining $\frac{n-1}{2}$ copies of the cycle graph C_3 , with a common vertex. Friendship graph F_4 is shown in the following figure.

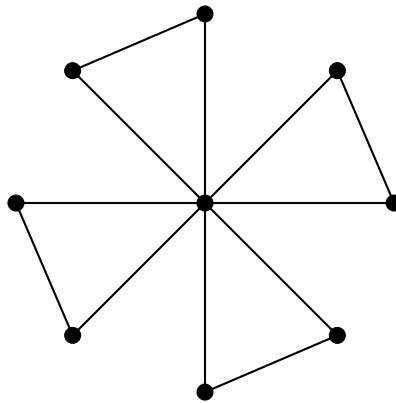


Figure 1.24: The Friendship graph F_4

1.8.15 Planar Graph

A *planar graph*, G , is a graph that can be drawn in the plane in such a way that pairs of edges intersect only at vertices, if at all. In other words, it can be drawn in such a way that no edges cross each other. If G has no such representation, G is called *nonplanar*. A drawing of a planar graph G in the plane in which edges intersect only at vertices is called a *planar representation* (or a *planar embedding*) of G .

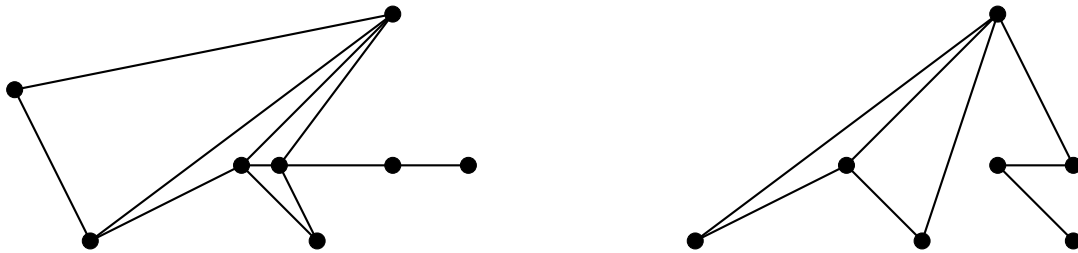


Figure 1.25: *Examples of planar graphs*

1.8.16 Strongly Regular Graph

Let $G = (V, E)$ be a regular graph with v vertices and degree k . Then G is a *strongly regular graph* if there are also integers λ and μ such that[11]:

- every two adjacent vertices have λ common neighbours;
- every two non-adjacent vertices have μ common neighbours.

A graph of this kind is sometimes denoted by $srg(v, k, \lambda, \mu)$.

1.8.17 The Line Graph of the Complete graph

The *line graph* of a graph G , denoted by $L(G)$, is defined as a graph that has the following properties:

- there is a vertex in $L(G)$ for every edge of G ;
- two vertices of $L(G)$ are adjacent if and only if they correspond to two edges of G with a common end vertex.

The line graph of a complete graph $L(K_n)$ has $p = \frac{n(n-1)}{2}$ vertices, and also the number of edges q of $L(K_n)$ is half the sum of the squares of degrees of the vertices of K_n minus the number of edges of K_n (see Brualdi [12]). Thus:

$$q = \frac{n(n-1)^2}{2} - \frac{n(n-1)}{2}$$
$$\Rightarrow q = \frac{n(n-1)(n-2)}{2}.$$

Chapter 2

LINEAR ALGEBRA AND METHODS OF FINDING EIGENVALUES

2.1 Introduction

In this chapter we review certain basic concepts from linear algebra to be applied in graph theory. We consider only real matrices. There are two important square matrices commonly associated to graphs: the adjacency matrix of the graph, and the (finite or combinatorial) Laplacian. Algebraic methods are applied to problems about graphs; This is in contrast to geometric, combinatoric, or algorithmic approaches. We illustrate a few techniques of finding eigenvalues of graphs by applying them to determine the eigenvalues of some classes of graphs discussed in chapter 1.

2.2 Basic Linear Algebra

The topics of linear equations, matrices, vectors, and of the algebraic structure known as a vector space, are intimately linked, and this area of mathematics is known as linear algebra. In this section we present the main results on vector spaces and matrices that will be needed in the rest of the dissertation. The notation and terminology of [25](J. M. Harris, J. L. Hirst. and M. Mosinghoff, *Combinatorics and Graph Theory*) will be used.

2.2.1 Matrices

A *Matrix* is any rectangular array of numbers. If a matrix A has m rows and n columns, we call A an $m \times n$ matrix. We refer to $m \times n$ as the *order* of the matrix. A typical $m \times n$ matrix A may be written as

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

The number in the i th row and j th column of A is called the ij th element of A and is written a_{ij} .

Sometimes we use the notation $A = (a_{ij})$ to indicate that A is the matrix whose ij th element is a_{ij} .

A matrix for which $m = n$ is a *square matrix* of order n .

The *diagonal* of a square matrix $A = (a_{ij})$ consists of the entries a_{ij} down the leading (top-left to bottom-right) diagonal.

2.2.2 Operations on Matrices

The Scalar Multiple of a Matrix

Given any matrix $A = (a_{ij})$ and any number k (a *number* is sometimes referred to as a *scalar*), we can define the *scalar multiple* $kA = (ka_{ij})$; note that $1A = A$.

Addition of two Matrices

Let $A = (a_{ij})$ and $B = (b_{ij})$ be two matrices with the same order (say, $m \times n$). We define their *sum* $A + B$ to be the matrix $C = (c_{ij})$, where $c_{ij} = a_{ij} + b_{ij}$; matrix addition is commutative and associative.

Matrix Multiplication

Given an $m \times k$ matrix $A = (a_{ij})$ and a $k \times n$ matrix $B = (b_{ij})$, we define their *product* AB to be the $m \times n$ matrix $C = (c_{ij})$, where $c_{ij} = \sum_k a_{ik}b_{kj}$.

Matrix multiplication is associative, but not commutative in general. The matrix product AA is written A^2 , with similar notation for higher powers of A .

Kronecker Product of two Matrices

Given two matrices $A = (a_{ij})$ and $B = (b_{ij})$ of the same size, we define their *Kronecker product* $A \otimes B$ to be the matrix $C = (c_{ij})$, where $c_{ij} = a_{ij}b_{ij}$.

The transpose of a Matrix

Given an $m \times n$ matrix

$$A = (a_{ij}) = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

we can interchange the rows and columns to form the $n \times m$ matrix

$$A^T = (a_{ji}) = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix}$$

called its *transpose*. It follows that

$$(A^T)^T = A \text{ and } (kA)^T = k(A)^T, \text{ for any scalar } k,$$

and that, for matrices A and B of appropriate sizes,

$$(A + B)^T = A^T + B^T \text{ and } (AB)^T = B^T A^T.$$

Trace of a square matrix

The *trace* $tr(A)$ of a square matrix A is the sum of the diagonal entries of A . In other words, the *trace* of the square matrix $A = (a_{ij})$ is defined as

$$tr(A) = \sum_{i=1}^n a_{ii}.$$

For matrices A and B of appropriate sizes,

$$tr(A + B) = tr(A) + tr(B) \text{ and } tr(AB) = tr(BA).$$

Convergence of a sequence of matrices

Let $A^{(1)}, A^{(2)}, A^{(3)}, \dots$ be a sequence of matrices in $\mathbb{R}^{m \times n}$. We say that the sequence of matrices *converges* to a matrix $A \in \mathbb{R}^{m \times n}$ if the sequence $A_{ij}^{(k)}$ of real numbers converges to A_{ij} for every pair $1 \leq i \leq m, 1 \leq j \leq n$, as k approaches infinity. That is, a sequence of matrices converges if the sequences given by each entry of matrix all converge.

2.2.3 Types of Matrices

A zero matrix.

A *zero matrix* O is a matrix in which each entry is 0; for matrices A and O of the same size, $A + O = O + A = A$.

An *all-1 matrix* J is a matrix in which each entry is 1.

For example, below we have

$$O_{2,3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ a zero matrix and } J_{2,3} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \text{ an all-1 matrix.}$$

A symmetric matrix.

A square matrix $A = (a_{ij})$ is *symmetric* if $A^T = A$ and *anti-symmetric* or *skew-symmetric* if $A^T = -A$

A **symmetric minor** of a square matrix A is a submatrix B obtaining by deleting some rows and the corresponding columns.

Diagonal matrix.

A *diagonal matrix* is a square matrix in which every non-diagonal entry is 0, and is denoted by $diag(a_{11}, a_{22}, \dots, a_{nn})$.

The *identity matrix* I is the diagonal matrix with 1s on its diagonal; for square matrices A and I of the same order, $AI = IA = A$.

A *permutation matrix* is a matrix obtained from I by permuting the rows or columns.

An **upper triangular matrix** is a square matrix in which every entry below and to the left of the diagonal is 0; a *lower triangular matrix* is defined similarly.

A circulant matrix

A *circulant matrix* $A = (a_{ij})$ is an $n \times n$ matrix in which each successive row is obtained by moving the preceding row by one position to the right; thus, for each i and j , $a_{ij} = a_{i+1, j+1}$, where the subscripts are taken modulo n .

Inverse of a matrix

A square matrix A is invertible if there is a matrix B for which $AB = BA = I$; the matrix B is

the *inverse* of A , denoted by A^{-1} . Note that $(A^{-1})^{-1} = A$, and that for square matrices A and B of the same order, $(AB)^{-1} = B^{-1}A^{-1}$.

Orthogonal matrix

An *orthogonal matrix* A is a symmetric matrix, where $A^{-1} = A^T$, where the columns are orthogonal, and have unit length.

2.2.4 The QR decomposition of a matrix

The *QR decomposition* of a matrix A is the representation of A as a product

$$A = QR$$

where Q is an orthogonal matrix and R is an upper triangular matrix with positive diagonal entries.

2.2.5 Quadratic forms

A *quadratic form* is an expression of the form $q(x) = x^T Ax$, where x is a column vector and A is a symmetric matrix; for example,

$$q(x) = 2x_1^2 + 3x_2^2 - 4x_3^2 + x_1x_2 - 6x_1x_3$$

is a quadratic form corresponding to the symmetric matrix

$$A = \begin{bmatrix} 2 & \frac{1}{2} & -3 \\ \frac{1}{2} & 3 & 0 \\ -3 & 0 & -4 \end{bmatrix}.$$

A quadratic form q is *positive definite* if $q(x) > 0$ and *positive semidefinite* if $q(x) \geq 0$, for every non-zero vector x .

2.3 Eigenvalues and Eigenvector

Eigenvalues and eigenvectors play an important part in the applications of linear algebra.

2.3.1 Definitions

Eigenvalues, Eigenvector and Spectrum

Let A be an $n \times n$ real matrix. An eigenvector of A is a vector such that Ax is parallel to x ; in other words, $Ax = \lambda x$ for some real or complex number λ . This number λ is called the eigenvalue of A belonging to eigenvector v . Clearly λ is an eigenvalue of the matrix A if and only if $\det(A - \lambda I) = 0$. This is an algebraic equation of degree n for λ , and hence has n roots (with multiplicity).

The *spectrum* of A , denoted by $\text{Spec}(A)$, is the set of eigenvalues of A .

If the matrix A is symmetric, then its eigenvalues and eigenvectors are particularly well behaved. All the eigenvalues are real. Furthermore, there is an orthogonal basis v_1, \dots, v_n of the space consisting of eigenvectors of A , so that the corresponding eigenvalues $\lambda_1, \dots, \lambda_n$ are precisely

the roots of $\det(A - \lambda I) = 0$. We may assume that $|v_1| = \dots = |v_n| = 1$; then A can be written as

$$A = \sum_{i=1}^n \lambda_i v_i v_i^T.$$

Another way of saying this is that every symmetric matrix can be written as $P^T D P$, where P is an orthogonal matrix and D is a diagonal matrix. The eigenvalues of A are just the diagonal entries of D .

Characteristic polynomial

If A is a square matrix, then the polynomial

$$P_A(\lambda) = \det(A - \lambda I)$$

is the *characteristic polynomial* of A and the equation

$$\det(A - \lambda I) = 0$$

is its *characteristic equation*. The roots of this equation are the *eigenvalues* of A ; a repeated root is a *multiple eigenvalue*, and a non-repeated root is a *simple eigenvalue*.

Trace of matrix

The *trace* of A is the sum of the eigenvalues of A , each taken with the same multiplicity as it occurs among the roots of the equation $\det(A - \lambda I) = 0$.

The $A(G)$ -coronal of a graph G

Let G be a graph on n vertices, and $A(G)$ its adjacency matrix. The matrix $xI - A(G)$ is invertible because $\det(xI - A(G)) = P_{A(G)}(x) \neq 0$. The $A(G)$ -*coronal*, $\Gamma_{A(G)}(x)$ of G is defined to be the sum of the entries of the matrix $(xI - A(G))^{-1}$. This can be calculated as

$$\Gamma_{A(G)}(x) = \mathbf{1}_n^T (xI - A(G))^{-1} \mathbf{1}_n$$

where $\mathbf{1}_n$ is a vector with all entries equal to 1 (see C. McLeman and E. McNicholas [63]).

2.3.2 Naive method of finding the eigenvalues

Procedure of finding the eigenvalues of the $n \times n$ matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

and their associated eigenvectors:

1. Solve for the real roots of the characteristic equation $f(\lambda) = \det(A - \lambda I) = 0$. These real roots $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of A .

2. Solve for the homogeneous system $(A - \lambda_i I)x = 0$, $i = 1, 2, \dots, n$. The nontrivial (nonzero) solutions are the eigenvectors associated with the eigenvalues λ_i .

Theorem 2.2.1 Let x_1, x_2, \dots, x_k be the eigenvectors of a $n \times n$ matrix A associated with distinct eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_k$, respectively, $k \leq n$. Then, x_1, x_2, \dots, x_k are linearly independent.

Corollary 2.2.1 If a $n \times n$ matrix A has n distinct eigenvalues, then A has n linearly independent eigenvectors.

Theorem 2.2.2 (Interlacing eigenvalues) Let A be an $n \times n$ symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, and B be an $(n - k) \times (n - k)$ symmetric minor of A with eigenvalues $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-k}$. Then

$$\lambda_i \leq \mu_i \leq \lambda_{i+k}.$$

2.3.3 Important properties

1. Suppose A is an $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ (including the repeats if there is any). Then:

- (i) $\det(A) = \prod_{i=1}^n \lambda_i = \lambda_1 \cdot \lambda_2 \cdot \dots \cdot \lambda_n$
(ii) $\text{tr}(A) = (\sum_{i=1}^n a_{ii}) = \lambda_1 + \lambda_2 + \dots + \lambda_n$

2. Suppose A is an $n \times n$ matrix with an eigenvalue λ and associated eigenvector x . Then:

- (i) A^{-1} (the inverse of A if it exists) has an eigenvalue $\frac{1}{\lambda}$ with associated eigenvector x .
(ii) the matrix $(A - kI)$ has an eigenvalue $(\lambda - k)$ and associated eigenvector x . Here k is any real number.

3. Let A be an $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$. Then:

- (i) $2A$ has eigenvalues $2\lambda_1, 2\lambda_2, \dots, 2\lambda_n$,
(ii) A^2 has eigenvalues $\lambda_1^2, \lambda_2^2, \dots, \lambda_n^2$.

4. *The Cayley-Hamilton Theorem.* If

$$P_A(\lambda) = \det(A - \lambda I) = \lambda^n + c_{n-1}\lambda^{n-1} + \dots + c_1\lambda + c_0$$

is the characteristic polynomial of A , then

$$P_A(A) = A^n + c_{n-1}A^{n-1} + \dots + c_1A + c_0I = 0.$$

2.3.4 Diagonalisation

An $n \times n$ matrix A is said to be diagonalizable if there is an invertible matrix P such that the result of the transformation $D = P^{-1}AP$ is a diagonal matrix. The product $D = P^{-1}AP$ is a diagonal matrix, and its nonzero entries are the eigenvalues of A . The matrix P is formed by eigenvectors of A .

2.3.5 Power of a matrix

If an $n \times n$ matrix A is diagonalizable then

$$A^k = PD^kP^{-1}.$$

Note that $D^k = \text{diag}(\lambda_1^k, \lambda_2^k, \dots, \lambda_n^k)$, with $\lambda_1, \lambda_2, \dots, \lambda_n$ the eigenvalues of A .

2.4 Semidefinite matrices

A square matrix A is called *positive semidefinite*, if it is symmetric and all of its eigenvalues are non-negative. This property is denoted by $A \succeq 0$. And a symmetric $n \times n$ matrix A is *positive definite*, we write $A \succ 0$, if all of its eigenvalues are positive.

Proposition 2.4.1 Let A be a real symmetric $n \times n$ matrix, the following are equivalent:

- (i) A is positive semidefinite;
- (ii) The quadratic form $x^T Ax$ is non-negative for every $x \in \mathbb{R}^n$;
- (iii) The determinant of every symmetric minor of A is non-negative.

Proposition 2.4.2 If two matrices A and B are positive semidefinite, then $\text{tr}(AB) \geq 0$, and $\text{tr}(AB) = 0$ iff $AB = 0$.

Proposition 2.4.3 A matrix A is positive semidefinite iff $AB \geq 0$ for every positive semidefinite matrix B .

2.5 Eigenvalues of Graphs

For a graph $G = (V, E)$ with n vertices, we define its eigenvalues as the eigenvalues of its adjacency matrix $A(G) = (a_{ij})_{i,j=1}^n$.

2.5.1 Theorem used for finding Eigenvalues

We apply the Lollipop theorem to find eigenvalues in general way of special graphs defined in chapter 1.

Theorem 2.5.1 (Lollipop Theorem) Let x_i be a vertex of degree one in the graph G on n vertices, and let x_j be the vertex adjacent to x_i . Let G_1 be the subgraph obtained from G by deleting the vertex x_i , and let G_2 be the subgraph obtained from G by deleting both vertices x_i and x_j . Then

$$P_{A(G)}(\lambda) = \lambda P_{A(G_1)}(\lambda) - P_{A(G_2)}(\lambda)$$

See Bian[8]

Proof Without loss of generality, let $i < j$, so row i comes before row j in

$$P_{A(G)}(\lambda) = \det(A(G) - \lambda I).$$

Then we have,

$$\begin{aligned} (A(G) - \lambda I)_{i,i} &= \lambda; \\ (A(G) - \lambda I)_{i,j} &= -1; \end{aligned}$$

$$(A(G) - \lambda I)_{i,j} = 0 \text{ for } 1 \leq k \leq n \text{ and } k \neq i \text{ and } k \neq j.$$

Expand the determinant of $(A(G) - \lambda I)$ along the i th row, where there are only two nonzero entries as defined above. Then,

$$P_{A(G)}(\lambda) = (-1)^{i+j} \lambda M_{i,i} + (-1)^{i+j} (-1) M_{i,j}$$

now,

$$M_{i,i} = \det(A(G_1) - \lambda I)$$

so,

$$P_{A(G)}(\lambda) = \lambda P_{A(G_1)}(\lambda) + (-1)^{i+j+1} M_{i,j}.$$

Now expand $M_{i,j}$ along the i th column, which only has one nonzero entry of -1 in the $(j-1)$ th row as x_i has degree one and is only adjacent to x_j . So,

$$\begin{aligned} P_{A(G)}(\lambda) &= \lambda P_{A(G_1)}(\lambda) + (-1)^{i+j+1} (-1)^{i+j-1} (-1) \det(A(G_2) - \lambda I) \\ &= \lambda P_{A(G_1)}(\lambda) - P_{A(G_2)}(\lambda) \end{aligned}$$

□

2.5.2 Eigenvalues of a graph which is the join of two graphs

1) Eigenvalues of a graph which is the join of two graphs whose adjacency matrices are both circulant matrices

The following theorem gives the eigenvalues and eigenvectors of a matrix which is the adjacency matrix of the join of two graphs, whose adjacency matrices are both circulant matrices.

Theorem 2.5.2 Let

$$U_k^T = (I\rho_{m,k}^1 \quad I\rho_{m,k}^2 \quad \dots \quad I\rho_{m,k}^{(m-1)})$$

and

$$V_j^T = (I\rho_{n,j}^1 \quad I\rho_{n,j}^2 \quad \dots \quad I\rho_{n,j}^{(n-1)})$$

where

$$\rho_{m,k} = e^{\frac{2\pi k}{m}} \text{ for } 1 \leq k \leq m-1 \text{ and } \rho_{n,j} = e^{\frac{2\pi j}{n}} \text{ for } 1 \leq j \leq n-1.$$

Let square matrices $A = (a_1, a_2, \dots, a_m)$ and $B = (b_1, b_2, \dots, b_n)$ be two circulant matrices. Then

1. $A \oplus B = \begin{bmatrix} A & J_{m,n} \\ (J_{m,n})^T & B \end{bmatrix}$
2. $CSET(A \oplus B) = \{W_1, W_2, \dots, W_{m+n}\}$ ($CSET(A \oplus B)$: Set of eigenvectors of $A \oplus B$)

where

$$W_k^T = (0_{1,m}, V_k^T) \text{ if } 1 \leq k \leq n-1;$$

$$W_{n+k}^T = (U_k^T, 0_{1,n}) \text{ if } 1 \leq k \leq m-1;$$

$$\{W_n^T, W_{n+m}^T\} = \{(J_{1,m}, \alpha J_{1,n}) \setminus n\alpha^2 + \alpha(d_A - d_B) - m = 0\}$$

where $d_A = a_1 + a_2 + \dots + a_m$ and $d_B = b_1 + b_2 + \dots + b_n$

3. The eigenvalues λ_k of $A \oplus B$ are given by:

$$\lambda_k = b_1 + b_2\rho_n^k + b_3\rho_n^{2k} + \cdots + b_n\rho_n^{(n-1)k} \text{ for } 1 \leq k \leq n-1;$$

$$\lambda_{k+n} = a_1 + a_2\rho_m^k + a_3\rho_m^{2k} + \cdots + a_m\rho_m^{(m-1)k} \text{ for } 1 \leq k \leq m-1;$$

$$\{\lambda_n, \lambda_{n+m}\} = \{n\alpha + d_A \setminus n\alpha^2 + \alpha(d_A - d_B) - m = 0\}$$

See Gross and Yellen[23], Lee and Yeh[31]

Proof To show that $W_k^T = (0_{1,m}, V_k^T)$ is not an eigenvector for $k = 0$, we let

$$C = A \oplus B = \begin{bmatrix} A & J_{m,n} \\ (J_{m,n})^T & B \end{bmatrix}$$

so that,

$$CW_0^T = \begin{bmatrix} A & J_{m,n} \\ (J_{m,n})^T & B \end{bmatrix} (0_{1,m}, V_0^T) = \begin{bmatrix} A & J_{m,n} \\ (J_{m,n})^T & B \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} m \\ m \\ \cdot \\ d_b \\ d_b \\ \cdot \\ d_b \end{bmatrix} = \lambda(0_{1,m}, V_0^T) = \lambda \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 1 \end{bmatrix},$$

which means $m = 0$ is impossible. Therefore $W_k^T = (0_{1,m}, V_k^T)$ is not an eigenvector for $k = 0$.

To show that

$$W_j^T = (0_{1,j}, V_j^T) = (000 \cdots 001\rho_{n,j}^1 \ \rho_{n,j}^2 \cdots \rho_{n,j}^{(n-1)})^T; 1 \leq j \leq n-1$$

is an eigenvector of C , consider:

$$CW_j^T = \begin{bmatrix} A & J_{m,n} \\ (J_{m,n})^T & B \end{bmatrix} (000 \cdots 001\rho_{n,j}^1 \ \rho_{n,j}^2 \cdots \rho_{n,j}^{(n-1)})^T.$$

The first m rows look like:

$$\sum_{k=0}^{n-1} \rho_{n,j}^k \sum_{k=0}^{n-1} \rho_{n,j}^k \cdots \sum_{k=0}^{n-1} \rho_{n,j}^k.$$

Then, from Corollary 2.1.1 of Jessop's thesis (see[28]),

$$\sum_{k=0}^{n-1} \rho_{n,j}^k = 0, \text{ so the first } m \text{ rows of } CW_j^T \text{ are } 0.$$

The next n rows look like:

$$b_1 + b_2\rho_{n,j}^1 + b_3\rho_{n,j}^2 + \cdots + b_n\rho_{n,j}^{(n-1)}; 1 \leq j \leq n-1$$

which, from Theorem 2.1.1 of Jessop's thesis (see[28]), is the eigenvalue corresponding to eigenvector

$$(1, \rho_{n,j}^1, \rho_{n,j}^2, \dots, \rho_{n,j}^{(n-1)}); \text{ for } 1 \leq j \leq n-1.$$

Thus we have proved that

$$W_j^T = (0_{1,m}, V_j^T) = (000 \dots 001\rho_{n,j}^1 \rho_{n,j}^2 \dots \rho_{n,j}^{(n-1)})^T; \text{ for } 1 \leq j \leq n-1$$

is an eigenvector of $C = A \oplus B$.

Applying the same method, we can show that $W_{n+j}^T = (U_j^T, 0_{1,n})$ for $1 \leq j \leq m-1$ are eigenvectors of $C = A \oplus B$.

To determine the first set of eigenvalues of $A \oplus B$, we set $\underline{v} = (0_{1,m}, \underline{x}^T)^T$ where $\underline{x}^T = (x_1, x_2, \dots, x_n)$ and solve for $(A \oplus B)\underline{v} = \lambda\underline{v}$. We specifically select \underline{v} to be of this form as we understand the join of subgraphs A and B , and this vector isolates the edges in B .

Solving $(A \oplus B)\underline{v} = \lambda\underline{v}$, we get

$$\begin{bmatrix} A_{m,m} & J_{m,n} \\ (J_{m,n})^T & B_{n,n} \end{bmatrix} \begin{bmatrix} 0_{m,1} \\ \underline{x}_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} 0_{m,1} \\ \underline{x}_{n,1} \end{bmatrix} \Rightarrow \begin{bmatrix} J_{m,n}\underline{x}_{n,1} \\ B_{n,n}\underline{x}_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} 0_{m,1} \\ \underline{x}_{n,1} \end{bmatrix}.$$

Solving $B\underline{x} = \lambda\underline{x}$, we get eigenvalues of B , which are, as per Theorem 2.1.1 of Jessop's thesis (see[28])

$$\lambda_k = b_1 + b_2\rho_j + b_3\rho_j^2 + \dots + b_m\rho_j^{n-1}; 1 \leq k \leq n-1.$$

To determine the next set of eigenvalues of $A \oplus B$, we set $\underline{v} = (\underline{x}^T, 0_{1,n})^T$ where $\underline{x}^T = (x_1, x_2, \dots, x_n)$ and solve for $(A \oplus B)\underline{v} = \lambda\underline{v}$. We specifically select \underline{v} to be of this form as we understand the join of subgraphs A and B , and this vector isolates the edges in A .

Solving $(A \oplus B)\underline{v} = \lambda\underline{v}$, we get

$$\begin{bmatrix} A_{m,m} & J_{m,n} \\ (J_{m,n})^T & B_{n,n} \end{bmatrix} \begin{bmatrix} \underline{x}_{m,1} \\ 0_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} \underline{x}_{m,1} \\ 0_{n,1} \end{bmatrix} \Rightarrow \begin{bmatrix} A_{m,m}\underline{x}_{m,1} \\ (J_{m,n})^T\underline{x}_{m,1} \end{bmatrix} = \lambda \begin{bmatrix} \underline{x}_{m,1} \\ 0_{n,1} \end{bmatrix}.$$

Solving $A\underline{x} = \lambda\underline{x}$, we get eigenvalues of A , which are, as per Theorem 2.1.1 of Jessop's thesis(see[28])

$$\lambda_{n+k} = a_1 + a_2\rho_j + a_3\rho_j^2 + \dots + a_m\rho_j^{m-1}; 1 \leq k \leq m-1.$$

To find the eigenvalues λ_n and λ_{n+m} of $A \oplus B$, we solve $(A \oplus B)\underline{v} = \lambda\underline{v}$, where $\underline{v} = (J_{1,m}, \alpha J_{1,n})^T$. The edges between the two graphs A and B , which form the join between the subgraphs, are significant in the determining of the conjugate eigen-pair of the adjacency matrix of the resultant graph. We use the factor of α in the vector \underline{v} to assist in obtaining the conjugate eigenvalues as follows:

$$\begin{bmatrix} A_{m,m} & J_{m,n} \\ (J_{m,n})^T & B_{n,n} \end{bmatrix} \begin{bmatrix} J_{m,1} \\ \alpha_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} J_{m,1} \\ \alpha_{n,1} \end{bmatrix} \Rightarrow \begin{bmatrix} (d_A + n\alpha)_{m,1} \\ (m + \alpha d_B)_{n,1} \end{bmatrix} = \lambda \begin{bmatrix} J_{m,1} \\ \alpha J_{n,1} \end{bmatrix}.$$

$$d_A + n\alpha = \lambda$$

$$m + \alpha d_B = \lambda\alpha.$$

Therefore,

$$m + \alpha d_B = (d_A + n\alpha)\alpha \Rightarrow n\alpha^2 + \alpha(d_A - d_B) - m = 0 \Rightarrow \alpha = \frac{-(d_A - d_B) \pm \sqrt{(d_A - d_B)^2 + 4nm}}{2n}$$

So, the conjugate pair of eigenvalues are

$$\lambda = n \left(\frac{-(d_A - d_B) \pm \sqrt{(d_A - d_B)^2 + 4nm}}{2n} \right) + d_A \quad \square$$

2) Eigenvalues of a graph which is the join of two regular graphs

Theorem 2.5.3. (see R. P. Varghese and K. R. Kumar [64])

Let G_i be a k_i -regular graph on n_i vertices and m_i edges, for $i = 1, 2$. Then the spectrum of $G_1 \diamond G_2$ consists of

- (i) $\lambda_j(G_2)$, for $j = 2, \dots, n_2$;
- (ii) $\frac{\lambda_j(G_1) \pm \sqrt{(\lambda_j(G_1) + 2)^2 + 4(k_1 - 1)}}$, for $j = 2, \dots, n_1$;
- (iii) 0 (with multiplicity $(m_1 - n_1)$);
- (iv) Three roots of the equation $x^3 - (k_1 + k_2)x^2 + (k_1k_2 - 2k_1 - n_1n_2)x + 2k_1k_2 = 0$.

Proof. We just have to prove that

$$P_{A(G_1 \diamond G_2)}(x) = P_{A(G_2)}(x)x^{m_1 - n_1}(x^2 - k_1x - 2k_1 - n_1x\Gamma_{A(G_2)}(x)) \prod_{i=2}^{n_1} (x^2 - \lambda_i x - (\lambda_i + k_1))$$

where,

$$\Gamma_{A(G_2)}(x) = 1_n^T (xI - A(G_2))^{-1} 1_n$$

is the $A(G_2)$ -coronal of G_2 (see section 2.3.1).

In fact, the adjacency matrix $A = A(G_1 \diamond G_2)$ of $G_1 \diamond G_2$ can be written (by a proper labeling of vertices) as

$$A = \begin{bmatrix} A_1 & R & J_{n_1 \times n_2} \\ R^T & O_{m_1} & O_{m_1 \times n_2} \\ J_{n_2 \times n_1} & O_{n_2 \times n_1} & A_2 \end{bmatrix}$$

where $A_1 = A(G_1)$ and $A_2 = A(G_2)$ are the adjacency matrix of G_1 and G_2 respectively, and R is the incidence matrix of G_1 .

The characteristic polynomial of $G_1 \diamond G_2$ is

$$\begin{aligned} P_{A(G_1 \diamond G_2)}(x) &= \begin{vmatrix} xI_{n_1} - A_1 & -R & -J_{n_1 \times n_2} \\ -R^T & xI_{m_1} & O_{m_1 \times n_2} \\ -J_{n_2 \times n_1} & O_{n_2 \times n_1} & xI_{n_2} - A_2 \end{vmatrix} \\ &= \det(xI_{n_2} - A_2) \det(S) \end{aligned}$$

where

$$\begin{aligned} S &= \begin{bmatrix} xI_{n_1} - A_1 & -R \\ -R^T & xI_{m_1} \end{bmatrix} - \begin{bmatrix} -J_{n_1 \times n_2} \\ O \end{bmatrix} (xI_{n_2} - A_2)^{-1} \begin{bmatrix} -J_{n_2 \times n_1} & O \end{bmatrix} \\ &= \begin{bmatrix} xI_{n_1} - A_1 & -R \\ -R^T & xI_{m_1} \end{bmatrix} - \begin{bmatrix} \Gamma_{A_2}(x) J_{n_1 \times n_1} & O \\ O & O \end{bmatrix} \\ &= \begin{bmatrix} xI_{n_1} - A_1 - \Gamma_{A_2}(x) J_{n_1 \times n_1} & -R \\ -R^T & xI_{m_1} \end{bmatrix}; \end{aligned}$$

So, the determinant of S is

$$\begin{aligned}
\det(S) &= \det(xI_{m_1})\det(xI_{n_1} - A_1 - \Gamma_{A_2}(x)J_{n_1 \times n_1} - R(xI_{m_1})^{-1}R^T) \\
&= x^{m_1}\det\left(xI_{n_1} - A_1 - \Gamma_{A_2}(x)J - \frac{RR^T}{x}\right) \\
&= x^{m_1}\det\left(xI_{n_1} - \left(A_1 + \frac{RR^T}{x}\right) - \Gamma_{A_2}(x)J\right) \\
&= x^{m_1}\det\left(xI_{n_1} - \left(A_1 + \frac{RR^T}{x}\right)\right)(1 - \Gamma_{A_2}(x)\Gamma_{A_1 + \frac{RR^T}{x}}(x))
\end{aligned}$$

G_1 is k_1 -regular and the row sum of RR^T is $2k_1$. Row sum of $A_1 + \frac{RR^T}{x}$ is $k_1 + \frac{2k_1}{x}$;

$$\Gamma_{A_1 + \frac{RR^T}{x}}(x) = \frac{n_1}{x - k_1 - \frac{2k_1}{x}} = \frac{xn_1}{x^2 - xk_1 - 2k_1}.$$

So,

$$\begin{aligned}
\det(S) &= x^{m_1}\det\left(xI_{n_1} - A_1 - \frac{A_1 + k_1I_{n_1}}{x}\right)(1 - \Gamma_{A_2}(x)\frac{xn_1}{x^2 - xk_1 - 2k_1}) \\
&= x^{m_1-n_1}\det(x^2I_{n_1} - xA_1 - A_1 - k_1I_{n_1})\left(\frac{x^2 - xk_1 - 2k_1 - xn_1\Gamma_{A_2}(x)}{x^2 - xk_1 - 2k_1}\right) \\
&= x^{m_1-n_1}\left(\frac{x^2 - xk_1 - 2k_1 - xn_1\Gamma_{A_2}(x)}{x^2 - xk_1 - 2k_1}\right)\prod_{i=1}^{n_1}(x^2 - \lambda_i x - (\lambda_i + k_1)).
\end{aligned}$$

Using the property that $\lambda_i(G_1) = k_1$; Then,

$$\det(S) = x^{m_1-n_1}(x^2 - k_1x - 2k_1 - n_1x\Gamma_{A_2}(x))\prod_{i=1}^{n_1}(x^2 - \lambda_i x - (\lambda_i + k_1)).$$

Finally, we get

$$P_{A(G_1 \diamond G_2)}(x) = P_{A(G_2)}(x)x^{m_1-n_1}(x^2 - k_1x - 2k_1 - n_1x\Gamma_{A(G_2)}(x))\prod_{i=2}^{n_1}(x^2 - \lambda_i x - (\lambda_i + k_1)). \quad \square$$

2.5.3 Eigenvalues of Complete Graphs

Generally, the complete graph K_n has an adjacency matrix $A(K_n)$ which is given bellow as

$$A(K_n) = (a_{ij}) = \begin{bmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 0 \end{bmatrix}.$$

where $a_{ij} = 1$ when $i \neq j$; $a_{ij} = 0$ when $i = j$.

lemma 2.5.1 Let H_n be the $n \times n$ matrix, with $n \geq 2$, such that

$$H_n = \begin{bmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{bmatrix}_{n \times n}, \text{ then } \det(H_n) \equiv \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix} = (-1)(\lambda+1)^{n-1}.$$

Proof By induction, assume

$$P_n = \begin{bmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{bmatrix}_{n \times n}, \text{ then}$$

$$\text{For } n = 2, H_2 = \begin{bmatrix} -1 & -1 \\ -1 & \lambda \end{bmatrix} \Rightarrow \det(H_2) \equiv \begin{vmatrix} -1 & -1 \\ -1 & \lambda \end{vmatrix} = -\lambda - 1 = (-1)(\lambda + 1)^1$$

$$\text{For } n = 3, H_3 = \begin{bmatrix} -1 & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{bmatrix} \text{ and,}$$

$$\begin{aligned} \det(H_3) &\equiv \begin{vmatrix} -1 & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{vmatrix} = - \begin{vmatrix} \lambda & -1 \\ -1 & \lambda \end{vmatrix} + \begin{vmatrix} -1 & -1 \\ -1 & \lambda \end{vmatrix} - \begin{vmatrix} -1 & \lambda \\ -1 & -1 \end{vmatrix} \\ &= - \begin{vmatrix} \lambda & -1 \\ -1 & \lambda \end{vmatrix} + \begin{vmatrix} -1 & -1 \\ -1 & \lambda \end{vmatrix} + \begin{vmatrix} -1 & -1 \\ -1 & \lambda \end{vmatrix} \\ &= - \begin{vmatrix} \lambda & -1 \\ -1 & \lambda \end{vmatrix} + 2 \begin{vmatrix} -1 & -1 \\ -1 & \lambda \end{vmatrix} = -\det(P_2) + 2\det(H_2) \\ &= -1(\lambda^2 - 1) + 2(-\lambda - 1) \\ &= (-1)(\lambda + 1)^2 \end{aligned}$$

For $n = 4$, $H_4 = \begin{bmatrix} -1 & -1 & -1 & -1 \\ -1 & \lambda & -1 & -1 \\ -1 & -1 & \lambda & -1 \\ -1 & -1 & -1 & \lambda \end{bmatrix}$ and,

$$\begin{aligned} \det(H_4) &\equiv \begin{vmatrix} -1 & -1 & -1 & -1 \\ -1 & \lambda & -1 & -1 \\ -1 & -1 & \lambda & -1 \\ -1 & -1 & -1 & \lambda \end{vmatrix} = - \begin{vmatrix} \lambda & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{vmatrix} + 3 \begin{vmatrix} -1 & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{vmatrix} = -\det(P_3) + 3\det(H_3) \\ &= -(\lambda\det(P_2) + 2\det(H_2)) + 3\det(H_3) \\ &= -(\lambda(\lambda^2 - 1) - 2(\lambda + 1)) - 3(\lambda + 1)^2 \\ &= -(\lambda(\lambda^2 - 1) - 2(\lambda + 1) + 3(\lambda + 1)^2) \\ &= -(\lambda + 1)(\lambda^2 + 2\lambda + 1) \\ &= -(\lambda + 1)(\lambda + 1)^2 \\ &= (-1)(\lambda + 1)^3 \end{aligned}$$

Assume the hypothesis it is true for $n = k$, i.e. $\det(H_k) = (-1)(\lambda + 1)^{k-1}$.

Then, for $n = k + 1$, we have,

$$H_{k+1} = \begin{bmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{bmatrix}_{(k+1) \times (k+1)}$$

and then, expanding along the first row,

$$\begin{aligned} \det(H_{k+1}) &\equiv \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{(k+1) \times (k+1)} \\ &= (-1) \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{k \times k} + (-1)(-1)[(k+1) - 1] \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{k \times k} \end{aligned}$$

The first term is obtained from the expansion of the first column (in the first row) and the second term is from the the $[(k+1) - 1]$ identical terms obtained from the expansion of the second to $[(k+1) - 1]th$ columns.

$$\text{Let } P_k = \lambda I - A(K_k) = \begin{bmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{bmatrix}_{k \times k} \quad \text{and } H_k = \begin{bmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{bmatrix}_{k \times k}.$$

Then,

$$\begin{aligned} \det(H_{k+1}) &= -\det(P_k) + k\det(H_k) \\ &= -[\lambda\det(P_{k-1}) + (k-1)\det(H_{k-1})] + k\det(H_k) \\ &= -[\lambda^2\det(P_{k-2}) + \lambda(k-2)\det(H_{k-2}) + (k-1)\det(H_{k-1})] + k\det(H_k) \\ &= -[\lambda^3\det(P_{k-3}) + \lambda^2(k-3)\det(H_{k-3}) + \lambda(k-2)\det(H_{k-2}) + (k-1)\det(H_{k-1})] + k\det(H_k) \end{aligned}$$

Now, the leading λ must have power $(k-2)$ so that we get $\det(P_{k-(k-2)})$ and $\det(H_{k-(k-2)})$ which are both known. so, continuing,

$$\begin{aligned} \det(H_{k+1}) &= -[\lambda^{k-2}\det(P_{k-(k-2)}) + \lambda^{k-3}2\det(H_2) + \lambda^{k-4}3\det(H_3) + \lambda^{k-5}4\det(H_4) + \cdots \\ &\quad \cdots + \lambda^2(k-3)\det(H_{k-3}) + \lambda(k-2)\det(H_{k-2}) + (k-1)\det(H_{k-1})] + k\det(H_k) \end{aligned}$$

Substituting $\det(P_2) = \lambda^2 - 1 = (\lambda + 1)(\lambda - 1)$ and $\det(H_k) = -(\lambda + 1)^{k-1}$ for all $k \leq n$, we get

$$\begin{aligned} \det(H_{k+1}) &= -[\lambda^{k-2}(\lambda + 1)(\lambda - 1) - \lambda^{k-3}2(\lambda + 1) - \lambda^{k-4}3(\lambda + 1)^2 - \lambda^{k-5}4(\lambda + 1)^3 + \cdots \\ &\quad \cdots - \lambda^2(k-3)(\lambda + 1)^{k-4} - \lambda(k-2)(\lambda + 1)^{k-3} - (k-1)(\lambda + 1)^{k-2}] - k(\lambda + 1)^{k-1} \end{aligned}$$

Factorizing $(\lambda + 1)$ out of the k terms in the square brackets, we get

$$\begin{aligned} \det(H_{k+1}) &= -(\lambda + 1)[(\lambda^{k-2}(\lambda - 1) - \lambda^{k-3}2 - \lambda^{k-4}3(\lambda + 1) - \lambda^{k-5}4(\lambda + 1)^2 + \cdots \\ &\quad \cdots - \lambda^2(k-3)(\lambda + 1)^{k-5} - \lambda(k-2)(\lambda + 1)^{k-4} - (k-1)(\lambda + 1)^{k-3}] - k(\lambda + 1)^{k-1} \end{aligned}$$

Working with the first two terms in square brackets, we get

$$\begin{aligned}
\det(H_{k+1}) &= -(\lambda + 1)[(\lambda^{k-3}(\lambda^2 - \lambda) - \lambda^{k-3}2 - \lambda^{k-4}3(\lambda + 1)^1 - \lambda^{k-5}4(\lambda + 1)^2 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-5} - \lambda(k-2)(\lambda + 1)^{k-4} - (k-1)(\lambda + 1)^{k-3}] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)[(\lambda^{k-3}(\lambda^2 - \lambda - 2) - \lambda^{k-4}3(\lambda + 1)^1 - \lambda^{k-5}4(\lambda + 1)^2 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-5} - \lambda(k-2)(\lambda + 1)^{k-4} - (k-1)(\lambda + 1)^{k-3}] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)[(\lambda^{k-3}(\lambda + 1)(\lambda - 2) - \lambda^{k-4}3(\lambda + 1)^1 - \lambda^{k-5}4(\lambda + 1)^2 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-5} - \lambda(k-2)(\lambda + 1)^{k-4} - (k-1)(\lambda + 1)^{k-3}] - k(\lambda + 1)^{k-1}
\end{aligned}$$

Taking out the next factor of $(\lambda + 1)$ from inside the square brackets, we get

$$\begin{aligned}
\det(H_{k+1}) &= -(\lambda + 1)^2[(\lambda^{k-3}(\lambda - 2) - \lambda^{k-4}3 - \lambda^{k-5}4(\lambda + 1)^1 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-6} - \lambda(k-2)(\lambda + 1)^{k-5} - (k-1)(\lambda + 1)^{k-4}] - k(\lambda + 1)^{k-1}
\end{aligned}$$

Working with the first two terms in square brackets, we get (*)

$$\begin{aligned}
\det(H_{k+1}) &= -(\lambda + 1)^2[(\lambda^{k-4}(\lambda^2 - 2\lambda) - \lambda^{k-4}3 - \lambda^{k-5}4(\lambda + 1)^1 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-6} - \lambda(k-2)(\lambda + 1)^{k-5} - (k-1)(\lambda + 1)^{k-4}] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^2[(\lambda^{k-4}(\lambda^2 - 2\lambda - 3) - \lambda^{k-5}4(\lambda + 1)^1 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-6} - \lambda(k-2)(\lambda + 1)^{k-5} - (k-1)(\lambda + 1)^{k-4}] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^2[(\lambda^{k-4}(\lambda + 1)(\lambda - 3) - \lambda^{k-5}4(\lambda + 1)^1 + \dots \\
&\quad \dots - \lambda^2(k-3)(\lambda + 1)^{k-6} - \lambda(k-2)(\lambda + 1)^{k-5} - (k-1)(\lambda + 1)^{k-4}] - k(\lambda + 1)^{k-1}
\end{aligned}$$

Note that the first term in the square brackets comprises of $(\lambda + 1)\lambda^{k-t}(\lambda - (t - 1))$.

We do the step (*) above a total of $(k - 3)$ times, tacking out the factor $(\lambda + 1)^{k-3}$ to get

$$\det(H_{k+1}) = -(\lambda + 1)^{k-3}[\lambda(\lambda + 1)(\lambda - (k - 2)) - (k - 1)(\lambda + 1)] - k(\lambda + 1)^{k-1}$$

Note that the power of λ in the first term in the square brackets is $(k - 2) - (k - 3) = 1$ and the power of $(\lambda + 1)$ in the second term in the square brackets is also $(k - 2) - (k - 3) = 1$.

Simplifying, we get

$$\begin{aligned}
\det(H_{k+1}) &= -(\lambda + 1)^{k-3}[(\lambda + 1)(\lambda^2 - \lambda(k - 2) - (k - 1))] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^{k-2}[(\lambda^2 - \lambda(k - 2) - (k - 1))] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^{k-2}[(\lambda - 1)(\lambda - (k - 1))] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^{k-1}[(\lambda - (k - 1))] - k(\lambda + 1)^{k-1} \\
&= -(\lambda + 1)^{k-1}[(\lambda - (k - 1)) - k] \\
&= -(\lambda + 1)^{k-1}[(\lambda + 1)] \\
&= -(\lambda + k)^k
\end{aligned}$$

This concludes the proof, by induction, that

$$\det(H_n) = (-1)(\lambda + 1)^{n-1}, \text{ for all } n \geq 2. \quad \square$$

Theorem 2.5.4 Any complete graph K_n has the eigenvalues $(n - 1)$, with multiplicity 1, and -1 , with multiplicity $(n - 1)$. Hence

$$P_{A(K_n)}(\lambda) \equiv \det(\lambda I - A(K_n)) = (\lambda - (n - 1))(\lambda + 1)^{n-1}.$$

Proof By induction,

$$\text{Let } A(K_n) = \begin{bmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 0 \end{bmatrix}_{n \times n} \quad \text{be the adjacency matrix of the complete graph } K_n$$

For $n = 2$,

$$A(K_2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\begin{aligned}
\det(\lambda I - A(K_2)) &= \begin{vmatrix} \lambda & -1 \\ -1 & \lambda \end{vmatrix} \\
&= \lambda^2 - 1 \\
&= (\lambda + 1)(\lambda - 1)
\end{aligned}$$

Note that the eigenvalues of $A(K_2)$ are $\lambda = -1$ (multiplicity $(2 - 1) = 1$) and $\lambda = (2 - 1) = 1$ (multiplicity 1).

Assume the hypothesis it true for $n = k$, i.e.,

$$\det(\lambda I - A(K_k)) = \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{k \times k}$$

$$= (\lambda + 1)^{k-1}(\lambda - (k - 1))$$

i.e., $\lambda = -1$, (multiplicity $(k - 1)$), and $\lambda = (k - 1)$ (multiplicity 1)

Then, for $n = k + 1$,

$$\det(\lambda I - A(K_{k+1})) = \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{(k+1) \times (k+1)}$$

$$= \lambda \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{k \times k} + k \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & -1 & \cdots & -1 \\ -1 & -1 & \lambda & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \lambda \end{vmatrix}_{k \times k}$$

$$= \lambda \det(\lambda I - A(K_k)) + k \det(H_k)$$

Now applying the inductive hypothesis for $\det(\lambda I - A(K_k))$, and Lemma 2.5.1 for $\det(H_k)$, we get

$$\begin{aligned} \det(\lambda I - A(K_{k+1})) &= \lambda(\lambda + 1)^{k-1}(\lambda - (k - 1)) + k(-1)(\lambda + 1)^{k-1} \\ &= (\lambda + 1)^{k-1}(\lambda^2 - \lambda(k - 1) - k) \\ &= (\lambda + 1)^{k-1}(\lambda + 1)(\lambda - k) \\ &= (\lambda + 1)^k(\lambda - k) \end{aligned}$$

i.e., $\lambda = -1$ (multiplicity $(k + 1) - 1$) and $\lambda = (k + 1) - 1$ (multiplicity 1).

so we have proved that $\lambda = -1$ (multiplicity $(n - 1)$), and $\lambda = n - 1$ (multiplicity 1), are the eigenvalues of the adjacency matrix of the complete graph $A(K_n)$. And the characteristic polynomial is $P_{A(K_n)}(\lambda) = (\lambda + 1)^{n-1}(\lambda - (n - 1))$. \square

2.5.4 Eigenvalues of Complete Bipartite Graphs

Let $K_{m,n}$ be the complete bipartite graph on $(m+n)$ vertices, with partition (V_1, V_2) , where $|V_1| = m$ and $|V_2| = n$.

Theorem 2.5.5 The eigenvalues of $K_{m,n}$ are 0 (with multiplicity $(m+n-2)$), $+\sqrt{mn}$ (with multiplicity 1), and $-\sqrt{mn}$ (with multiplicity 1). Hence

$$P_{A(K_{m,n})}(\lambda) = \lambda^{m+n-2}(\lambda - \sqrt{mn})(\lambda + \sqrt{mn}).$$

Proof

The adjacency matrix of $K_{m,n}$ can be written as the block matrix

$$A(K_{m,n}) = \begin{bmatrix} O_{m,m} & J_{m,n} \\ (J_{m,n})^T & O_{n,n} \end{bmatrix}$$

This matrix has rank 2, since the first m rows are the same, the last n rows are the same, and the first and the last rows are linearly independent. Thus $K_{m,n}$ has nullity $(m+n-2)$, and hence has eigenvalues 0 with multiplicity $m+n-2$. See Anton[4].

Now let $\underline{v} \in \mathbb{R}^{m+n}$ be the vector whose first m entries are x and last n entries are y , i.e., $\underline{v} = (x, x, \dots, x, y, y, \dots, y)$ with x occurring m times, and y occurring n times. The edges jointing the two partitions of the bipartite graph are significant in determining the eigenvalues, and suggest the splitting of the eigenvector into two parts relating to the bipartition. this definition of \underline{v} facilitates finding the eigenvalues as follows

$A(K_{m,n})\underline{v} = \begin{bmatrix} O_{m,m} & J_{m,n} \\ (J_{m,n})^T & O_{n,n} \end{bmatrix} \underline{v} = (ny, ny, \dots, ny, mx, mx, \dots, mx)$ with ny occurring x times, and mx occurring n times. To get eigenvalues, we solve $A\underline{v} = \lambda\underline{v}$. so,

$$(ny, \dots, ny, mx, \dots, mx) = \lambda(x, \dots, x, y, \dots, y) = (\lambda x, \dots, \lambda x, \lambda y, \dots, \lambda y)$$

whit λx occurring m times, and λy occurring n times.

Therefore $ny = \lambda x$ and $mx = \lambda y$. So,

$$n \left(\frac{mx}{\lambda} \right) = \lambda x \Rightarrow \lambda^2 = mn \Rightarrow \lambda = \pm\sqrt{mn}.$$

Hence the eigenvalues of $A(K_{m,n})$ are 0 (multiplicity $m+n-2$), \sqrt{mn} (multiplicity 1) and $-\sqrt{mn}$ (multiplicity 1); And

$$P_{A(K_{m,n})}(\lambda) = \lambda^{m+n-2}(\lambda - \sqrt{mn})(\lambda + \sqrt{mn})$$

is the characteristic polynomial of $A(K_{m,n})$. □

2.5.5 Eigenvalues of star Graphs

Theorem 2.5.6 The eigenvalues of the star graph with $m = n-1$ rays of length 1 on n vertices, denoted $S_{n-1,1}$, are: 0 (with multiplicity $n-2$), $\sqrt{n-1}$ (with multiplicity 1) and $-\sqrt{n-1}$ (with multiplicity 1). Hence

$$P_{A(S_{m,1})}(\lambda) = \lambda^{n-2}(\lambda - \sqrt{n-1})(\lambda + \sqrt{n-1})$$

is the characteristic polynomial of the adjacency matrix of the star graph $S_{n-1, 1}$.

Proof By induction.

The theorem is true for a star graph with rays of length 1 on 2 and 3 vertices (See[25]).

Assume

$$\det(\lambda I - A_{S_{(n-1)}}) = \lambda^{n-3}(\lambda^2 - (n-2))$$

where $\lambda^{n-3}(\lambda^2 - (n-2))$ is the characteristic polynomial of a star graph on $n-1$ vertices. The characteristic polynomial of the star graph of rays of length 1 on n vertices is

$$\det(\lambda I - A_{S_n}) = \begin{vmatrix} \lambda & -1 & -1 & -1 & \cdots & -1 \\ -1 & \lambda & 0 & 0 & \cdots & 0 \\ -1 & 0 & \lambda & 0 & \cdots & 0 \\ -1 & 0 & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & \cdots & \lambda \end{vmatrix}.$$

Using cofactor expansion along the second row, we have the determinant as:

$$\begin{aligned} \det(\lambda I - A_{S_{(n-1)}}) &= M_{21} + \lambda M_{22} \\ &= \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ 0 & \lambda & 0 & \cdots & 0 \\ 0 & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda \end{vmatrix} + \lambda \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & 0 & \cdots & 0 \\ -1 & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \cdots & \lambda \end{vmatrix} \end{aligned}$$

It is obvious that M_{22} is the determinant of the matrix $(\lambda I - A_{S_{(n-1)}})$. Now let M_{21} be B . Then,

$$B = \begin{vmatrix} -1 & -1 & -1 & \cdots & -1 \\ 0 & \lambda & 0 & \cdots & 0 \\ 0 & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda \end{vmatrix}$$

Using cofactor expansion of B along the first column, we get

$$B = (-1)M_{11} = (-1) \begin{vmatrix} \lambda & 0 & \cdots & 0 \\ 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda \end{vmatrix}.$$

But $M_{11} = \det(\lambda I_{n-2})$, where I_{n-2} is the $n-2$ identity matrix. Therefore, $B = -\lambda^{n-2}$ and

$$\begin{aligned} \det(\lambda I - A_{S_n}) &= -(-1)(-\lambda^{n-2}) + \lambda \det(\lambda I - A_{S_{(n-1)}}) \\ &= \lambda \det(\lambda I - A_{S_{(n-1)}}) - \lambda^{n-2}. \end{aligned}$$

Using the inductive hypothesis, we have

$$\begin{aligned}
\det(\lambda I - A_{S_n}) &= \lambda(\lambda^{n-3}(\lambda^2 - (n-2))) - \lambda^{n-2} \\
&= \lambda^{n-2}(\lambda^2 - (n-2)) - \lambda^{n-2} \\
&= \lambda^{n-2}(\lambda^2 - (n-2) - 1) \\
&= \lambda^{n-2}(\lambda^2 - n + 1) \\
&= \lambda^{n-2}(\lambda^2 - (n-1))
\end{aligned}$$

Now, let

$$\begin{aligned}
\det(\lambda I - A_{S_n}) = 0 &\Rightarrow \lambda^{n-2}(\lambda^2 - (n-1)) = 0 \\
&\Rightarrow \lambda^{n-2} = 0 \text{ or } \lambda^2 - (n-1) = 0 \\
&\Rightarrow \lambda = 0 \text{ (multiplicity } n-2) \text{ or } \lambda = \pm\sqrt{n-1}
\end{aligned}$$

Thus by induction the eigenvalues of a star graph of rays of length 1 on n vertices are: $\lambda = 0$ (multiplicity $n-2$), $\lambda = \sqrt{n-1}$ (multiplicity 1) and $\lambda = -\sqrt{n-1}$ (multiplicity 1). \square

Theorem 2.5.7 The eigenvalues of the star graph $S_{m,2}$ with $m = \frac{n-1}{2}$ rays of length 2 on n vertices are: 1 and -1 , each of multiplicity $m-1 = \frac{n-3}{2}$, one eigenvalue 0, and two eigenvalues

$$\lambda = \pm\sqrt{m+1} = \pm\sqrt{\frac{n+1}{2}}.$$

Hence

$$P_{A(S_{m,2})}(\lambda) = \lambda(\lambda-1)^{\frac{n-3}{2}}(\lambda+1)^{\frac{n-3}{2}}\left(\lambda - \sqrt{\frac{n+1}{2}}\right)\left(\lambda + \sqrt{\frac{n+1}{2}}\right)$$

is the characteristic polynomial of the adjacency matrix of the star graph $S_{\frac{n-1}{2}, 2}$.

Proof

The adjacency matrix of a star graph $S_{m,2}$ with $m = \frac{n-1}{2}$ rays of length 2 on n vertices is

$$A(S_{m,2}) = \begin{bmatrix} O_{1,1} & J_{1,m} & O_{1,m} \\ J_{m,1} & O_{m,m} & I_{m,m} \\ O_{m,1} & I_{m,m} & O_{m,m} \end{bmatrix}_{(2m+1) \times (2m+1)}.$$

The characteristic polynomial is

$$\begin{aligned}
\det(\lambda I - A(S_{m,2})) &= \begin{vmatrix} \lambda & -J_{1,m} & O_{1,m} \\ -J_{m,1} & \lambda I_{m,m} & -I_{m,m} \\ O_{m,1} & -I_{m,m} & \lambda I_{m,m} \end{vmatrix}_{(2m+1) \times (2m+1)} \\
&= \begin{vmatrix} \lambda & -1 & -J_{1,m-1} & 0 & O_{1,m-1} \\ -1 & \lambda & O_{1,m-1} & -1 & O_{1,m-1} \\ -J_{m-1,1} & O_{m-1,1} & \lambda I_{m-1,m-1} & O_{m-1,1} & -I_{m-1,m-1} \\ 0 & -1 & O_{1,m-1} & \lambda & O_{m-1,1} \\ O_{m-1,1} & O_{m-1,1} & -I_{m-1,m-1} & O_{m-1,1} & \lambda I_{m-1,m-1} \end{vmatrix}
\end{aligned}$$

Expanding the determinant using the first row, we get

$$\det(\lambda I - A(S_{m,2})) = \lambda \begin{vmatrix} \lambda I_{m,m} & -I_{m,m} \\ -I_{m,m} & \lambda I_{m,m} \end{vmatrix}_{2m \times 2m} + m \begin{vmatrix} -1 & O_{1,m-1} & -1 & O_{1,m-1} \\ -J_{m-1,1} & \lambda I_{m-1,m-1} & O_{m-1,1} & -I_{m-1,m-1} \\ 0 & O_{1,m-1} & \lambda & O_{m-1,1} \\ O_{m-1,1} & -I_{m-1,m-1} & O_{m-1,1} & \lambda I_{m-1,m-1} \end{vmatrix}$$

There are m occurrences of the second term in the expression above, as the expansion of all the m nonzero entries in the first row yield the same minor as above, with alternating signs.

Now expanding the determinant of the second term using the $(m+1)$ th row, we get

$$\det(\lambda I - A(S_{m,2})) = \lambda \begin{vmatrix} \lambda I_{m,m} & -I_{m,m} \\ -I_{m,m} & \lambda I_{m,m} \end{vmatrix}_{2m \times 2m} + m(-1)^{m+1+m+1} \lambda \begin{vmatrix} -1 & O_{1,m-1} & O_{1,m-1} \\ -J_{m-1,1} & \lambda I_{m-1,m-1} & -I_{m-1,m-1} \\ O_{m-1,1} & -I_{m-1,m-1} & \lambda I_{m-1,m-1} \end{vmatrix}_{(2m-1) \times (2m-1)}$$

Now expanding the determinant in the second term using the first row, we get

$$\begin{aligned} \det(\lambda I - A(S_{m,2})) &= \lambda \begin{vmatrix} \lambda I_{m,m} & -I_{m,m} \\ -I_{m,m} & \lambda I_{m,m} \end{vmatrix}_{2m \times 2m} + m(-1)^{m+1+m+1} \lambda(-1) \begin{vmatrix} \lambda I_{m-1,m-1} & -I_{m-1,m-1} \\ -I_{m-1,m-1} & \lambda I_{m-1,m-1} \end{vmatrix}_{(2m-2) \times (2m-2)} \\ &\Rightarrow \det(\lambda I - A(S_{m,2})) \\ &= \lambda \begin{vmatrix} \lambda I_{m,m} & -I_{m,m} \\ -I_{m,m} & \lambda I_{m,m} \end{vmatrix}_{2m \times 2m} + m\lambda \begin{vmatrix} \lambda I_{m-1,m-1} & -I_{m-1,m-1} \\ -I_{m-1,m-1} & \lambda I_{m-1,m-1} \end{vmatrix}_{(2m-2) \times (2m-2)} \end{aligned}$$

The determinant in the first term comes from the circulant matrix with eigenvalues

$$\exp\left(\frac{2\pi i j}{2m}\right)^m; \quad 0 \leq j \leq 2m-1,$$

which yields eigenvalues: $\lambda = 1$ (multiplicity m) and $\lambda = -1$ (multiplicity m).

The determinant in the second term comes from the circulant matrix with eigenvalues

$$\left(\exp\left(\frac{2\pi i j}{2m-2}\right)\right)^{m-1}; \quad 0 \leq j \leq 2m-1,$$

which yields eigenvalues: $\lambda = 1$ (multiplicity $(m-1)$) and $\lambda = -1$ (multiplicity $(m-1)$).

This yields the characteristic polynomial of $A(S_{m,2})$:

$$\begin{aligned} \det(\lambda I - A(S_{m,2})) &= \lambda(\lambda-1)^m(\lambda+1)^m - m\lambda(\lambda-1)^{m-1}(\lambda+1)^{m-1} \\ &= \lambda(\lambda-1)^{m-1}(\lambda+1)^{m-1}((\lambda-1)(\lambda+1) - m) \\ &= \lambda(\lambda-1)^{m-1}(\lambda+1)^{m-1}(\lambda^2 - (m+1)). \end{aligned}$$

$$\Rightarrow \det(\lambda I - A(S_{m,2})) \equiv P_{A(S_{m,2})}(\lambda) = \lambda(\lambda - 1)^{m-1}(\lambda + 1)^{m-1}(\lambda^2 - (m + 1)).$$

Thus the eigenvalues of the adjacency matrix $A(S_{m,2})$ of a star graph with m rays of length 2 are:

- $\lambda = 0$ with multiplicity 1,
- $\lambda = 1$ with multiplicity $m - 1$,
- $\lambda = -1$ with multiplicity $m - 1$,
- $\lambda = \sqrt{m + 1}$ with multiplicity 1 and
- $\lambda = -\sqrt{m + 1}$ with multiplicity 1. □

2.5.6 Eigenvalues of the Cycle Graph

The adjacency matrix $A(C_n)$ of the cycle graph C_n on n vertices has the form:

$$A(C_n) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

Lemma 2.5.2 The linear homogeneous recurrence equation

$x_{i-1} + x_{i+1} = \lambda x_i$ for $2 \leq i \leq n - 1$, and initial conditions $x_0 = x_n$ and $x_{n+1} = x_1$ has solutions

$$\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right); 0 \leq j \leq n - 1 \text{ (See[28]).}$$

Theorem 2.5.8 Let $A(C_n)$ be the adjacency matrix of the cycle graph C_n . The eigenvalues of $A(C_n)$ are:

$$\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right); \text{ for } j = 0, 1, 2, 3, \dots, (n - 1), \text{ for } n \geq 3.$$

Proof Let $\underline{x}_n = (x_1, x_2, \dots, x_n)$ be the eigenvector. Then,

$$A(C_n)\underline{x}_n = \lambda_n \underline{x}_n$$

$$\Rightarrow \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix} = \lambda_n \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} x_2 + x_n \\ x_1 + x_3 \\ x_2 + x_4 \\ x_3 + x_5 \\ \vdots \\ x_{n-3} + x_{n-1} \\ x_{n-2} + x_n \\ x_1 + x_{n-1} \end{bmatrix} = \lambda_n \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix}$$

i.e., $x_{i-1} + x_{i+1} = \lambda_n x_i$ for $1 \leq i \leq n$, and initial conditions $x_0 = x_n$ and $x_{n+1} = x_1$

From Lemma 2.5.2, this linear homogeneous recurrence equation has solution

$$\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right); 0 \leq j \leq n-1.$$

Therefore, the eigenvalues of the adjacency matrix of the cycle graph C_n on n vertices are

$$\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right); 0 \leq j \leq n-1 \text{ for } n \geq 3. \quad \square$$

2.5.7 Eigenvalues of the Path Graph

The adjacency matrix $A(P_n)$ of the path graph P_n has the form:

$$A(P_n) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

Lemma 2.5.3 The linear homogeneous recurrence relation

$$x_{i-1} + x_{i+1} = \lambda x_i \text{ for } 2 \leq i \leq n-1, \text{ and initial conditions } x_0 = 0 \text{ and } x_{n+1} = 0$$

has solutions $\lambda_j = 2\cos\left(\frac{\pi j}{n+1}\right); 1 \leq j \leq n$ (See[28]).

Theorem 2.5.9 Let $A(P_n)$ be the adjacency matrix of the path graph P_n . The eigenvalue of $A(P_n)$ are:

$$\lambda_j = 2\cos\left(\frac{\pi j}{n+1}\right); \text{ for } j = 1, 2, \dots, n \text{ and } n \geq 2.$$

Proof Let $\underline{x}_n = (x_1, x_2, \dots, x_n)$ be the eigenvector. Then,

$$A(P_n)\underline{x}_n = \lambda_n \underline{x}_n$$

$$\Rightarrow \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix} = \lambda_n \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} x_2 \\ x_1 + x_3 \\ x_2 + x_4 \\ x_3 + x_5 \\ \vdots \\ x_{n-3} + x_{n-1} \\ x_{n-2} + x_n \\ x_{n-1} \end{bmatrix} = \lambda_n \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix}$$

i.e., $x_{i-1} + x_{i+1} = \lambda_n x_i$ for $1 \leq i \leq n$, and initial conditions $x_0 = 0$ and $x_{n+1} = 0$

From Lemma 2.5.3, this linear homogeneous recurrence equation has solution

$$\lambda_j = 2\cos\left(\frac{\pi j}{n+1}\right); 1 \leq j \leq n.$$

Therefore, the eigenvalues of the adjacency matrix of the path graph P_n on n vertices are

$$\lambda_j = 2\cos\left(\frac{\pi j}{n+1}\right); 1 \leq j \leq n \text{ for } n \geq 2. \quad \square$$

2.5.8 Eigenvalues of the Wheel Graph

corollary 2.5.1. The eigenvalues of the wheel graph W_n on n vertices, $n \geq 4$, are: $0, 1 \pm \sqrt{n}$ (each with multiplicity 1), and $\lambda_j = 2\cos\frac{2\pi j}{n-1}; j = 1, \dots, n-2$ (each with multiplicity 1)

Proof. Since the wheel graph W_n is the join of two regular graphs $G_1 = K_1$ and $G_2 = C_{n-1}$, we use the theorem 2.5.3. $G_1 = K_1$ is 0-regular on 1 vertex, so, $k_1 = 0$ and $n_1 = 1$; $G_2 = C_{n-1}$ is 2-regular on $n-1$ vertices, so, $k_2 = 2$ and $n_2 = n-1$. $W_n = K_1 \diamond C_{n-1}$.

We know that, K_1 has as eigenvalue $\lambda = 0$, and the eigenvalues of the cycle graph C_{n-1} are : $\lambda_j = 2\cos\frac{2\pi j}{n-1}; j = 0, \dots, n-2$ (each with multiplicity 1). Then the spectrum of $W_n = K_1 \diamond C_{n-1}$ consists of

(i) $\lambda_j = 2\cos\frac{2\pi j}{n-1}; j = 1, \dots, n-2;$

(ii) $\frac{0 \pm \sqrt{(0+2)^2 + 4(0-1)}}{2} = 0;$

(iii) Three roots of the equation $x^3 - (0+2)x^2 + (0-0-1(n-1))x + 0 = 0$.

$\Rightarrow x^3 - 2x^2 + (n-1)x = 0 \Rightarrow x = 0$ and $x = 1 \pm \sqrt{n}$. □

2.5.9 Eigenvalues of the Dual-star Graph

Let $D_u S_n$ be the dual star graph defined as two star graphs with m rays of length 1 (each on $\frac{n}{2}$ vertices) joined by an edge (its center edge) connecting their centers. This graph has 4 nonzero eigenvalues found as solutions of the following equation (see Winter and Jessop [51]):

$$x^4 - (2m + 1)x^2 + m^2 = 0 \Rightarrow x^4 - (n - 1)x^2 + \frac{(n - 2)^2}{4} = 0 \Rightarrow x^2 = \frac{(n - 1) \pm \sqrt{2n - 3}}{2}$$

$$x = \pm \sqrt{\frac{(n - 1) + \sqrt{2n - 3}}{2}} \text{ or } x = \pm \sqrt{\frac{(n - 1) - \sqrt{2n - 3}}{2}}$$

Thus, the eigenvalues of the dual star graph $D_u S_n$ are:

$$\lambda_1 = \sqrt{\frac{(n - 1) + \sqrt{2n - 3}}{2}}, \lambda_2 = -\sqrt{\frac{(n - 1) + \sqrt{2n - 3}}{2}},$$

$$\lambda_3 = \sqrt{\frac{(n - 1) - \sqrt{2n - 3}}{2}} \text{ and } \lambda_4 = -\sqrt{\frac{(n - 1) - \sqrt{2n - 3}}{2}}$$

each with multiplicity 1.

2.5.10 Eigenvalues of the Lollipop Graph

In previously published papers, there is an error on the application of lollipop theorem for finding the eigenvalues of the lollipop graph. The characteristic polynomial is incorrect and must be $(\lambda + 1)^{n-3}[\lambda^3 - \lambda^2(n - 3) - \lambda(n - 1) + (n - 3)]$.

Theorem 2.5.10. let G be the lollipop graph on n vertices, denoted by LP_n , comprising of the complete graph K_{n-1} on $(n - 1)$ vertices, joined to a single end vertex x_2 by an edge $x_1 x_2$, with $n \geq 3$. And let G' be the subgraph of G induced by removing the vertex x_1 , and let G'' be the subgraph of G by removing the vertex x_2 . Then the eigenvalues of G are:

$$\lambda = -1 \text{ (multiplicity } n - 3).$$

Proof. The bulk of this proof is my original work.

We use the Lollipop theorem (see Theorem 2.5.1).

$$P_{A(G)}(\lambda) = \lambda P_{A(G')}(\lambda) - P_{A(G'')}(\lambda)$$

$$P_{A(LP_n)}(\lambda) = \lambda P_{A(K_{n-1})}(\lambda) - P_{A(K_{n-2})}(\lambda)$$

$$= \lambda(\lambda + 1)^{n-2}(\lambda - (n - 2)) - (\lambda + 1)^{n-3}(\lambda - (n - 3))$$

$\Rightarrow P_{A(LP_n)}(\lambda) = (\lambda + 1)^{n-3}[\lambda^3 - \lambda^2(n - 3) - \lambda(n - 1) + (n - 3)]$ is the characteristic polynomial of the adjacency matrix of LP_n .

we have $(\lambda + 1)^{n-3} = 0$ and $\lambda^3 - \lambda^2(n - 3) - \lambda(n - 1) + (n - 3) = 0$.

$$(i) \quad (\lambda + 1)^{n-3} = 0 \Rightarrow \lambda = -1 \text{ (multiplicity } n - 3)$$

(ii) To solve the cubic equation $\lambda^3 - \lambda^2(n-3) - \lambda(n-1) + (n-3) = 0$, we apply the substitution

$$\lambda = y + \frac{n-3}{3},$$

multiplying out and simplifying, to obtain

$$y^3 + \left[1 - n - \frac{(n-3)^2}{3}\right]y + \left[n - 3 - \frac{2(n-3)^3}{27} - \frac{(n-3)(n-1)}{3}\right] = 0.$$

$$\Rightarrow y^3 + Ay = B$$

where

$$A = \left[1 - n - \frac{(n-3)^2}{3}\right] = \frac{1}{3}(3n - n^2 - 6)$$

$$B = -\left[n - 3 - \frac{2(n-3)^3}{27} - \frac{(n-3)(n-1)}{3}\right] = \frac{(n-3)}{27}(2n^2 - 3n - 18).$$

We find s and t so that

$$3st = A \tag{1}$$

$$s^3 - t^3 = B. \tag{2}$$

It turns out that $y = s - t$ will be a solution of the equation $y^3 + Ay = B$.

Solving the equation (1) for s and substituting into (2) yields:

$$\left(\frac{A}{3t}\right)^3 - t^3 = B.$$

Simplifying, this turns into the equation

$$t^6 + Bt^3 - \frac{A^3}{27} = 0,$$

which using the substitution $u = t^3$ becomes the quadratic equation

$$u^2 + Bu - \frac{A^3}{27} = 0.$$

Using the quadratic formula, we obtain that

$$u = t^3 = \frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}.$$

and

$$t = \sqrt[3]{\frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}}.$$

By equation (2),

$$s^3 = B + t^3 = B + \frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}};$$

$$\Rightarrow s = \sqrt[3]{B + \frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}}.$$

So that

$$y = s - t = \sqrt[3]{B + \frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}} - \sqrt[3]{\frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}};$$

and the solution to our original cubic equation is given by

$$\lambda = y + \frac{n-3}{3} = \sqrt[3]{B + \frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}} - \sqrt[3]{\frac{-3\sqrt{3}B \pm \sqrt{27B^2 + 4A^3}}{6\sqrt{3}}} + \frac{n-3}{3};$$

i.e

$$\lambda = \sqrt[3]{\frac{B}{2} \pm \frac{1}{6\sqrt{3}}\sqrt{27B^2 + 4A^3}} - \sqrt[3]{\frac{-B}{2} \pm \frac{1}{6\sqrt{3}}\sqrt{27B^2 + 4A^3}} + \frac{n-3}{3};$$

where

$$A = \frac{1}{3}(3n - n^2 - 6)$$

$$B = \frac{(n-3)}{27}(2n^2 - 3n - 18).$$

Notice that, for

$$A = \frac{1}{3}(3n - n^2 - 6)$$

$$B = \frac{(n-3)}{27}(2n^2 - 3n - 18);$$

$$27B^2 + 4A^3 < 0, \text{ for all } n \geq 3.$$

Therefore, we obtain two imaginary roots.

Furthermore, using *Cardan formula* for finding a root of polynomial $y^3 + Ay + B$; if

$$4A^3 + 27B^2 \geq 0,$$

we have

$$y = \sqrt[3]{-\frac{B}{2} - \frac{1}{2}\sqrt{\frac{4A^3 + 27B^2}{27}}} + \sqrt[3]{-\frac{B}{2} + \frac{1}{2}\sqrt{\frac{4A^3 + 27B^2}{27}}};$$

i.e

$$y = \sqrt[3]{-\frac{B}{2} - \frac{1}{6\sqrt{3}}\sqrt{4A^3 + 27B^2}} + \sqrt[3]{-\frac{B}{2} + \frac{1}{6\sqrt{3}}\sqrt{4A^3 + 27B^2}};$$

where

$$A = \frac{1}{3}(3n - n^2 - 6)$$

$$B = -\frac{1}{27}((n-3)(2n^2 - 3n - 18)) = \frac{(n-3)}{27}(3n - 2n^2 + 18);$$

So that,

$$\lambda = y + \frac{n-3}{3}.$$

But, in our case,

$$4A^3 + 27B^2 < 0.$$

Thus, this root, λ , is also imaginary. Finally, we have only one real root:

$$\lambda = -1(\text{ multiplicity } n-3).$$

□

2.5.11 Eigenvalues of the Line Graph of the complete graph K_n

The line graph of the complete graph K_n denoted by $L(K_n)$ has $p = \frac{n(n-1)}{2}$ vertices (see Brualdi[12]). The number q of edges is the sum of the square of the degrees minus the number of edges of K_n . Thus,

$$q = \frac{n(n-1)^2}{2} - \frac{n(n-1)}{2} = \frac{n(n-1)(n-2)}{2}.$$

Also,

$$2n^2 - 6n = \frac{4n(n-1)}{2} - 4n = 4p - 4n \Rightarrow n^2 - n - 2p = 0 \Rightarrow n = \frac{1 \pm \sqrt{1+8p}}{2} = \frac{1 + \sqrt{1+8p}}{2}.$$

Lemma 2.5.4. Suppose that G is a k -regular graph of order n . Then the characteristic polynomial of $L(G)$ is

$$P_{A(L(G))}(\lambda) = (\lambda + 2)^{n(k-2)/2} P_{A(G)}(\lambda - k + 2).$$

Theorem 2.5.11. The Eigenvalues of the Line Graph of the complete graph K_n are: $\lambda = -2$, with multiplicity $\frac{n(n-3)}{2}$; $\lambda = 2n-4$, with multiplicity 1, and $\lambda = n-4$, with multiplicity $(n-1)$.

Proof. applying Lemma 2.5.4, since K_n is a $(n-1)$ -regular graph of order n , we have

$$\begin{aligned} P_{A(L(K_n))}(\lambda) &= (\lambda + 2)^{n(n-1-2)/2} P_{A(K_n)}(\lambda - (n-1) + 2) \\ &= (\lambda + 2)^{n(n-3)/2} P_{A(K_n)}(\lambda - n + 3) \\ &= (\lambda + 2)^{n(n-3)/2} ((\lambda - n + 3) - (n-1))((\lambda - n + 3) + 1)^{n-1} \\ &= (\lambda + 2)^{n(n-3)/2} (\lambda - (2n-4))(\lambda - (n-4))^{n-1} \quad \square \end{aligned}$$

2.5.12 Eigenvalues of The Friendship Graph

Theorem 2.5.12. The eigenvalues of a friendship graph F_p on n vertices, where $p = \frac{n-1}{2}$, are $\lambda = -1$ (with multiplicity p), $\lambda = 1$ (with multiplicity $(p-1)$), $\lambda = \frac{1 \pm \sqrt{1+8p}}{2}$ (with multiplicity 1 each).

See M.R. Rajesh Kanna And All [35], and J. R. Vermette [43].

Proof. The adjacency matrix of a friendship F_p is

$$A(F_p) = \begin{bmatrix} 0 & 1 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 0 & 1 & \cdots & 1 & 1 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 1 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 1 & 0 & \cdots & 1 & 0 \end{bmatrix}_{(2p+1) \times (2p+1)}.$$

The characteristic equation of $A(F_p)$ is

$$(\lambda + 1)^p(\lambda - 1)^{p-1}(\lambda^2 - \lambda - 2p) = 0.$$

Eigenvalues are $\lambda = -1$ (with multiplicity p), $\lambda = 1$ (with multiplicity $(p-1)$), $\lambda = \frac{1 \pm \sqrt{1+8p}}{2}$ (with multiplicity 1 each)

2.6 Spectra of graphs with end vertices appended to each vertex in a graph

In this section, we determinate the spectra of graphs obtained by appending h end vertex to all vertices of a defined class of graphs called the *base graph*.

Let the generalized sun graph $SG(h,p)$ be a graph which consists of the base graph G on p vertices, with h end vertices appended to each of the p vertices in the graph G . Then the graph $SG(h,p)$ has $n = p(h+1)$ vertices, and the $n \times n$ adjacency matrix of $SG(h,p)$ is:

$$A(SG(h,p)) = \begin{bmatrix} A(G) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{bmatrix}.$$

And

$$\det(A(SG(h,p))) = \begin{vmatrix} A(G) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{vmatrix} = \begin{cases} 1 & \text{for } h = 1 \text{ and } p \text{ even} \\ -1 & \text{for } h = 1 \text{ and } p \text{ odd} \\ 0 & \text{otherwise.} \end{cases}$$

See Winter and Jessop[53]

Theorem 2.6.1

If α_j are the eigenvalues of $A(G)$, $1 \leq j \leq p$, then

$$\lambda_{2j-1} = \frac{\alpha_j + \sqrt{\alpha_j^2 + 4h}}{2} \text{ and } \lambda_{2j} = \frac{\alpha_j - \sqrt{\alpha_j^2 + 4h}}{2}$$

are two eigenvalues of $A(SG(h,p))$, $1 \leq j \leq p$. The remaining $p(h-1)$ eigenvalues of $A(SG(h,p))$ are $\lambda = 0$.

See Winter and Jessop[53]

2.6.1 Eigenvalues of the L-regular caterpillar Graph and the Caterpillar Graph

A caterpillar graph is denoted by $CT(k,l)$ where k and l denote the number of vertices on the path and the number of pendent edges respectively. This graph will have $n = k(l+1)$ vertices

and the adjacency matrix of the caterpillar graph is an $n \times n$ matrix, and takes the general form:

$$A(CT(k,l)) = \begin{bmatrix} A(P_k) & I_{k,k} & I_{k,k} & \cdots & I_{k,k} \\ I_{k,k} & O_{k,k} & O_{k,k} & \cdots & O_{k,k} \\ I_{k,k} & O_{k,k} & O_{k,k} & \cdots & O_{k,k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ I_{k,k} & O_{k,k} & O_{k,k} & \cdots & O_{k,k} \end{bmatrix},$$

where $I_{k,k}$ is repeated l times horizontally and l times vertically.

Lemma 2.6.1. The Laplacian eigenvalues of the caterpillar graph $CT(k,l)$ are $\lambda = 1$, with multiplicity $k(l-1)$ and the eigenvalues of the $(2k) \times (2k)$ matrix

$$G(l) = \begin{bmatrix} A(l) & F & & & \\ F & B(l) & F & & \\ & F & \ddots & \ddots & \\ & & \ddots & B(l) & F \\ & & & F & A(l) \end{bmatrix},$$

where $A(l) = \begin{bmatrix} 1 & \sqrt{l} \\ \sqrt{l} & l+1 \end{bmatrix}$, $B(l) = \begin{bmatrix} 1 & \sqrt{l} \\ \sqrt{l} & l+2 \end{bmatrix}$, and $F = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.

The eigenvalues of $G(l)$ are

$$\lambda_j = \frac{1}{2} \left[l+3 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right] \text{ and}$$

$$\lambda_{k+j} = \frac{1}{2} \left[l+3 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right]$$

where $\sigma_j = 2\cos \left[\frac{(k+1-j)\pi}{k} \right]$ for $j = 1, \dots, k$.

See Rojo[37].

Lemma 2.6.2. If G is a bipartite graph and if λ is a nonzero Laplacian eigenvalue of G then $\lambda - 2$ is an eigenvalue of $L(G)$ (see Rojo[37]).

Proof. Since $CT(k,l)$ is a bipartite graph, the eigenvalues of $L(CT(k,l))$ can be derived from the Laplacian eigenvalues of $CT(k,l)$ (see Lemma 2.6.1 for these eigenvalues), namely:

$$\lambda_i = \lambda - 2 = 1 - 2 = -1 \text{ with multiplicity } k(l-1),$$

$$\lambda_j = \lambda_i - 2 = \frac{1}{2} \left[l-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l)} \right],$$

where

$$\sigma_j = 2\cos \left[\frac{(k+1-j)\pi}{k} \right], \text{ for } 2 \leq j \leq k \text{ and}$$

$$\mu_{k+j} = \lambda_j - 2 = \frac{1}{2} \left[l-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l)} \right],$$

where

$$\sigma_j = 2\cos \left[\frac{(k+1-j)\pi}{k} \right], \text{ for } 1 \leq j \leq k. \quad \square$$

2.6.2 Eigenvalues of the Complete Sun Graph

Let $CompSun(h,p)$ be the complete sun graph which consists of the complete graph K_p , with h end vertices appended to each of the p vertices in K_p . Then $CompSun(h,p)$ has $n = (h+1)p$ vertices and $p\left(\frac{p-1}{2} + h\right)$ edges. Then the $(n \times n)$ adjacency matrix of $CompSun(h,p)$ is:

$$A(CompSun(h,p)) = \begin{bmatrix} A(K_p) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{n,n} & \cdots & O_{n,n} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{n,n} & \cdots & O_{n,n} \end{bmatrix}.$$

See Winter and Jessop [53].

Theorem 2.6.2. The eigenvalues of $CompSun(h,p)$ are

$$\lambda = \frac{-1 \pm \sqrt{1+4h}}{2} \text{ with multiplicity } (p-1),$$

$$\lambda = \frac{(p-1) \pm \sqrt{(p-1)^2 + 4h}}{2} \text{ with multiplicity } 1, \text{ and}$$

$$\lambda = 0 \text{ with multiplicity } p(h-1).$$

Proof. The eigenvalues of $A(K_p)$ are $\alpha = -1$ with multiplicity $p-1$, and $\alpha = p-1$ with multiplicity 1. See Jessop [28]. Therefore, from Theorem 2.6.1, the eigenvalues of $CompSun(h,p)$ are

$$\lambda = \frac{-1 \pm \sqrt{1+4h}}{2} \text{ with multiplicity } (p-1),$$

$$\lambda = \frac{(p-1) \pm \sqrt{(p-1)^2 + 4h}}{2} \text{ with multiplicity } 1,$$

And the remaining $p(h+1) - 2p = p(h-1)$ eigenvalues of $CompSun(h,p)$ are 0. □

2.6.3 Eigenvalues of the Complete Split-bipartite Sun Graph

Let $BipSun(h,p)$ be the complete split-bipartite sun graph which consists of the complete split-bipartite graph $K_{\frac{p}{2}, \frac{p}{2}}$, with h end vertices appended to each of the p vertices in $K_{\frac{p}{2}, \frac{p}{2}}$. Then $BipSun(h,p)$ has $n = (h+1)p$ vertices and $\frac{p^2}{4} + ph$ edges. Then the $(n \times n)$ adjacency matrix of $BipSun(h,p)$ is:

$$A(BipSun(h,p)) = \begin{bmatrix} A(K_{\frac{p}{2}, \frac{p}{2}}) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{bmatrix}.$$

See Winter and Jessop [53].

Theorem 2.6.3. The eigenvalues of $BipSun(h,p)$ are

$$\lambda = \frac{p \pm \sqrt{p^2 + 16h}}{4} \text{ with multiplicity } 1,$$

$$\lambda = \frac{(-p \pm \sqrt{p^2 + 16h})}{4} \text{ with multiplicity } 1,$$

$$\lambda = \pm\sqrt{h} \text{ with multiplicity } p - 2, \text{ and}$$

$$\lambda = 0 \text{ with multiplicity } p(h - 1).$$

Proof. The eigenvalues of $K_{\frac{p}{2}, \frac{p}{2}}$ are $\alpha = \pm\frac{p}{2}$ with multiplicity 1, and $\alpha = 0$ with multiplicity $p - 2$. See Jessop [28]. Therefore, from Theorem 2.6.1, the eigenvalues of $BipSun(h,p)$ are

$$\lambda = \frac{\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 + 4h}}{2} = \frac{p \pm \sqrt{p^2 + 16h}}{4} \text{ with multiplicity } 1,$$

$$\lambda = \frac{\frac{-p}{2} \pm \sqrt{\left(\frac{-p}{2}\right)^2 + 4h}}{2} = \frac{-p \pm \sqrt{p^2 + 16h}}{4} \text{ with multiplicity } 1,$$

$$\lambda = \frac{(0) \pm \sqrt{(0)^2 + 4h}}{2} = \pm\sqrt{h} \text{ with multiplicity } p - 2.$$

And the remaining $p(h+1) - 2p = p(h-1)$ eigenvalues of $BipSun(h,p)$ are 0. □

2.6.4 Eigenvalues of the Wheel Sun Graph

Let $WheelSun(h,p)$ be the wheel sun graph which consists of the wheel graph W_p , with h end vertices appended to each of the p vertices in W_p . Then $WheelSun(h,p)$ has $n = (h + 1)p$ vertices and $(h + 2)(p - 1) + h$ edges. Then the $(n \times n)$ adjacency matrix of $WheelSun(h,p)$ is:

$$A(WheelSun(h,p)) = \begin{bmatrix} A(W_p) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{bmatrix}.$$

See Winter and Jessop [53].

Theorem 2.6.4. The eigenvalues of $A(WheelSun(h,p))$ are

$$\lambda = \cos\left(\frac{2\pi k}{p-1}\right) \pm \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h} \text{ where } k = 1, \dots, p-2,$$

$$\lambda = \frac{(1 + \sqrt{p}) \pm \sqrt{(1 + \sqrt{p})^2 + 4h}}{2} \text{ with multiplicity 1 each,}$$

$$\lambda = \frac{(1 - \sqrt{p}) \pm \sqrt{(1 - \sqrt{p})^2 + 4h}}{2} \text{ with multiplicity 1 each, and}$$

$$\lambda = 0 \text{ with multiplicity } p(h-1).$$

Proof. The eigenvalues of $A(W_p)$ are $\alpha = 2\cos\left(\frac{2\pi k}{p-1}\right)$ $1 \leq k \leq p-2$, and $\alpha = 1 \pm \sqrt{p}$ with multiplicity 1. See Jessop [28]. Therefore, from Theorem 2.6.1, the eigenvalues of $A(WheelSun(h,p))$ are

$$\lambda = \frac{2\cos\left(\frac{2\pi k}{p-1}\right) \pm \sqrt{\left(2\cos\left(\frac{2\pi k}{p-1}\right)\right)^2 + 4h}}{2} = \cos\left(\frac{2\pi k}{p-1}\right) \pm \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h}, \quad 1 \leq k \leq p-2,$$

$$\lambda = \frac{(1 + \sqrt{p}) \pm \sqrt{(1 + \sqrt{p})^2 + 4h}}{2} \text{ with multiplicity 1, and}$$

$$\lambda = \frac{(1 - \sqrt{p}) \pm \sqrt{(1 - \sqrt{p})^2 + 4h}}{2} \text{ with multiplicity 1.}$$

The remaining $p(h+1) - 2p = p(h-1)$ eigenvalues of $A(WheelSun(h,p))$ are 0. □

2.6.5 Eigenvalues of the Star Sun Graph

Let $StarSun(h,p)$ be the star sun graph which consists of the star graph $S_{p-1,1}$, with h end vertices appended to each of the p vertices in $S_{p-1,1}$. Then $StarSun(h,p)$ has $n = (h+1)p$ vertices and $(h+1)(p-1) + h$ edges. Then the $(n \times n)$ adjacency matrix of $StarSun(h,p)$ is:

$$A(StarSun(h,p)) = \begin{bmatrix} A(S_{p-1,1}) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{bmatrix}.$$

See Winter and Jessop [53].

Theorem 2.6.5. The eigenvalues of $A(\text{StarSun}(h,p))$ are

$$\lambda = \frac{\sqrt{p-1} \pm \sqrt{p-1+4h}}{2} \text{ with multiplicity } 1,$$

$$\lambda = \frac{-\sqrt{p-1} \pm \sqrt{p-1+4h}}{2} \text{ with multiplicity } 1,$$

$$\lambda = \pm\sqrt{h} \text{ with multiplicity } (p-2), \text{ and}$$

$$\lambda = 0 \text{ with multiplicity } p(h-1).$$

Proof. The eigenvalues of $A(S_{p-1,1})$ are $\alpha = \pm\sqrt{p-1}$, with multiplicity 1 and $\alpha = 0$, with multiplicity $p-2$. See Jessop [28]. Therefore, from Theorem 2.6.1, the eigenvalues of $A(\text{StarSun}(h,p))$ are

$$\begin{aligned} \lambda &= \frac{\sqrt{p-1} \pm \sqrt{(\sqrt{p-1})^2 + 4h}}{2} \\ &= \frac{\sqrt{p-1} \pm \sqrt{p-1+4h}}{2} \text{ with multiplicity } 1, \end{aligned}$$

$$\begin{aligned} \lambda &= \frac{-\sqrt{p-1} \pm \sqrt{(-\sqrt{p-1})^2 + 4h}}{2} \\ &= \frac{-\sqrt{p-1} \pm \sqrt{p-1+4h}}{2} \text{ with multiplicity } 1, \end{aligned}$$

$$\begin{aligned} \lambda &= \frac{0 \pm \sqrt{(0)^2 + 4h}}{2} \\ &= \pm\sqrt{h} \text{ with multiplicity } p-2, \end{aligned}$$

The remaining $p(h+1) - 2p = p(h-1)$ eigenvalues of $A(\text{StarSun}(h,p))$ are 0. □

2.6.6 Eigenvalues of the Cycle Sun Graph

Let $\text{CycleSun}(h,p)$ be the cycle sun graph which consists of the cycle graph C_p , with h end vertices appended to each of the p vertices in C_p . Then $\text{CycleSun}(h,p)$ has $n = (h+1)p$ vertices and $(h+1)p$ edges. Then the $(n \times n)$ adjacency matrix of $\text{CycleSun}(h,p)$ is:

$$A(\text{CycleSun}(h,p)) = \begin{bmatrix} A(C_p) & I_{p,p} & \cdots & I_{p,p} \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \\ \vdots & \vdots & \ddots & \vdots \\ I_{p,p} & O_{p,p} & \cdots & O_{p,p} \end{bmatrix}.$$

See Winter and Jessop [53].

Theorem 2.6.6. The eigenvalues of $A(\text{CycleSun}(h,p))$ are

$$\lambda = \cos\left(\frac{2\pi k}{p}\right) \pm \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h}, \text{ where } k = 0, 1, \dots, p-1, \text{ and}$$

$$\lambda = 0 \text{ with multiplicity } p(h-1).$$

Proof. The eigenvalues of $A(C_p)$ are $\alpha = 2\cos\left(\frac{2\pi k}{p}\right)$ $0 \leq k \leq p-1$. See Jessop [28]. Therefore, from Theorem 2.6.1, the eigenvalues of $A(\text{CycleSun}(h,p))$ are

$$\lambda = \frac{2\cos\left(\frac{2\pi k}{p}\right) \pm \sqrt{\left(2\cos\left(\frac{2\pi k}{p}\right)\right)^2 + 4h}}{2} = \cos\left(\frac{2\pi k}{p}\right) \pm \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h}, \quad 0 \leq k \leq p-1.$$

The remaining $p(h+1)-2p = p(h-1)$ eigenvalues of $A(\text{CycleSun}(h,p))$ are 0. □

2.7 Eigenvalues of Complement of regular graph

We remind that the *complement* \overline{G} of the graph G is the graph with the same vertex set as G , where two distinct vertices are adjacent whenever they are nonadjacent in G ; And a graph G is called *regular* of degree k , when every vertex has precisely k neighbors.

Lemma 2.7.1 (see [17] and [19]). If G is k -regular, with n vertices, and $k = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the eigenvalues of G , then the eigenvalues of its complement, \overline{G} , are $n-1-k, -1-\lambda_n, \dots, -1-\lambda_2$.

Theorem 2.7.1 (see [19]). If G is a regular graph of degree k (or a k -regular) with n vertices, then

$$P_{A(\overline{G})}(\lambda) = (-1)^n \frac{\lambda - n + k + 1}{\lambda + k + 1} P_{A(G)}(-\lambda - 1)$$

where $P_{A(\overline{G})}$ is the characteristic polynomial of the complement, \overline{G} , of the graph G .

Proof. From lemma 2.7.1 above

$$P_{A(G)}(\lambda) = (\lambda - k) \prod_{i=2}^n (\lambda - \lambda_i)$$

and

$$P_{A(\overline{G})}(\lambda) = (\lambda - (n-1-k)) \prod_{i=2}^n (\lambda - (-1 - \lambda_i)).$$

We have:

$$\begin{aligned} P_{A(\overline{G})}(\lambda) &= (\lambda - n + 1 + k) \prod_{i=2}^n (\lambda + 1 + \lambda_i) \\ &= (-1)^n (\lambda - n + k + 1) (-1) \prod_{i=2}^n (-\lambda - 1 - \lambda_i) \end{aligned}$$

$$\begin{aligned} P_{A(G)}(-\lambda - 1) &= (-\lambda - 1 - k) \prod_{i=2}^n (-\lambda - 1 - \lambda_i) \\ \implies (-1) \prod_{i=2}^n (-\lambda - 1 - \lambda_i) &= \frac{P_{A(G)}(-\lambda - 1)}{\lambda + 1 + k}. \end{aligned}$$

So that:

$$P_{A(\overline{G})}(\lambda) = (-1)^n \frac{\lambda - n + k + 1}{\lambda + k + 1} P_{A(G)}(-\lambda - 1) \quad \square$$

Example 2.7.1. We use the formula above to find the formula for the spectra of complete graphs. The complement of a complete graph K_n is a graph of n isolated vertices. Let \overline{K}_n denote the complement of a complete graph on n vertices. The adjacency matrix of \overline{K}_n is:

$$A(\overline{K}_n) = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Thus, the characteristic polynomial of the complement of K_n is $P_n = \lambda^n$ and the eigenvalues are $\lambda = 0$ (with multiplicity n).

Let $P_{A(\overline{G})}(\lambda)$ be the characteristic polynomial of K_n and $P_{A(G)}(\lambda)$ be the characteristic polynomial of the complement of K_n . We have:

$$\begin{aligned} P_{A(\overline{G})}(\lambda) &= (-1)^n \frac{\lambda - n + k + 1}{\lambda + k + 1} P_{A(G)}(-\lambda - 1) \\ P_{A(K_n)}(\lambda) &= (-1)^n \frac{\lambda - n + k + 1}{\lambda + k + 1} P_{A(\overline{K}_n)}(-\lambda - 1) \\ &= (-1)^n \frac{\lambda - n + 1}{\lambda + 1} P_{A(\overline{K}_n)}(-\lambda - 1) \quad (k = 0, \text{ because } \overline{K}_n \text{ is 0-regular}) \\ P_{A(K_n)}(\lambda) &= \frac{\lambda - n + 1}{\lambda + 1} P_{A(\overline{K}_n)}(\lambda + 1) \\ &= \frac{\lambda - n + 1}{\lambda + 1} (\lambda + 1)^n \\ &= (\lambda - n + 1)(\lambda + 1)^{n-1}. \end{aligned}$$

Since

$$P_{A(K_n)}(\lambda) = (\lambda - (n - 1))(\lambda + 1)^{n-1}$$

any complete graph K_n has the eigenvalues $(n - 1)$, with multiplicity 1, and -1 , with multiplicity $(n - 1)$.

Example 2.7.2. Eigenvalues of the complement of the Cycle graph

The cycle graph, C_n , is a 2-regular graph. And, let \overline{C}_n be its complement, with $n \geq 3$, then \overline{C}_n is $(n - 3)$ -regular graph, and has as eigenvalues:

$$n - 3, \quad -1 - 2 \cos\left(\frac{2\pi j}{n}\right);$$

$j = 1, \dots, (n - 1)$, each with multiplicity 1.

2.8 Conclusion

This chapter is devoted to define eigenvalues of graph and how we apply this to the adjacency matrix of graph. We presented different techniques used to find the eigenvalues for certain classes of graphs so that we can determine their energies in the next chapter. Some techniques use the definition of the eigenvalues of the adjacency matrix of a graph while others used known results or theorems such as lollipop theorem. And we showed that we can use the idea of complements to find the spectrum of some regular graphs as a complete graph.

Chapter 3

ENERGY OF CLASSES OF GRAPHS

3.1 Introduction

The energy of graph was first defined by Ivan Gutman in 1978 [24]. However, the motivation for his definition appeared much earlier, in the 1930's, when Erich Hückel proposed the famous Hückel Molecular Orbital Theory.

The energy of graph is defined as the sum of absolute values of the eigenvalues of the adjacency matrix of the graph in consideration. This quantity is studied in the context of spectral graph theory.

Given the importance of the energy of graph in chemical context, finding a simple expression for the energy of a class of graphs is necessary and can be trivial, especially if the eigenvalues are integral (for the complete graph, for example). We determine the energy of different classes of graphs using the eigenvalues determined in the previous chapter.

Definition 3.1.1

The *energy* of graph G is the sum of the absolute values of the adjacency matrix of G , i.e., for an n - vertex graph G , with adjacency matrix A , having eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, the energy of G , denoted by $E(G)$, is defined as:

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

Lemma 3.1.1 If $\{\lambda_i : \lambda_i > 0\}$ are all the positive eigenvalues of a graph G , and $\{\lambda_i : \lambda_i < 0\}$ all its negative eigenvalues. Then, the energy of G is

$$E(G) = 2 \sum \{\lambda_i : \lambda_i > 0\} = -2 \sum \{\lambda_i : \lambda_i < 0\}.$$

Proof. let $\lambda_1, \lambda_2, \dots, \lambda_s$ be all the positive eigenvalues, and $\lambda_{s+1}, \dots, \lambda_n$ all the negative eigenvalues. We have

$$\begin{aligned} E(G) &= \sum_{i=1}^n |\lambda_i| \Rightarrow \sum_{i=1}^s \lambda_i = - \sum_{i=s+1}^n \lambda_i = \frac{E(G)}{2}. \\ \Rightarrow E(G) &= 2 \sum_{i=1}^s \lambda_i = -2 \sum_{i=s+1}^n \lambda_i \quad \square \end{aligned}$$

3.2 Analytical Methods to obtain the Energy of Graphs

This section is based on the article by Winter and Jessop[52]. We require the following results for the analysis of the energy of paths, cycles and wheels.

Theorem 3.2.1 (See Winter and Jessop [52]).

Let $n \geq 2$.

1. For n even, then

$$\sum_{j=1}^{\frac{n}{2}} 2\cos\left(\frac{\pi j}{n}\right) = \cot\left(\frac{\pi}{2n}\right) - 1;$$

2. For n odd, then

$$\sum_{j=1}^{\frac{n-1}{2}} 2\cos\left(\frac{\pi j}{n}\right) = \operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1;$$

3. For n odd and $n = 2t + 1$, for t even, then

$$\sum_{j=1}^{\frac{n-1}{4}} 2\cos\left(\frac{2\pi j}{n}\right) = \frac{1}{2}\operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1 \text{ and}$$

4. For n odd and $n = 2t + 1$, for t odd and $t > 1$, then

$$\sum_{j=1}^{\frac{n-3}{4}} 2\cos\left(\frac{2\pi j}{n}\right) = \frac{1}{2}\operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1.$$

Proof

1. Let

$$C = \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{\pi j}{n}\right); \quad S = \sum_{j=1}^{\frac{k}{2}} 2\sin\left(\frac{\pi j}{n}\right), \text{ we suppose } k \text{ is even,}$$

and

$$\gamma = \cos\left(\frac{\pi}{n}\right) + i\sin\left(\frac{\pi}{n}\right);$$

so that

$$\gamma^{\frac{k}{2}} = \left[\cos\left(\frac{\pi}{n}\right) + i\sin\left(\frac{\pi}{n}\right)\right]^{\frac{k}{2}} = \cos\left(\frac{\pi k}{n}\right) + i\sin\left(\frac{\pi k}{n}\right).$$

Then

$$\begin{aligned} C + iS &= \left(2\cos\frac{\pi}{n} + 2i\sin\frac{\pi}{n}\right) + \left(2\cos\frac{2\pi}{n} + 2i\sin\frac{2\pi}{n}\right) + \cdots + \left(2\cos\frac{\pi k}{n} + 2i\sin\frac{\pi k}{n}\right) \\ &= 2\gamma + 2\gamma^2 + \cdots + 2\gamma^{\frac{k}{2}} \\ &= 2\gamma\left(1 + \gamma + \cdots + \gamma^{\frac{k}{2}-1}\right) \\ &= 2\gamma\frac{1 - \gamma^{\frac{k}{2}}}{1 - \gamma} \end{aligned}$$

$$\begin{aligned}
&= 2\gamma \frac{\left[1 - \left(\cos\left(\frac{\pi k}{n}\right) + i\sin\left(\frac{\pi k}{n}\right)\right)\right]}{\left(1 - \cos\left(\frac{\pi}{n}\right)\right) - i\sin\left(\frac{\pi}{n}\right)} \\
&= 2 \left(\cos\frac{\pi}{n} + i\sin\frac{\pi}{n}\right) \frac{\left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{\left(1 - \cos\frac{\pi}{n}\right) - i\sin\frac{\pi}{n}} \times \frac{\left(1 - \cos\frac{\pi}{n}\right) + i\sin\frac{\pi}{n}}{\left(1 - \cos\frac{\pi}{n}\right) + i\sin\frac{\pi}{n}} \\
&= 2 \frac{\left[\cos\frac{\pi}{n} + i\sin\frac{\pi}{n}\right] \left[\left(1 - \cos\frac{\pi}{n}\right) + i\sin\frac{\pi}{n}\right] \left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{\left(1 - \cos\frac{\pi}{n}\right)^2 + \sin^2\frac{\pi}{n}} \\
&= \frac{2 \left[\left(\cos\frac{\pi}{n} - 1\right) + i\left(\sin\frac{\pi}{n} - \cos\frac{\pi}{n}\sin\frac{\pi}{n} + \cos\frac{\pi}{n}\sin\frac{\pi}{n}\right)\right] \left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{2 - 2\cos\frac{\pi}{n}} \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) + i\sin\frac{\pi}{n}\right] \left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{1 - \cos\frac{\pi}{n}} \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) + i\sin\frac{\pi}{n}\right] \left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{1 - \left(\cos^2\frac{\pi}{2n} - \sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) + i\sin\frac{\pi}{n}\right] \left[\left(1 - \cos\left(\frac{\pi k}{n}\right)\right) - i\sin\left(\frac{\pi k}{n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)}
\end{aligned}$$

Taking the real parts:

$$\begin{aligned}
C &= \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{\pi j}{n}\right) \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) \left(1 - \cos\left(\frac{\pi k}{n}\right)\right) + \left(\sin\frac{\pi}{n}\right) \sin\left(\frac{\pi k}{n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi k}{n}\right) + \cos\left(\frac{\pi k}{n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)}
\end{aligned}$$

For $k = n$, we get

$$\begin{aligned}
C &= \sum_{j=1}^{\frac{n}{2}} 2\cos\left(\frac{\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi}{2}\right) + \cos\left(\frac{\pi}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\cos^2\frac{\pi}{2n} - \sin^2\frac{\pi}{2n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[-2\sin^2\frac{\pi}{2n} + \sin\left(\frac{\pi}{n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[-2\sin^2\frac{\pi}{2n} + 2\sin\left(\frac{\pi}{2n}\right)\cos\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \cot\left(\frac{\pi}{2n}\right) - 1.
\end{aligned}$$

This gives result (1) of theorem 3.2.1.

2. Recall from Theorem 3.2.1, result (1), that

$$\begin{aligned}
C &= \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi k}{n 2}\right) + \cos\left(\frac{\pi k}{n 2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)}
\end{aligned}$$

For $k = n - 1$, we get

$$\begin{aligned}
C &= \sum_{j=1}^{\frac{n-1}{2}} 2\cos\left(\frac{\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi}{n} \frac{n-1}{2}\right) + \cos\left(\frac{\pi}{n} \frac{n-1}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} \frac{n+1}{2}\right) + \cos\left(\frac{\pi}{n} \frac{n-1}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) - \left(-\sin\left(\frac{\pi}{2n}\right)\right) + \left(\sin\left(\frac{\pi}{2n}\right)\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[\left(\cos\frac{\pi}{n} - 1\right) + 2\sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \frac{\left[-2\sin^2\left(\frac{\pi}{2n}\right) + 2\sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)} \\
&= \operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1.
\end{aligned}$$

3. Recall from Theorem 3.2.1, result (1), that

$$C = \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{\pi j}{n}\right) = \frac{\left[\cos\frac{\pi}{n} - 1 - \cos\left(\frac{\pi}{n} + \frac{\pi}{n} \frac{k}{2}\right) + \cos\left(\frac{\pi}{n} \frac{k}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{2n}\right)}$$

So let

$$\begin{aligned}
D &= \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{2\pi j}{n}\right), \text{ then} \\
D &= \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{2\pi j}{n}\right) = \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi}{n} + \frac{2\pi}{n} \frac{k}{2}\right) + \cos\left(\frac{2\pi}{n} \frac{k}{2}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)}
\end{aligned}$$

For $k = \frac{n-1}{2}$, we get

$$\begin{aligned}
D &= \sum_{j=1}^{\frac{n-1}{4}} 2\cos\left(\frac{2\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi}{n} + \frac{2\pi}{n}\frac{n-1}{4}\right) + \cos\left(\frac{2\pi}{n}\frac{n-1}{4}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi}{n}\frac{n+3}{4}\right) + \cos\left(\frac{2\pi}{n}\frac{n-1}{4}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= \frac{\left[-2\sin^2\frac{\pi}{n} - \left(\cos\frac{\pi}{2}\cos\frac{3\pi}{2n} - \sin\frac{\pi}{2}\sin\frac{3\pi}{2n}\right) + \left(\cos\frac{\pi}{2}\cos\frac{\pi}{2n} + \sin\frac{\pi}{2}\sin\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{3\pi}{2n}\right) + \sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{\pi}{n} + \frac{\pi}{2n}\right) + \sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\frac{\pi}{n}\cos\frac{\pi}{2n} + \cos\frac{\pi}{n}\sin\frac{\pi}{2n} + \sin\frac{\pi}{2n}\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[2\sin\frac{\pi}{2n}\cos\frac{\pi}{2n}\cos\frac{\pi}{2n} + \sin\frac{\pi}{2n}(\cos\frac{\pi}{n} + 1)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[2\sin\frac{\pi}{2n}\cos\frac{\pi}{2n}\cos\frac{\pi}{2n} + \sin\frac{\pi}{2n}(\cos^2\frac{\pi}{2n} - \cos^2\frac{\pi}{2n} + 1)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[2\sin\left(\frac{\pi}{2n}\right)\cos\left(\frac{\pi}{2n}\right)\cos\left(\frac{\pi}{2n}\right) + \sin\left(\frac{\pi}{2n}\right)2\cos^2\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[4\sin\left(\frac{\pi}{2n}\right)\cos^2\left(\frac{\pi}{2n}\right)\right]}{\left(8\sin^2\left(\frac{\pi}{2n}\right)\cos^2\left(\frac{\pi}{2n}\right)\right)} \\
&= \frac{1}{2}\operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1.
\end{aligned}$$

4. Recall from theorem 3.2.1, result (3), that

$$\begin{aligned}
D &= \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{2\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi}{n} + \frac{2\pi k}{n \cdot 2}\right) + \cos\left(\frac{2\pi k}{n \cdot 2}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)}
\end{aligned}$$

For $k = \frac{n-3}{2}$, we get

$$\begin{aligned}
D &= \sum_{j=1}^{\frac{n-3}{4}} 2\cos\left(\frac{2\pi j}{n}\right) \\
&= \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi}{n} + \frac{2\pi n-3}{n \cdot 4}\right) + \cos\left(\frac{2\pi n-3}{n \cdot 4}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= \frac{\left[\cos\frac{2\pi}{n} - 1 - \cos\left(\frac{2\pi n+1}{n \cdot 4}\right) + \cos\left(\frac{2\pi n-3}{n \cdot 4}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= \frac{\left[-2\sin^2\frac{\pi}{2} - \left(\cos\frac{\pi}{2}\cos\frac{\pi}{2n} - \sin\frac{\pi}{2}\sin\frac{\pi}{2n}\right) + \left(\cos\frac{\pi}{2}\cos\frac{3\pi}{2n} + \sin\frac{\pi}{2}\sin\frac{3\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{\pi}{2n}\right) + \sin\left(\frac{3\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{\pi}{2n}\right) + \sin\left(\frac{\pi}{n}\right)\cos\left(\frac{\pi}{2n}\right) + \cos\left(\frac{\pi}{n}\right)\sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{\pi}{2n}\right) + 2\sin\left(\frac{\pi}{2n}\right)\cos^2\left(\frac{\pi}{2n}\right) + \left(\cos^2\left(\frac{\pi}{2n}\right) - \sin^2\left(\frac{\pi}{2n}\right)\right)\sin\left(\frac{\pi}{2n}\right)\right]}{\left(2\sin^2\frac{\pi}{n}\right)}
\end{aligned}$$

$$\begin{aligned}
&= -1 + \frac{\left[\sin\left(\frac{\pi}{2n}\right) + 2\sin\left(\frac{\pi}{2n}\right)\cos^2\left(\frac{\pi}{2n}\right) + \left(\cos^2\left(\frac{\pi}{2n}\right) - \left(1 - \cos^2\frac{\pi}{2n}\right)\right)\sin\left(\frac{\pi}{2n}\right) \right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{\left[\sin\left(\frac{\pi}{2n}\right) + 2\sin\left(\frac{\pi}{2n}\right)\cos^2\left(\frac{\pi}{2n}\right) + \left(2\cos^2\left(\frac{\pi}{2n}\right) - 1\right)\sin\left(\frac{\pi}{2n}\right) \right]}{\left(2\sin^2\frac{\pi}{n}\right)} \\
&= -1 + \frac{4\sin\frac{\pi}{2n}\cos^2\frac{\pi}{2n}}{8\sin^2\frac{\pi}{2n}\cos^2\frac{\pi}{2n}} \\
&= \frac{1}{2}\operatorname{cosec}\frac{\pi}{2n} - 1. \quad \square
\end{aligned}$$

3.2.1 Energy of The Path Graph

Let P_n be the path on n vertices, and with $n - 1$ edges.

Lemma 3.2.1. The eigenvalues of the path graph P_n are $\lambda_j = 2\cos\left(\frac{\pi j}{n+1}\right)$; $1 \leq j \leq n$ (each with multiplicity 1) for $n \geq 2$ (See Jessop [28] and section 2.5.7).

Theorem 3.2.2. The energy of the path is for :

1. n even,

$$E(P_n) = \sum_{j=1}^n \left| 2\cos\left(\frac{\pi j}{n+1}\right) \right| = 2 \left[\operatorname{cosec}\frac{\pi}{2(n+1)} - 1 \right];$$

2. n odd,

$$E(P_n) = \sum_{j=1}^n \left| 2\cos\left(\frac{\pi j}{n+1}\right) \right| = 2 \left[\cot\frac{\pi}{2(n+1)} - 1 \right]$$

Proof

As per Lemma 3.2.1, the eigenvalues of the path graph P_n are $\lambda_j = 2\cos\frac{\pi j}{n+1}$; $1 \leq j \leq n$, so

$$E(P_n) = \sum_{j=1}^n |\lambda_j| = \sum_{j=1}^n \left| 2\cos\left(\frac{\pi j}{n+1}\right) \right|.$$

1. Now let n be even, i.e. $n = 2t$, $t \in \mathbb{N}$. Then

$$\begin{aligned}
E(P_n) &= \sum_{j=1}^n \left| 2\cos\left(\frac{\pi j}{n+1}\right) \right| \\
&= \sum_{j=1}^{2t} \left| 2\cos\left(\frac{\pi j}{2t+1}\right) \right|
\end{aligned}$$

$$\begin{aligned}
&= \sum_{j=1}^t \left[\left| 2\cos\left(\frac{\pi j}{2t+1}\right) \right| + \left| 2\cos\left(\frac{\pi(2t+1-j)}{2t+1}\right) \right| \right] \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+1}\right) \right| + 2 \left| \cos\left(\frac{\pi(2t+1)}{2t+1}\right) \cos\left(\frac{\pi j}{2t+1}\right) + \sin\left(\frac{\pi(2t+1)}{2t+1}\right) \sin\left(\frac{\pi j}{2t+1}\right) \right| \right] \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+1}\right) \right| + 2 \left| \cos(\pi) \cos\left(\frac{\pi j}{2t+1}\right) + \sin(\pi) \sin\left(\frac{\pi j}{2t+1}\right) \right| \right] \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+1}\right) \right| + 2 \left| -\cos\left(\frac{\pi j}{2t+1}\right) \right| \right]
\end{aligned}$$

Now $\frac{j}{2t+1} < 0.5$ for $1 \leq j \leq t$, so $\cos\left(\frac{\pi j}{2t+1}\right) \geq 0$. Therefore

$$\begin{aligned}
E(P_n) &= \sum_{j=1}^t \left[2\cos\left(\frac{\pi j}{2t+1}\right) + 2\cos\left(\frac{\pi j}{2t+1}\right) \right] \\
&= 2 \sum_{j=1}^t 2\cos\left(\frac{\pi j}{2t+1}\right) \\
&= 2 \sum_{j=1}^{\frac{n}{2}} 2\cos\left(\frac{\pi j}{n+1}\right)
\end{aligned}$$

Setting $k = n + 1$, we get

$$E(P_n) = 2 \sum_{j=1}^{\frac{k-1}{2}} 2\cos\left(\frac{\pi j}{k}\right)$$

Now applying result 2 from Theorem 3.2.1, we get

$$\begin{aligned}
E(P_n) &= 2 \left(\operatorname{cosec}\left(\frac{\pi}{2k}\right) - 1 \right) \\
&= 2 \left(\operatorname{cosec}\frac{\pi}{2(n+1)} - 1 \right)
\end{aligned}$$

2. Now let n be odd, i.e. $n = 2t + 1$, $t \in \mathbb{N}$. Then

$$\begin{aligned}
E(P_n) &= \sum_{j=1}^n \left| 2\cos\left(\frac{\pi j}{n+1}\right) \right| \\
&= \sum_{j=1}^{2t+1} \left| 2\cos\left(\frac{\pi j}{2t+2}\right) \right| \\
&= \sum_{j=1}^t \left[\left| 2\cos\left(\frac{\pi j}{2t+2}\right) \right| + \left| 2\cos\left(\frac{\pi(2t+2-j)}{2t+2}\right) \right| \right] + \left| 2\cos\left(\frac{\pi(t+1)}{2t+2}\right) \right| \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+2}\right) \right| + 2 \left| \cos\left(\frac{\pi(2t+2)}{2t+2}\right) \cos\left(\frac{\pi j}{2t+2}\right) + \sin\left(\frac{\pi(2t+2)}{2t+2}\right) \sin\left(\frac{\pi j}{2t+2}\right) \right| \right] \\
&\quad + 2\cos\left(\frac{\pi}{2}\right) \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+2}\right) \right| + 2 \left| \cos(\pi) \cos\left(\frac{\pi j}{2t+2}\right) + \sin(\pi) \sin\left(\frac{\pi j}{2t+2}\right) \right| \right] \\
&= \sum_{j=1}^t \left[2 \left| \cos\left(\frac{\pi j}{2t+2}\right) \right| + 2 \left| -\cos\left(\frac{\pi j}{2t+2}\right) \right| \right]
\end{aligned}$$

Now $\frac{j}{2t+2} < 0.5$ for $1 \leq j \leq t$, so $\cos\left(\frac{\pi j}{2t+2}\right) \geq 0$. Therefore

$$\begin{aligned}
E(P_n) &= \sum_{j=1}^t \left[2\cos\left(\frac{\pi j}{2t+2}\right) + 2\cos\left(\frac{\pi j}{2t+2}\right) \right] \\
&= 2 \sum_{j=1}^t 2\cos\left(\frac{\pi j}{2t+2}\right) \\
&= 2 \sum_{j=1}^{\frac{n-1}{2}} 2\cos\left(\frac{\pi j}{n+1}\right)
\end{aligned}$$

Setting $k = n + 1$, we get

$$\begin{aligned}
E(P_n) &= 2 \sum_{j=1}^{\frac{k-2}{2}} 2\cos\left(\frac{\pi j}{k}\right) \\
&= 2 \sum_{j=1}^{\frac{k}{2}-1} 2\cos\left(\frac{\pi j}{k}\right) + 2\cos\left(\frac{\pi k}{2k}\right) \\
&= 2 \sum_{j=1}^{\frac{k}{2}} 2\cos\left(\frac{\pi j}{k}\right)
\end{aligned}$$

Now applying result 1 from Theorem 3.2.1, we get

$$\begin{aligned}
E(P_n) &= 2 \left(\cot\left(\frac{\pi}{2k}\right) - 1 \right) \\
&= 2 \left(\cot\frac{\pi}{2(n+1)} - 1 \right) \quad \square
\end{aligned}$$

3.2.2 Energy of The Cycle Graph

Let C_n be the cycle graph on n vertices, and with n edges.

Lemma 3.2.2. The eigenvalues of the cycle graph C_n are $\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right); j = 0, \dots, n-1$ (each with multiplicity 1), for $n \geq 3$ (See Jessop [27] and section 2.5.6)

The following observation will be used to solve Theorem 3.2.3 below

Lemma 3.2.3

$$2 \left[\cos\frac{\pi}{2t+1} + \cos\frac{3\pi}{2t+1} + \dots + \cos\frac{(2t-1)\pi}{2t+1} \right] = 2 \sum_{r=1}^t \cos\frac{\pi(2t-2r+1)}{2t+1} = 1; t = 1, 2, \dots$$

(See Winter, Jessop and Adewusi [48]).

Theorem 3.2.3 (see Winter and Jessop [52])

1. Let $q \in \mathbb{N}$ and $n = 4q + 1$, then

$$\sum_{j=q+1}^{2q} \left| \cos\left(\frac{2\pi j}{n}\right) \right| = \sum_{j=1}^q \left| \cos\left(\frac{2\pi j}{n}\right) \right| + \frac{1}{2}.$$

2. Let $q \in \mathbb{N}$ and $n = 4q + 3$, then

$$\sum_{j=q+1}^{2q+1} \left| \cos\left(\frac{2\pi j}{n}\right) \right| = \sum_{j=1}^q \left| \cos\left(\frac{2\pi j}{n}\right) \right| + \frac{1}{2}.$$

Proof

1. From Lemma 3.2.2, for n odd and t even, i.e. $n = 2t + 1$, $t = 2q$, and $n = 4q + 1$; and for $q = 1, 2, \dots$, we have

$$2 \sum_{r=1}^t \cos \left(\frac{\pi(2t - 2r + 1)}{2t + 1} \right) = 1; \quad t = 2, 3, 4, \dots$$

$$\Rightarrow \sum_{r=1}^{2q} \cos \left(\frac{\pi(4q - 2r + 1)}{4q + 1} \right) = \frac{1}{2};$$

$$\Rightarrow \left[\cos \frac{\pi}{4q+1} + \cos \frac{3\pi}{4q+1} + \cos \frac{5\pi}{4q+1} + \dots + \cos \frac{(2q-1)\pi}{4q+1} \right] +$$

$$\left[\cos \frac{(2q+1)\pi}{4q+1} + \cos \frac{(2q+3)\pi}{4q+1} + \cos \frac{(2q+5)\pi}{4q+1} + \dots + \cos \frac{(4q-1)\pi}{4q+1} \right] = [A] + [B] = \frac{1}{2}$$

where

$$A = \cos \frac{\pi}{4q+1} + \cos \frac{3\pi}{4q+1} + \cos \frac{5\pi}{4q+1} + \dots + \cos \frac{(2q-1)\pi}{4q+1} \quad (q \text{ terms}), \text{ and}$$

$$B = \cos \frac{(2q+1)\pi}{4q+1} + \cos \frac{(2q+3)\pi}{4q+1} + \cos \frac{(2q+5)\pi}{4q+1} + \dots + \cos \frac{(4q-1)\pi}{4q+1} \quad (q \text{ terms}).$$

All terms in [A] are positive. Now

$$A = \cos \frac{\pi}{4q+1} + \cos \frac{3\pi}{4q+1} + \cos \frac{5\pi}{4q+1} + \dots + \cos \frac{(2q-1)\pi}{4q+1}$$

$$= \cos \frac{((4q+1) - 4q)\pi}{4q+1} + \cos \frac{((4q+1) - (4q-2))\pi}{4q+1} + \cos \frac{((4q+1) - (4q-4))\pi}{4q+1} + \dots$$

$$+ \cos \frac{((4q+1) - (2q+2))\pi}{4q+1}$$

$$= -\cos \frac{(4q)\pi}{4q+1} - \cos \frac{(4q-2)\pi}{4q+1} - \cos \frac{(4q-4)\pi}{4q+1} - \dots - \cos \frac{(2q+2)\pi}{4q+1}$$

$$A = - \sum_{j=q+1}^{2q} \cos \frac{2\pi j}{4q+1}$$

$$B = \cos \frac{(2q+1)\pi}{4q+1} + \cos \frac{(2q+3)\pi}{4q+1} + \cos \frac{(2q+5)\pi}{4q+1} + \dots + \cos \frac{(4q-1)\pi}{4q+1}$$

$$= \cos \frac{((4q+1) - (2q))\pi}{4q+1} + \cos \frac{((4q+1) - (2q-2))\pi}{4q+1} + \cos \frac{((4q+1) - (2q-4))\pi}{4q+1} + \dots$$

$$+ \cos \frac{((4q+1) - (2))\pi}{4q+1}$$

$$= -\cos \frac{(2q)\pi}{4q+1} - \cos \frac{(2q-2)\pi}{4q+1} - \cos \frac{(2q-4)\pi}{4q+1} - \dots - \cos \frac{(2)\pi}{4q+1}$$

$$B = -C$$

Where

$$C = \cos \frac{(2q)\pi}{4q+1} + \cos \frac{(2q-2)\pi}{4q+1} + \cos \frac{(2q-4)\pi}{4q+1} + \cdots + \cos \frac{(2)\pi}{4q+1} = \sum_{j=1}^q \cos \frac{(2j)\pi}{4q+1}$$

and all term in C are positive. Therefore

$$A + B = \frac{1}{2} \Rightarrow A = C + \frac{1}{2}.$$

Then

$$- \sum_{j=q+1}^{2q} \cos \frac{2\pi j}{4q+1} = \sum_{j=1}^q \cos \frac{2\pi j}{4q+1} + \frac{1}{2}$$

Taking absolute values of both sides, we get

$$\sum_{j=q+1}^{2q} \left| \cos \frac{2\pi j}{4q+1} \right| = \sum_{j=1}^q \left| \cos \frac{2\pi j}{4q+1} \right| + \frac{1}{2}$$

2. From Lemma 3.2.2, for n odd and t odd, i.e. $n = 2t + 1$, $t = 2q + 1$, and $n = 4q + 3$; and for $q = 1, 2, \dots$, we have

$$2 \sum_{r=1}^t \cos \left(\frac{\pi(2t - 2r + 1)}{2t + 1} \right) = 1; \quad t = 3, 4, 5 \dots$$

$$\Rightarrow \sum_{r=1}^{2q+1} \cos \left(\frac{\pi(4q + 2 - 2r + 1)}{4q + 3} \right) = \frac{1}{2};$$

$$\Rightarrow \left[\cos \frac{\pi}{4q+3} + \cos \frac{3\pi}{4q+3} + \cos \frac{5\pi}{4q+3} + \cdots + \cos \frac{(2q+1)\pi}{4q+3} \right] +$$

$$\left[\cos \frac{(2q+3)\pi}{4q+3} + \cos \frac{(2q+5)\pi}{4q+3} + \cos \frac{(2q+7)\pi}{4q+3} + \cdots + \cos \frac{(4q+1)\pi}{4q+3} \right] = [A] + [B] = \frac{1}{2}$$

where

$$A = \cos \frac{\pi}{4q+3} + \cos \frac{3\pi}{4q+3} + \cos \frac{5\pi}{4q+3} + \cdots + \cos \frac{(2q+1)\pi}{4q+3} \quad (q+1 \text{ terms}), \text{ and}$$

$$B = \cos \frac{(2q+3)\pi}{4q+3} + \cos \frac{(2q+5)\pi}{4q+3} + \cos \frac{(2q+7)\pi}{4q+3} + \cdots + \cos \frac{(4q+1)\pi}{4q+3} \quad (q \text{ terms}).$$

All terms in $[A]$ are positive. Indeed, the first term in A is $\cos \frac{\pi}{4q+3}$ which is positive, since

$\frac{\pi}{4q+3}$ is clearly in the first quadrant; the last term is $\cos \frac{(2q+1)\pi}{4q+3}$, this is positive, because

$$0 < \frac{(2q+1)\pi}{4q+3} < \frac{2q\pi}{4q+3} < \frac{2q\pi}{4q} = \frac{1}{2}\pi.$$

So $\cos \frac{(2q+1)\pi}{4q+3}$ is in the first quadrant as well. Hence $\cos \frac{(2q+1)\pi}{4q+3} > 0$

Now

$$\begin{aligned}
A &= \cos \frac{\pi}{4q+3} + \cos \frac{3\pi}{4q+3} + \cos \frac{5\pi}{4q+3} + \cdots + \cos \frac{(2q+1)\pi}{4q+3} \\
&= \cos \frac{((4q+3) - (4q+2))\pi}{4q+3} + \cos \frac{((4q+3) - (4q))\pi}{4q+3} + \cos \frac{((4q+3) - (4q-2))\pi}{4q+3} + \cdots \\
&\quad + \cos \frac{((4q+3) - (2q+2))\pi}{4q+3} \\
&= -\cos \frac{(4q+2)\pi}{4q+3} - \cos \frac{(4q)\pi}{4q+3} - \cos \frac{(4q-2)\pi}{4q+3} - \cdots - \cos \frac{(2q+2)\pi}{4q+3}
\end{aligned}$$

$$A = - \sum_{j=q+1}^{2q+1} \cos \frac{2\pi j}{4q+3}$$

$$\begin{aligned}
B &= \cos \frac{(2q+3)\pi}{4q+3} + \cos \frac{(2q+5)\pi}{4q+3} + \cos \frac{(2q+7)\pi}{4q+3} + \cdots + \cos \frac{(4q+1)\pi}{4q+3} \\
&= \cos \frac{((4q+3) - (2q))\pi}{4q+3} + \cos \frac{((4q+3) - (2q-2))\pi}{4q+3} + \cos \frac{((4q+3) - (2q-4))\pi}{4q+3} + \cdots \\
&\quad + \cos \frac{((4q+3) - (2))\pi}{4q+3} \\
&= -\cos \frac{(2q)\pi}{4q+3} - \cos \frac{(2q-2)\pi}{4q+3} - \cos \frac{(2q-4)\pi}{4q+3} - \cdots - \cos \frac{(2)\pi}{4q+3}
\end{aligned}$$

$$B = -C$$

Where

$$C = \cos \frac{(2q)\pi}{4q+3} + \cos \frac{(2q-2)\pi}{4q+3} + \cos \frac{(2q-4)\pi}{4q+3} + \cdots + \cos \frac{(2)\pi}{4q+3} = \sum_{j=1}^q \cos \frac{(2j)\pi}{4q+3}$$

and all terms in C are positive. Therefore

$$\begin{aligned}
A + B &= \frac{1}{2} \\
\Rightarrow A &= C + \frac{1}{2} \\
\Rightarrow - \sum_{j=q+1}^{2q+1} \cos \frac{2\pi j}{4q+3} &= \sum_{j=1}^q \cos \frac{2\pi j}{4q+3} + \frac{1}{2}
\end{aligned}$$

Taking absolute values of both sides, we get

$$\sum_{j=q+1}^{2q+1} \left| \cos \frac{2\pi j}{4q+3} \right| = \sum_{j=1}^q \left| \cos \frac{2\pi j}{4q+3} \right| + \frac{1}{2}$$

□

Theorem 3.2.4. The energy of the cycle graph C_n is given by:

1. For n even, and $n = 2t$,

1.1 For t even, then

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4\cot\left(\frac{\pi}{n}\right).$$

1.2 For t odd, then

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4\operatorname{cosec}\left(\frac{\pi}{n}\right).$$

2. For n odd, and $n = 2t + 1$,

2.1 For t even, then

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

2.2 For t odd, then

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

Proof. From Lemma 3.2.2, the eigenvalues of the cycle graph C_n are $\lambda_j = 2\cos\frac{2\pi j}{n}; j = 0, 1, \dots, n-1$, so

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

1. Now let n be even, i.e. $n = 2t$. Then

$$\begin{aligned} E(C_n) &= \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\ &= \sum_{j=0}^{2t-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\ &= 2 \left[\left| \cos\left(\frac{0}{n}\right) \right| + \left| \cos\left(\frac{2\pi}{n}\right) \right| + \left| \cos\left(\frac{4\pi}{n}\right) \right| + \dots + \left| \cos\left(\frac{2\pi t}{n}\right) \right| \right] \\ &\quad + 2 \left[\left| \cos\left(\frac{2\pi(t+1)}{n}\right) \right| + \dots + \left| \cos\left(\frac{2\pi(2t-1)}{n}\right) \right| \right] \\ &= 2 \sum_{k=0}^{t-1} \left[\left| \cos\left(\frac{2\pi k}{n}\right) \right| + \left| \cos\left(\frac{2\pi(k+t)}{n}\right) \right| \right] \\ &= 2 \sum_{k=0}^{t-1} \left[\left| \cos\left(\frac{2\pi k}{2t}\right) \right| + \left| \cos\left(\frac{2\pi k}{2t} + \frac{2\pi t}{2t}\right) \right| \right] \end{aligned}$$

$$\begin{aligned}
&= 2 \sum_{k=0}^{t-1} \left[\left| \cos \left(\frac{2\pi k}{2t} \right) \right| + \left| \cos \left(\frac{2\pi k}{2t} \right) \cos(\pi) - \sin \left(\frac{2\pi k}{2t} \right) \sin(\pi) \right| \right] \\
&= 2 \sum_{k=0}^{t-1} \left[\left| \cos \left(\frac{2\pi k}{2t} \right) \right| + \left| -\cos \left(\frac{2\pi k}{2t} \right) \right| \right] \\
&= 2 \sum_{k=0}^{t-1} \left| 2\cos \left(\frac{2\pi k}{2t} \right) \right| \\
&\Rightarrow E(C_n) = 2 \sum_{k=0}^{t-1} \left| 2\cos \left(\frac{2\pi k}{2t} \right) \right|
\end{aligned}$$

Now,

$$\begin{aligned}
E(C_n) &= \sum_{j=0}^{2t-1} \left| 2\cos \left(\frac{2\pi j}{n} \right) \right| \\
&= 2 \sum_{k=0}^{t-1} \left| 2\cos \left(\frac{2\pi k}{2t} \right) \right| \\
&= 2 \sum_{k=0}^{t-1} \left| 2\cos \left(\frac{\pi k}{t} \right) \right| \\
&= 2 \left[|2\cos(0)| + \sum_{k=1}^{t-1} \left| 2\cos \left(\frac{\pi k}{t} \right) \right| \right] \\
&= 2 \left[2 + \sum_{k=1}^{t-1} \left| 2\cos \left(\frac{\pi k}{t} \right) \right| \right] \\
&\Rightarrow E(C_n) = 2 \left[2 + \sum_{k=1}^{t-1} \left| 2\cos \left(\frac{\pi k}{t} \right) \right| \right]
\end{aligned}$$

Set $l = t - 1$, then

$$E(C_n) = 2 \left[2 + \sum_{k=1}^l \left| 2\cos \left(\frac{\pi k}{l+1} \right) \right| \right].$$

1.1 For t even and l odd, we have from Theorem 3.2.1 result 2,

$$\sum_{k=1}^l \left| 2\cos \left(\frac{\pi k}{l+1} \right) \right| = 2 \left(\cot \left(\frac{\pi}{2(l+1)} \right) - 1 \right)$$

So

$$\begin{aligned}
E(C_n) &= 2 \left[2 + \sum_{k=1}^l \left| 2\cos \left(\frac{\pi k}{l+1} \right) \right| \right] \\
&= 2 \left[2 + 2 \left(\cot \left(\frac{\pi}{2(l+1)} \right) - 1 \right) \right] \\
&= 4 \left[1 + \cot \left(\frac{\pi}{2t} \right) - 1 \right] \\
&= 4\cot \left(\frac{\pi}{2t} \right) \\
&= 4\cot \left(\frac{\pi}{n} \right) \\
&\Rightarrow E(C_n) = 4\cot \left(\frac{\pi}{n} \right)
\end{aligned}$$

1.2 For t odd and l even, we have from Theorem 3.2.1 result 1,

$$\sum_{k=1}^l \left| 2\cos \left(\frac{\pi k}{l+1} \right) \right| = 2 \left(\operatorname{cosec} \left(\frac{\pi}{2(l+1)} \right) - 1 \right)$$

So

$$\begin{aligned}
E(C_n) &= 2 \left[2 + \sum_{k=1}^l \left| 2\cos \left(\frac{\pi k}{l+1} \right) \right| \right] \\
&= 2 \left[2 + 2 \left(\operatorname{cosec} \left(\frac{\pi}{2(l+1)} \right) - 1 \right) \right] \\
&= 4 \left[1 + \operatorname{cosec} \left(\frac{\pi}{2t} \right) - 1 \right] \\
&= 4\operatorname{cosec} \left(\frac{\pi}{2t} \right) \\
&= 4\operatorname{cosec} \left(\frac{\pi}{n} \right) \\
&\Rightarrow E(C_n) = 4\operatorname{cosec} \left(\frac{\pi}{n} \right)
\end{aligned}$$

2. Now let n be odd, i.e. $n = 2t + 1$. Then

$$\begin{aligned}
E(C_n) &= \sum_{j=0}^{2t} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\
&= \left| 2\cos\left(\frac{0}{n}\right) \right| + \sum_{j=1}^{2t} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\
&= \left| 2\cos\left(\frac{0}{n}\right) \right| + \sum_{j=1}^t \left[\left| 2\cos\left(\frac{2\pi j}{2t+1}\right) \right| + \left| 2\cos\left(\frac{2\pi(2t+1-j)}{2t+1}\right) \right| \right] \\
&= 2 + \sum_{j=1}^t \left[\left| 2\cos\left(\frac{2\pi j}{2t+1}\right) \right| + \left| 2\cos\left(2\pi - \frac{2\pi j}{2t+1}\right) \right| \right] \\
&= 2 + \sum_{j=1}^t \left[\left| 2\cos\left(\frac{2\pi j}{2t+1}\right) \right| + \left| 2\cos(2\pi)\cos\left(\frac{2\pi j}{2t+1}\right) + 2\sin(2\pi)\sin\left(\frac{2\pi j}{2t+1}\right) \right| \right] \\
&= 2 + \sum_{j=1}^t \left[\left| 2\cos\left(\frac{2\pi j}{2t+1}\right) \right| + \left| 2\cos\left(\frac{2\pi j}{2t+1}\right) \right| \right] \\
&= 2 + 2 \sum_{j=1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\
&\Rightarrow E(C_n) = 2 + 2 \sum_{j=1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right|
\end{aligned}$$

2.1 Now for t even, we get

$$\begin{aligned}
E(C_n) &= 2 + 2 \sum_{j=1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\
&= 2 + 2 \left[\sum_{j=1}^{\frac{t}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + \sum_{j=\frac{t}{2}+1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \right]
\end{aligned}$$

Now from Theorem 3.2.3, for t even ($t = 2q$ and $q \in \mathbb{N}$),

$$\sum_{j=\frac{t}{2}+1}^t \left| \cos\left(\frac{2\pi j}{n}\right) \right| = \sum_{j=1}^{\frac{t}{2}} \left| \cos\left(\frac{2\pi j}{n}\right) \right| + \frac{1}{2}.$$

so,

$$\begin{aligned} E(C_n) &= 2 + 2 \left[\sum_{j=1}^{\frac{t}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + \sum_{j=1}^{\frac{t}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + 1 \right] \\ &= 4 + 4 \sum_{j=1}^{\frac{t}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \end{aligned}$$

Now for $1 \leq j \leq \frac{t}{2}$, $2\cos\left(\frac{2\pi k}{n}\right) \geq 0$, so

$$E(C_n) = 4 + 4 \sum_{j=1}^{\frac{t}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4 + 4 \sum_{j=1}^{\frac{t}{2}} 2\cos\left(\frac{2\pi j}{n}\right) = 4 + 4 \sum_{j=1}^{\frac{n-1}{4}} 2\cos\left(\frac{2\pi j}{n}\right).$$

Now from Theorem 3.2.1 result 3,

$$\sum_{j=1}^{\frac{n-1}{4}} 2\cos\left(\frac{2\pi j}{n}\right) = \frac{1}{2} \operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1;$$

so

$$E(C_n) = 4 + 4 \left(\frac{1}{2} \operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1 \right) = 2 \operatorname{cosec}\left(\frac{\pi}{2n}\right).$$

2.2 Now for t odd, we get

$$\begin{aligned} E(C_n) &= 2 + 2 \sum_{j=1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \\ &= 2 + 2 \left[\sum_{j=1}^{\frac{t-1}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + \sum_{j=\frac{t-1}{2}+1}^t \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \right] \end{aligned}$$

Now from Theorem 3.2.3, for t odd ($t = 2q + 1$ and $q \in \mathbb{N}$),

$$\sum_{j=\frac{t-1}{2}+1}^t \left| \cos\left(\frac{2\pi j}{n}\right) \right| = \sum_{j=1}^{\frac{t-1}{2}} \left| \cos\left(\frac{2\pi j}{n}\right) \right| + \frac{1}{2}.$$

So,

$$\begin{aligned} E(C_n) &= 2 + 2 \left[\sum_{j=1}^{\frac{t-1}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + \sum_{j=1}^{\frac{t-1}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| + 1 \right] \\ &= 4 + 4 \sum_{j=1}^{\frac{t-1}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| \end{aligned}$$

Now for $1 \leq j \leq \frac{t}{2}$, $2\cos\left(\frac{2\pi k}{n}\right) \geq 0$, so

$$E(C_n) = 4 + 4 \sum_{j=1}^{\frac{t-1}{2}} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4 + 4 \sum_{j=1}^{\frac{t-1}{2}} 2\cos\left(\frac{2\pi j}{n}\right) = 4 + 4 \sum_{j=1}^{\frac{n-3}{4}} 2\cos\left(\frac{2\pi j}{n}\right).$$

Now from Theorem 3.2.1 result 4,

$$\sum_{j=1}^{\frac{n-3}{4}} 2\cos\left(\frac{2\pi j}{n}\right) = \frac{1}{2}\operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1;$$

so

$$E(C_n) = 4 + 4\left(\frac{1}{2}\operatorname{cosec}\left(\frac{\pi}{2n}\right) - 1\right) = 2\operatorname{cosec}\left(\frac{\pi}{2n}\right). \quad \square$$

3.2.3 Energy of The Wheel Graph

Theorem 3.2.5. (See Winter and Jessop [52])

The energy of the wheel graph W_n is

1. For n even,

$$E(W_n) = 2\sqrt{n} - 2 + 2\operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right).$$

2. For n odd, and $n = 2t + 1$,

- 2.1 For t even, then

$$E(W_n) = 2\sqrt{n} - 2 + 4\cot\left(\frac{\pi}{n-1}\right).$$

- 2.2 For t odd, then

$$E(W_n) = 2\sqrt{n} - 2 + 4\operatorname{cosec}\left(\frac{\pi}{n-1}\right).$$

Proof. We know (see corollary 2.5.1) that the eigenvalues of the wheel graph W_n are: $0, 1 \pm \sqrt{n}$ (each with multiplicity 1), and $\lambda_j = 2\cos\frac{2\pi j}{n-1}; j = 1, \dots, n-2$ (each with multiplicity 1).

For $n \geq 4$, we have

$$\begin{aligned} E(W_n) &= \sum_{i=1}^n |\lambda_i| \\ &= |0| + |1 + \sqrt{n}| + |1 - \sqrt{n}| + \sum_{j=1}^{n-2} \left| 2\cos\frac{2\pi j}{n-1} \right| \\ &= (1 + \sqrt{n}) + (-(1 - \sqrt{n})) + \sum_{j=1}^{n-2} \left| 2\cos\frac{2\pi j}{n-1} \right| \\ &= 1 + \sqrt{n} - 1 + \sqrt{n} + \sum_{j=1}^{n-2} \left| 2\cos\frac{2\pi j}{n-1} \right| \\ \Rightarrow E(W_n) &= 2\sqrt{n} + \sum_{j=1}^{n-2} \left| 2\cos\frac{2\pi j}{n-1} \right| \end{aligned}$$

Setting $k = n - 1$, then

$$\begin{aligned}
E(W_n) &= 2\sqrt{k+1} + \sum_{j=1}^{k-1} \left| 2\cos \frac{2\pi j}{k} \right| \\
&= 2\sqrt{k+1} + \sum_{j=0}^{k-1} \left| 2\cos \frac{2\pi j}{k} \right| - 2 \\
&= 2\sqrt{k+1} - 2 + \sum_{j=0}^{k-1} \left| 2\cos \frac{2\pi j}{k} \right|
\end{aligned}$$

From Theorem 3.2.4 we get

1. For n even, k odd,

$$\begin{aligned}
E(W_n) &= 2\sqrt{k+1} - 2 + \sum_{j=0}^{k-1} \left| 2\cos \frac{2\pi j}{k} \right| \\
&= 2\sqrt{k+1} - 2 + 2\operatorname{cosec} \left(\frac{\pi}{2k} \right) \\
&= 2\sqrt{n} - 2 + 2\operatorname{cosec} \left(\frac{\pi}{2(n-1)} \right) \\
\Rightarrow E(W_n) &= 2\sqrt{n} - 2 + 2\operatorname{cosec} \left(\frac{\pi}{2(n-1)} \right)
\end{aligned}$$

2. For n odd, k even, and $k = 2t$,

2.1 For t even, then

$$E(W_n) = 2\sqrt{k+1} - 2 + 4\cot \left(\frac{\pi}{k} \right)$$

Now $n = k + 1 = 2t + 1$, so n is odd. Therefore

$$E(W_n) = 2\sqrt{n} - 2 + 4\cot \left(\frac{\pi}{n-1} \right).$$

2.2 For t odd, then

$$E(W_n) = 2\sqrt{k+1} - 2 + 4\operatorname{cosec} \left(\frac{\pi}{k} \right).$$

Now $n = k + 1 = 2t + 1$, so n is odd. Therefore

$$E(W_n) = 2\sqrt{n} - 2 + 4\operatorname{cosec} \left(\frac{\pi}{n-1} \right). \quad \square$$

Lemma 3.2.4. For large values of n the following expressions behave in the following way:

1. $\lim_{n \rightarrow \infty} \left[\operatorname{cosec} \left(\frac{\pi}{n} \right) \right] \approx \frac{n}{\pi}$; n large
2. $\lim_{n \rightarrow \infty} \left[\cot \left(\frac{\pi}{n} \right) \right] \approx \frac{n}{\pi}$; n large.

Proof. we use the following results

$$(i) \quad \lim_{x \rightarrow 0^+} \sin x = x$$

$$(ii) \quad \lim_{x \rightarrow 0^+} \cos x = 1.$$

So,

$$\begin{aligned} 1. \lim_{n \rightarrow \infty} \left[\operatorname{cosec} \left(\frac{\pi}{n} \right) \right] &= \lim_{n \rightarrow \infty} \left[\frac{1}{\sin \left(\frac{\pi}{n} \right)} \right] \\ &\approx \frac{1}{\frac{\pi}{n}} \quad \text{from (i)} \\ &= \frac{n}{\pi} \end{aligned}$$

$$\begin{aligned} 2. \lim_{n \rightarrow \infty} \left[\cot \left(\frac{\pi}{n} \right) \right] &= \lim_{n \rightarrow \infty} \left[\frac{\cos \left(\frac{\pi}{n} \right)}{\sin \left(\frac{\pi}{n} \right)} \right] \\ &\approx \frac{1}{\frac{\pi}{n}} \quad \text{from (i) and (ii)} \\ &= \frac{n}{\pi} \end{aligned}$$

□

Theorem 3.2.6. For large n , the energy of paths, cycles and wheels (as classes denoted by \mathfrak{F}) is:

$$\lim_{n \rightarrow \infty} E(\mathfrak{F}) \approx \frac{4n}{\pi}$$

Proof

(1)- *Energy of the path graph P_n for large n :*

For n even,

$$\begin{aligned} E(P_n) &= \sum_{j=1}^n \left| 2 \cos \left(\frac{\pi j}{n+1} \right) \right| = 2 \left(\operatorname{cosec} \frac{\pi}{2(n+1)} - 1 \right) \\ \Rightarrow \lim_{n \rightarrow \infty} E(P_n) &= \lim_{n \rightarrow \infty} \left[2 \left(\operatorname{cosec} \frac{\pi}{2(n+1)} - 1 \right) \right] \approx \frac{2.2n}{\pi} = \frac{4n}{\pi} \end{aligned}$$

For n odd,

$$\begin{aligned} E(P_n) &= \sum_{j=1}^n \left| 2 \cos \left(\frac{\pi j}{n+1} \right) \right| = 2 \left(\cot \frac{\pi}{2(n+1)} - 1 \right) \\ \Rightarrow \lim_{n \rightarrow \infty} E(P_n) &= \lim_{n \rightarrow \infty} \left[2 \left(\cot \frac{\pi}{2(n+1)} - 1 \right) \right] \approx \frac{2.2n}{\pi} = \frac{4n}{\pi} \end{aligned}$$

Therefore, for large n , the energy of the path graph P_n is

$$\lim_{n \rightarrow \infty} [E(P_n)] \approx \frac{4n}{\pi}.$$

(2)- Energy of the cycle graph C_n for large n :

For n even, $n = 2t$ and t even,

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4\cot\left(\frac{\pi}{n}\right)$$

$$\Rightarrow \lim_{n \rightarrow \infty} E(C_n) = \lim_{n \rightarrow \infty} \left[4\cot\left(\frac{\pi}{n}\right) \right] = \frac{4n}{\pi}$$

For n even, $n = 2t$ and t odd,

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4\operatorname{cosec}\left(\frac{\pi}{n}\right)$$

$$\Rightarrow \lim_{n \rightarrow \infty} E(C_n) = \lim_{n \rightarrow \infty} \left[4\operatorname{cosec}\left(\frac{\pi}{n}\right) \right] = \frac{4n}{\pi}$$

For n odd, $n = 2t + 1$ and all t ,

$$E(C_n) = 2\operatorname{cosec}\left(\frac{\pi}{2n}\right)$$

$$\Rightarrow \lim_{n \rightarrow \infty} E(C_n) = \lim_{n \rightarrow \infty} \left[2\operatorname{cosec}\left(\frac{\pi}{2n}\right) \right] = \frac{4n}{\pi}$$

Therefore, for large n , the energy of the cycle graph C_n is

$$\lim_{n \rightarrow \infty} [E(C_n)] = \frac{4n}{\pi}.$$

(3)- Energy of the wheel graph W_n for large n :

For large n we have

$$\lim_{n \rightarrow \infty} [E(W_n)] = \lim_{n \rightarrow \infty} \left[2\sqrt{n} + \sum_{j=1}^{n-2} \left| 2\cos\frac{2\pi j}{n-1} \right| \right].$$

Set $k = n - 1$. Then

$$\begin{aligned} \lim_{n \rightarrow \infty} [E(W_n)] &= \lim_{k \rightarrow \infty} \left[2\sqrt{k+1} - 2 + \sum_{j=0}^{k-1} \left| 2\cos\frac{2\pi j}{k} \right| \right] \\ &= \lim_{k \rightarrow \infty} \left[2\sqrt{k+1} - 2 + E(C_k) \right] \\ &\approx \lim_{k \rightarrow \infty} [E(C_k)] \\ &= \lim_{n \rightarrow \infty} [E(C_n)] \\ &= \frac{4n}{\pi} \\ \Rightarrow \lim_{n \rightarrow \infty} [E(W_n)] &\approx \frac{4n}{\pi} \end{aligned}$$

Therefore, for large n , the energy of the wheel graph W_n is

$$\lim_{n \rightarrow \infty} [E(W_n)] \approx \frac{4n}{\pi}.$$

□

3.3 Energy of generalized sun graphs

Theorem 3.3.1 (See Winter and Jessop [52])

The energy of the generalized sun graph $SG(h,p)$ is

$$E(SG(h,p)) = \sum_{i=1}^p \sqrt{\alpha_j^2 + 4h}$$

where α_j are the eigenvalues of $A(G)$.

Proof. Let λ_j be the eigenvalues of $A(SG(h,p))$. Then

$$E(SG(h,p)) = \sum_{j=1}^{p(h+1)} |\lambda_j| = \sum_{j=1}^p \left[\left| \frac{\alpha_j + \sqrt{\alpha_j^2 + 4h}}{2} \right| + \left| \frac{\alpha_j - \sqrt{\alpha_j^2 + 4h}}{2} \right| \right]$$

Since

$$\frac{\alpha_j - \sqrt{\alpha_j^2 + 4h}}{2} < 0$$

we have

$$\left| \frac{\alpha_j - \sqrt{\alpha_j^2 + 4h}}{2} \right| = \frac{-\alpha_j + \sqrt{\alpha_j^2 + 4h}}{2}.$$

So that,

$$\begin{aligned} E(SG(h,p)) &= \sum_{j=1}^p \left[\frac{\alpha_j + \sqrt{\alpha_j^2 + 4h}}{2} + \frac{-\alpha_j + \sqrt{\alpha_j^2 + 4h}}{2} \right] \\ &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \end{aligned}$$

where α_j are the eigenvalues of $A(G)$.

□

3.3.1 Energy of Caterpillar Graph

Let $CT(k,l)$ be the caterpillar graph where k and l denote the number of vertices on the path and the number of pendant edges respectively. This graph has $n = k(l+1)$ vertices. Let $L(CT(k,l))$ be the line graph of $CT(k,l)$.

Theorem 3.3.2. (see winter and Jessop [52])

The energy of $L(CT(k,l))$ is

$$E(L(CT(k,l))) = k(l-1) + \sum_{j=2}^k \left| \frac{1}{2} \left(l-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right|$$

$$+ \sum_{j=2}^k \left| \frac{1}{2} \left(l-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right|$$

$$\text{where } \sigma_j = 2\cos\left(\frac{(k+1-j)\pi}{k}\right), \text{ for } j = 1, \dots, k.$$

Proof

The laplacian eigenvalues of the caterpillar graph $CT(k,l)$ are given by Lemma 2.6.1 and since $CT(k,l)$ is a bipartite graph, from Lemma 2.6.2, the eigenvalues of $L(CT(k,l))$ can be derived from the Laplacian eigenvalues of $CT(k,l)$, namely

$$\mu = \lambda - 2 = 1 - 2 = -1, \text{ with multiplicity } k(l-1)$$

$$\mu_j = \lambda_j - 2$$

$$= \frac{1}{2} \left(l-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right), \text{ where } \sigma_j = 2\cos\left(\frac{(k+1-j)\pi}{k}\right),$$

for $j = 2, \dots, k$, and

$$\mu_{k+j} = \lambda_j - 2$$

$$= \frac{1}{2} \left(l-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right), \text{ where } \sigma_j = 2\cos\left(\frac{(k+1-j)\pi}{k}\right),$$

for $j = 1, \dots, k$.

Therefore the energy of $L(CT(k,l))$ is

$$\begin{aligned}
E(L(CT(k,l))) &= \sum_{i=1}^n |\lambda_i| \\
&= k(l-1) + \sum_{j=2}^k \left| \frac{1}{2} \left(l-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right| \\
&\quad + \sum_{j=1}^k \left| \frac{1}{2} \left(l-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right|
\end{aligned}$$

$$\text{where } \sigma_j = 2\cos\left(\frac{(k+1-j)\pi}{k}\right), \text{ for } j = 1, \dots, k.$$

□

3.3.2 Energy of the Complete Sun Graph

Theorem 3.3.3. The energy of the complete sun graph is

$$E(CompSun(h,p)) = (p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}.$$

Proof. From Theorem 3.3.1,

$$\begin{aligned}
E(CompSun(h,p)) &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \text{ where } \alpha_j \text{ are the eigenvalues of } A(K_p) \\
&= (p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}.
\end{aligned}$$

□

3.3.3 Energy of the Complete Split-bipartite Sun Graph

Theorem 3.3.4. The energy of the complete split-bipartite sun graph is

$$E(BipSun(h,p)) = \sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}.$$

Proof. From Theorem 3.3.1,

$$\begin{aligned}
E(BipSun(h,p)) &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \text{ where } \alpha_j \text{ are the eigenvalues of } A(K_{\frac{p}{2}, \frac{p}{2}}) \\
&= \sqrt{\left(\frac{p}{2}\right)^2 + 4h} + \sqrt{\left(-\frac{p}{2}\right)^2 + 4h} + (p-2)\sqrt{4h} \\
&= \sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}.
\end{aligned}$$

□

3.3.4 Energy of the Wheel Sun Graph

Theorem 3.3.4. The energy of the wheel sun graph is

$$E(\text{WheelSun}(h,p)) = 2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}.$$

Proof. From Theorem 3.3.1,

$$\begin{aligned} E(\text{WheelSun}(h,p)) &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \text{ where } \alpha_j \text{ are the eigenvalues of } A(W_p) \\ &= \sum_{k=1}^{p-2} \sqrt{\left(2\cos\left(\frac{2\pi k}{p-1}\right)\right)^2 + 4h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}} \\ &= 2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}. \quad \square \end{aligned}$$

3.3.5 Energy of the Star Sun Graph

Theorem 3.3.5. The energy of the Star sun graph is

$$E(\text{StarSun}(h,p)) = 2\sqrt{p-1+4h} + 2(p-2)\sqrt{h}.$$

Proof. From Theorem 3.3.1,

$$\begin{aligned} E(\text{starSun}(h,p)) &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \text{ where } \alpha_j \text{ are the eigenvalues of } A(S_{p-1,1}) \\ &= \sqrt{(+\sqrt{p-1})^2 + 4h} + \sqrt{(-\sqrt{p-1})^2 + 4h} + (p-2)\sqrt{(0)^2 + 4h} \\ &= 2\sqrt{p-1+4h} + 2(p-2)\sqrt{h}. \quad \square \end{aligned}$$

3.3.6 Energy of the Cycle Sun Graph

Theorem 3.3.6. The energy of the cycle sun graph is

$$E(\text{CycleSun}(h,p)) = 2 \sum_{k=0}^{p-1} \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h}.$$

Proof. From Theorem 3.3.1,

$$\begin{aligned}
E(\text{CycleSun}(h,p)) &= \sum_{j=1}^p \sqrt{\alpha_j^2 + 4h} \text{ where } \alpha_j \text{ are the eigenvalues of } A(C_p) \\
&= \sum_{k=0}^{p-1} \sqrt{\left(2\cos\left(\frac{2\pi k}{p}\right)\right)^2 + 4h} \\
&= 2 \sum_{k=0}^{p-1} \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h}. \quad \square
\end{aligned}$$

3.4 Energy of some other Graphs

3.4.1 Energy of The Complete Graph

Let K_n be the complete graph on n vertices, and with $\frac{n(n-1)}{2}$ edges. The eigenvalues of the complete graph K_n on n vertices are $\lambda = 1$ (with multiplicity $(n-1)$), and $\lambda = (n-1)$ with multiplicity 1 (See Jessop [28] and section 2.5.3)

So the energy of the complete graph is

$$E(K_n) = 2(n-1).$$

For large n , the energy of the complete graph K_n is

$$\lim_{n \rightarrow \infty} [E(K_n)] \approx 2n.$$

3.4.2 Energy of The Complete Split-bipartite Graph $K_{\frac{n}{2}, \frac{n}{2}}$

Let $K_{\frac{n}{2}, \frac{n}{2}}$ be the complete split-bipartite graph on n vertices, and with $\frac{n^2}{4}$ edges. The eigenvalues of the complete split-bipartite Graph $K_{\frac{n}{2}, \frac{n}{2}}$ are $\lambda = 0$ (with multiplicity $n-2$) and $\lambda = \pm \frac{n}{2}$ (each with multiplicity 1). See Jessop [28].

So the energy of the complete split-bipartite graph is

$$E(K_{\frac{n}{2}, \frac{n}{2}}) = n.$$

For large n , the energy of the complete split-bipartite graph $K_{\frac{n}{2}, \frac{n}{2}}$ is

$$\lim_{n \rightarrow \infty} \left[E(K_{\frac{n}{2}, \frac{n}{2}}) \right] = n.$$

3.4.3 Energy of The Star Graph, with rays of length 1

Let $S_{n-1,1}$ be the star graph on n vertices, and with $n - 1$ rays of length 1, $n \geq 2$. The eigenvalues of the star graph $S_{n-1,1}$ are $\lambda = 0$ (with multiplicity $n - 2$) and $\lambda = \pm\sqrt{n-1}$ (each with multiplicity 1). See Jessop [28] and Theorem 2.5.6

So the energy of the star graph $S_{n-1,1}$ is

$$E(S_{n-1,1}) = 2\sqrt{n-1}.$$

For large n , the energy of the star graph $S_{n-1,1}$ is

$$\lim_{n \rightarrow \infty} [E(S_{n-1,1})] \approx 2\sqrt{n}.$$

3.4.4 Energy of The Star Graph, with rays of length 2

Let $S_{\frac{n-1}{2},2}$ be the star graph on n vertices, and with $\frac{n-1}{2}$ rays of length 2, $n \geq 3$. The eigenvalues of the star graph $S_{\frac{n-1}{2},2}$ are $\lambda = 0$ (with multiplicity 1), $\lambda = \pm 1$ (each with multiplicity $\frac{n-1}{2} - 1$) and $\lambda = \pm\sqrt{\frac{n-1}{2} + 1}$ (each with multiplicity 1). See Jessop [28] and Theorem 2.5.7

So the energy of the star graph $S_{\frac{n-1}{2},2}$ is

$$E(S_{\frac{n-1}{2},2}) = n - 3 + \sqrt{2(n+1)}$$

For large n , the energy of the star graph $S_{\frac{n-1}{2},2}$ is

$$\lim_{n \rightarrow \infty} [E(S_{\frac{n-1}{2},2})] \approx n + \sqrt{2n}.$$

3.4.5 Energy of The Dual Star Graph

Let $D_u S_n$ be the dual star graph. We know (see Winter and Jessop [51] and section 2.5.9.) that the eigenvalues of $D_u S_n$ are:

$$\lambda_1 = \sqrt{\frac{(n-1) + \sqrt{2n-3}}{2}}, \lambda_2 = -\sqrt{\frac{(n-1) + \sqrt{2n-3}}{2}},$$

$$\lambda_3 = \sqrt{\frac{(n-1) - \sqrt{2n-3}}{2}} \text{ and } \lambda_4 = -\sqrt{\frac{(n-1) - \sqrt{2n-3}}{2}}$$

each with multiplicity 1.

So the energy of the dual star graph $D_u S_n$ is

$$E(D_u S_n) = 2\sqrt{\frac{(n-1) + \sqrt{2n-3}}{2}} + 2\sqrt{\frac{(n-1) - \sqrt{2n-3}}{2}}.$$

For large n , the energy of the dual star graph $D_u S_n$ is

$$\lim_{n \rightarrow \infty} [E(D_u S_n)] \approx 2\sqrt{\frac{n + \sqrt{2n}}{2}} + 2\sqrt{\frac{n - \sqrt{2n}}{2}} \approx 2\sqrt{2n}.$$

3.4.6 Energy of The Lollipop Graph

Theorem 3.4.1. The energy of the lollipop graph LP_n is

$$E(LP_n) = n - 3.$$

Proof. The eigenvalues of the lollipop graph LP_n are $\lambda = -1$ (multiplicity $n - 3$); So, the energy of the lollipop graph LP_n is

$$\begin{aligned} E(LP_n) &= |(-1)|(n - 3) \\ &= n - 3. \end{aligned} \quad \square$$

3.4.7 Energy of The Friendship Graph

Theorem 3.4.2. The energy of a friendship graph F_p on n vertices, where $p = \frac{n-1}{2}$ is

$$E(F_p) = (2p - 1) + \sqrt{1 + 8p}.$$

See M.R. Rajesh Kanna and All [35]

Proof. Eigenvalues of F_p are $\lambda = -1$ (with multiplicity p), $\lambda = 1$ (with multiplicity $(p - 1)$), $\lambda = \frac{1 + \sqrt{1 + 8p}}{2}$ (with multiplicity 1) and $\lambda = \frac{1 - \sqrt{1 + 8p}}{2}$ (with multiplicity 1);

See Theorem 2.5.12 in section 2.5. The energy of the friendship graphs F_p is

$$\begin{aligned} E(F_p) &= |(-1)|p + |1|(p - 1) + \left| \frac{1 + \sqrt{1 + 8p}}{2} \right| + \left| \frac{1 - \sqrt{1 + 8p}}{2} \right| \\ &= (2p - 1) + \left| \frac{-1 - \sqrt{1 + 8p}}{2} \right| + \left| \frac{1 - \sqrt{1 + 8p}}{2} \right| = (2p - 1) + \left| \frac{-1}{2} + \frac{1}{2} - 2\frac{\sqrt{1 + 8p}}{2} \right| \\ &= (2p - 1) + \sqrt{1 + 8p}. \end{aligned} \quad \square$$

3.4.8 Energy of the Line Graph of the complete graph K_n

Let $L(K_n)$ be the Line Graph of the complete graph K_n . We know (see theorem 2.5.11), that the eigenvalues of $L(K_n)$ are: $\lambda = -2$, with multiplicity $\frac{n(n-3)}{2}$; $\lambda = 2n - 4$, with multiplicity 1, and $\lambda = n - 4$, with multiplicity $(n - 1)$. So that, the energy of $L(K_n)$, for $n \geq 5$, is

$$E(L(K_n)) = 2n^2 - 6n.$$

Proof.

$$\begin{aligned} E(L(K_n)) &= |-2|\frac{n(n-3)}{2} + |2n-4| + |n-4|(n-1) \\ &= n(n-3) + 2n-4 + (n-4)(n-1) \\ &= 2n^2 - 6n. \end{aligned} \quad \square$$

3.5 Energy of the complement of the cycle graph

The bulk of the proof is my own.

Theorem 3.5.1.[27] The energy of the complement of a cycle graph \overline{C}_n is

$$E(\overline{C}_n) = \begin{cases} 2 \left(\frac{2n-9}{3} + \sqrt{3} \cot \frac{\pi}{n} \right); & \text{for } n = 3k \\ 2 \left(\frac{2n-8}{3} + \frac{2 \sin \frac{\pi}{3} (1 - \frac{1}{n})}{\sin \frac{\pi}{n}} \right); & \text{for } n = 3k+1 \\ 2 \left(\frac{2n-10}{3} + \frac{2 \sin \frac{\pi}{3} (1 + \frac{1}{n})}{\sin \frac{\pi}{n}} \right); & \text{for } n = 3k+2. \end{cases} \quad (k \geq 1)$$

Proof.

We know by Example 2.7.2 that, the eigenvalues of the complement of a Cycle graph \overline{C}_n , on n vertices (with $n \geq 3$), are:

$$n-3, \quad -1 - 2 \cos \left(\frac{2\pi j}{n} \right), \quad j = 1, \dots, (n-1); \text{ each with multiplicity } 1.$$

So that

$$\begin{aligned} E(\overline{C}_n) &= |n-3| + \sum_{j=1}^{n-1} \left| -1 - 2 \cos \left(\frac{2\pi j}{n} \right) \right| \\ &= n-3 + \sum_{j=1}^{n-1} \left| -(1 + 2 \cos \left(\frac{2\pi j}{n} \right)) \right| \end{aligned}$$

$$\Rightarrow E(\overline{C}_n) = n-3 + \sum_{j=1}^{n-1} \left| -(1 + 2 \cos \left(\frac{2\pi j}{n} \right)) \right|. \quad (1)$$

$$\left| -(1 + 2 \cos \left(\frac{2\pi j}{n} \right)) \right| = \begin{cases} - \left(1 + 2 \cos \left(\frac{2\pi j}{n} \right) \right); & \text{if } - \left(1 + 2 \cos \left(\frac{2\pi j}{n} \right) \right) \geq 0 \\ 1 + 2 \cos \left(\frac{2\pi j}{n} \right); & \text{if } - \left(1 + 2 \cos \left(\frac{2\pi j}{n} \right) \right) \leq 0 \end{cases}$$

Case 1. $n = 3k \Rightarrow k = \frac{n}{3}$.

Then,

$$-(1 + 2 \cos \left(\frac{2\pi j}{n} \right)) \geq 0 \iff 1 + 2 \cos \left(\frac{2\pi j}{n} \right) \leq 0$$

$$\iff \cos \left(\frac{2\pi j}{n} \right) \leq -\frac{1}{2} \iff \frac{2\pi}{3} \leq \frac{2\pi j}{n} \leq \frac{4\pi}{3}$$

$$\iff \frac{1}{3} \leq \frac{j}{n} \leq \frac{2}{3} \iff \frac{n}{3} \leq j \leq \frac{2n}{3}.$$

$$\begin{aligned}
\text{Let } \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} (1 + 2 \cos \left(\frac{2\pi j}{n} \right)) &= \frac{n}{3} + 1 + \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \cos \left(\frac{2\pi j}{n} \right) \\
&= \frac{n+3}{3} + \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \cos \left(\frac{2\pi j}{n} \right) \\
\sum_{j=\frac{n}{3}}^{\frac{2n}{3}} (1 + 2 \cos \left(\frac{2\pi j}{n} \right)) &= \frac{n+3}{3} + \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \cos \left(\frac{2\pi j}{n} \right)
\end{aligned}$$

and

$$C = \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \cos \left(\frac{2\pi j}{n} \right); \quad S = \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \sin \left(\frac{2\pi j}{n} \right); \quad \gamma = \cos \frac{2\pi}{n} + i \sin \frac{2\pi}{n} \quad \text{so that } \gamma^j = \cos \frac{2\pi j}{n} + i \sin \frac{2\pi j}{n}.$$

Then

$$\begin{aligned}
C + iS &= 2 \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} \gamma^j = 2(\gamma^{\frac{n}{3}} + \gamma^{\frac{n}{3}+1} + \gamma^{\frac{n}{3}+2} + \dots + \gamma^{\frac{2n}{3}-1} + \gamma^{\frac{2n}{3}}) \\
&= 2\gamma^{\frac{n}{3}}(1 + \gamma + \gamma^2 + \dots + \gamma^{\frac{n}{3}-1} + \gamma^{\frac{n}{3}}) \\
&= 2\gamma^{\frac{n}{3}} \left(\frac{1 - \gamma^{\frac{n}{3}+1}}{1 - \gamma} \right); \quad \gamma \neq 1.
\end{aligned}$$

So

$$\begin{aligned}
C + iS &= 2 \left(\cos \left(\frac{2\pi}{n} \cdot \frac{n}{3} \right) + i \sin \left(\frac{2\pi}{n} \cdot \frac{n}{3} \right) \right) \left(\frac{1 - (\cos \frac{2\pi}{n} \cdot (\frac{n}{3} + 1) + i \sin \frac{2\pi}{n} \cdot (\frac{n}{3} + 1))}{1 - (\cos \frac{2\pi}{n} + i \sin \frac{2\pi}{n})} \right) \\
&= 2 \left(-\frac{1}{2} + \frac{\sqrt{3}}{2}i \right) \left(\frac{\left(1 + \frac{1}{2} \cos \frac{2\pi}{n} + \frac{\sqrt{3}}{2} \sin \frac{2\pi}{n} \right) + i \left(\frac{1}{2} \sin \frac{2\pi}{n} - \frac{\sqrt{3}}{2} \cos \frac{2\pi}{n} \right)}{(1 - \cos \frac{2\pi}{n}) - i \sin \frac{2\pi}{n}} \right)
\end{aligned}$$

$C + iS =$

$$2 \left(-\frac{1}{2} + \frac{\sqrt{3}}{2}i \right) \left(\frac{\left(1 + \frac{1}{2} \cos \frac{2\pi}{n} + \frac{\sqrt{3}}{2} \sin \frac{2\pi}{n} \right) + i \left(\frac{1}{2} \sin \frac{2\pi}{n} - \frac{\sqrt{3}}{2} \cos \frac{2\pi}{n} \right)}{(1 - \cos \frac{2\pi}{n})^2 + \sin^2 \frac{2\pi}{n}} \right) \left(\left(1 - \cos \frac{2\pi}{n} \right) + i \sin \frac{2\pi}{n} \right)$$

Let

$$\begin{aligned}
K &= \left(1 + \frac{1}{2} \cos \frac{2\pi}{n} + \frac{\sqrt{3}}{2} \sin \frac{2\pi}{n}\right) \left(1 - \cos \frac{2\pi}{n}\right) \\
iL &= i \left(1 + \frac{1}{2} \cos \frac{2\pi}{n} + \frac{\sqrt{3}}{2} \sin \frac{2\pi}{n}\right) \sin \frac{2\pi}{n} \\
iM &= i \left(\frac{1}{2} \sin \frac{2\pi}{n} - \frac{\sqrt{3}}{2} \cos \frac{2\pi}{n}\right) \left(1 - \cos \frac{2\pi}{n}\right) \\
N &= \left(\frac{\sqrt{3}}{2} \cos \frac{2\pi}{n} - \frac{1}{2} \sin \frac{2\pi}{n}\right) \sin \frac{2\pi}{n}
\end{aligned}$$

So,

$$\begin{aligned}
C + iS &= 2 \left(-\frac{1}{2} + \frac{\sqrt{3}}{2}i\right) \left(\frac{(K + N) + i(L + M)}{2 - 2 \cos \frac{2\pi}{n}}\right) \\
&= \frac{1}{2} \left(\frac{-(K + N) - \sqrt{3}(L + M)}{1 - \cos \frac{2\pi}{n}} + i \frac{\sqrt{3}(K + N) - (L + M)}{1 - \cos \frac{2\pi}{n}}\right).
\end{aligned}$$

Taking the real parts:

$$\begin{aligned}
C &= \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} 2 \cos \frac{2\pi j}{n} = \frac{1}{2} \left(\frac{-(K + N) - \sqrt{3}(L + M)}{1 - \cos \frac{2\pi}{n}}\right) \\
&= -\frac{1}{2} \frac{(K + \sqrt{3}M) + (N + \sqrt{3}L)}{1 - \cos \frac{2\pi}{n}} \\
&= -\frac{1}{2} \frac{(1 - \cos \frac{2\pi}{n} + \sqrt{3} \sin \frac{2\pi}{n})(1 - \cos \frac{2\pi}{n}) + (\sqrt{3} + \sqrt{3} \cos \frac{2\pi}{n} + \sin \frac{2\pi}{n}) \sin \frac{2\pi}{n}}{1 - \cos \frac{2\pi}{n}} \\
&= -\frac{1}{2} \left(\frac{2 - 2 \cos \frac{2\pi}{n} + 2\sqrt{3} \sin \frac{2\pi}{n}}{1 - \cos \frac{2\pi}{n}}\right) \\
&= -\left(\frac{1 - \cos \frac{2\pi}{n} + \sqrt{3} \sin \frac{2\pi}{n}}{1 - \cos \frac{2\pi}{n}}\right) \\
&= -\left(1 + \frac{2\sqrt{3} \cos \frac{\pi}{n} \sin \frac{\pi}{n}}{1 - (\cos^2 \frac{\pi}{n} - \sin^2 \frac{\pi}{n})}\right) \\
&= -\left(1 + \frac{2\sqrt{3} \cos \frac{\pi}{n} \sin \frac{\pi}{n}}{2 \sin^2 \frac{\pi}{n}}\right)
\end{aligned}$$

So, we get

$$C = -(1 + \sqrt{3} \cot \frac{\pi}{n}).$$

And

$$\sum_{j=\frac{n}{3}}^{\frac{2n}{3}} \left(1 + 2 \cos \frac{2\pi j}{n}\right) = \frac{n+3}{3} - \left(1 + \sqrt{3} \cot \frac{\pi}{n}\right).$$

The total sum of all the positive eigenvalues of \overline{C}_n is

$$\begin{aligned} n - 3 + \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} \left(-\left(1 + 2 \cos \frac{2\pi j}{n}\right)\right) &= n - 3 - \sum_{j=\frac{n}{3}}^{\frac{2n}{3}} \left(1 + 2 \cos \frac{2\pi j}{n}\right) \\ &= n - 3 - \left(\frac{n+3}{3} - \left(1 + \sqrt{3} \cot \frac{\pi}{n}\right)\right) \\ &= n - 3 + \left(1 + \sqrt{3} \cot \frac{\pi}{n}\right) - \frac{n+3}{3}; \\ &= \frac{2n-9}{3} + \sqrt{3} \cot \frac{\pi}{n}. \end{aligned}$$

Thus, using the lemma 3.1.1, the energy of the complement of a cycle graph, on n vertices with $n \geq 3$ and $n \equiv 0 \pmod{3}$ i.e $n = 3k$ with $k \geq 1$, is

$$E(\overline{C}_n) = 2 \left(\frac{2n-9}{3} + \sqrt{3} \cot \frac{\pi}{n}\right).$$

Similarly we can provide the other two cases: for $n = 3k + 1$ and $n = 3k + 2$, $k \geq 1$. □

3.6 Hyper-energetic graphs

A graph G , having energy greater than the complete graph K_n on the same number of vertices n , is called *hyper-energetic* i.e.

$$E(G) > 2(n-1) \text{ (see Stevanovic [41]).}$$

Example: The line graph $L(K_n)$ of the complete graph K_n is hyper-energetic for $n \geq 5$.

Because, we know (see section 3.4.8) that $E(L(K_n)) = 2n^2 - 6n$, and since $L(K_n)$ has $n(n-1)/2$ vertices, $E(K_{n(n-1)/2}) = 2(n(n-1)/2 - 1) = n^2 - n - 2$. So that

$$E(L(K_n)) = 2n^2 - 6n > n^2 - n - 2 = E(K_{n(n-1)/2}) \text{ for } n \geq 5.$$

3.7 Conclusion

Using the eigenvalues found in previous chapter, we have determined the energy of some classes of graphs studied in chapter 1. We analyzed the energies of the path graph, cycle graph and wheel graph on n vertices. We expressed the energy of cycles, paths and wheels in terms of simplified expressions using the cotangent or cosecant. We used the analytical methods.

Chapter 4

THE CHROMATIC NUMBER OF A GRAPH

In this Chapter, we give a brief history about the origin and the importance of the chromatic number. we give also the basic definitions on different types of colouring, and everything on finding the chromatic number of graphs.

In Graph theory, graph colouring is a special case of graph labeling. It is an assignment of labels traditionally called colours to the edges or vertices of a graph based on a set of specified criteria is known as graph colouring. In its simplest form, it is a way of colouring the vertices of a graph such that no two adjacent vertices share the same colour; this is called a Vertex colouring.

The chromatic idea can be translated to a molecular construction. So, the chromatic number associated with the molecular graph (the atoms are vertices and edges are bonds between the atoms) would involve the partitioning of the atoms into the smallest number of sets of like atoms so that like atoms are not bonded. For example, the water molecule H_2O has two hydrogen atoms bonded to an oxygen atom, the hydrogen atoms are not bonded, so that, the molecular graphic version would involve the chromatic number of 2, where the oxygen atom has a different colour to the hydrogen atoms which are assigned the same colour; While, the benzene ring molecule C_6H_6 has same atoms (carbon atoms) are bonded.



Figure 4.1. *Water molecule*

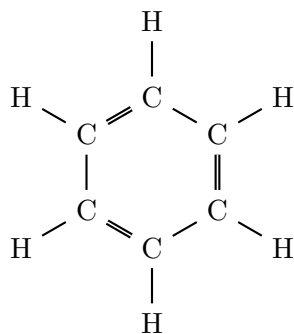


Figure 4.2. *The benzene ring molecule*

The other examples: the hydrogen sulfide molecule H_2S , the ammonia molecule H_3N , the methane molecule CH_4 have respectively two, three, four hydrogen atoms bonded to another atom, such that same atoms are not bonded.

The atoms bond to form molecules. And different atoms are forced to bond in order to get *stability*; Different atoms come together to achieve the noble gas configuration. This coming together and sharing of electron pairs leads to the formation of a chemical bond know as a covalent bond.

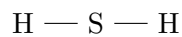


Figure 4.3. *The hydrogen sulfide molecule*

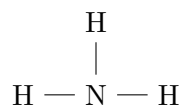


Figure 4.4. *The ammonia molecule*

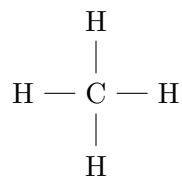


Figure 4.5. *The methane molecule*

A *covalent bond* is a shared pair of electrons between two different nonmetal atoms. These electrons can originate from one atom, or one electron can originate from each of the two atoms. The two electrons in the bond are attracted to both atomic nuclei and are shared between the two atoms. Two different atoms share the electrons because atoms (other than hydrogen and helium) are most stable when surrounded by eight electrons (an octet), which means that an atom with a full octet of electrons has lower energy (is more stable) than one without a full octet (See Winter, Mayala and Namayanja [56] and Wiswesser [57]).

4.1 Origin of Chromatic Theory

Chromatic Theory goes back to a problem, posed some 152 years ago, relating to the colouring of maps, either real or imaginary. The condition postulated was that countries with a common border line (and not just a border point) should receive different colours.

The question was, "How many colours are needed to cover all the different maps imaginable?" The practical answer turned out to be four at most, but this was only proved theoretically by K. Appel and W. Haken some 40 years ago. The first proof was published in 1976 as a 140 pages document with microfiche of some 1482 cases, after many hundreds of hours of computer work.

Apart from being an exercise in abstract thinking, what practical application does this have? The chromatic theory brings one immediate application to mind. If you want to make a timetable for an exam, one common condition is that you cannot have two papers written by students at the same time if one or more of the students has to write both papers. If you rephrase the

problem correctly it turn out to be a simple colouring matter. The idea of using the minimum number of colors then translates to, "What is the minimum number of session you need to set up the timetable?"

4.2 Vertex colouring

Vertex colouring is the following optimization problem: given a graph G , how many colours are required to colour its vertices in such a way no two adjacent vertices receive the same colour? The required number of colours is called the chromatic number of G and is denoted by $\chi(G)$.

Although the chromatic number is one of the most studied parameters in graph theory, no formula exists for the chromatic number of an arbitrary graph. Thus, for the most part, one must be content with supplying bounds for the chromatic number of graphs.

4.2.1 Definitions

Definition 4.1. A (*vertex*) *colouring* of a graph G is a mapping $\phi : V(G) \rightarrow S$. The elements of S are called *colours*; the vertices of one colour form a *colour class*. If $|S| = k$, we say that ϕ is a *k-colouring* (often we use $S = \{1, \dots, k\}$).

Definition 4.2. A *k-colouring* of a graph G is a vertex colouring of G that uses k colours.

Definition 4.3. A vertex colouring is *proper* if adjacent vertices have different colours.

Definition 4.4. A graph G is said to be *k-colourable* if it has a proper k-colouring.

Definition 4.5. The *Chromatic number* $\chi(G)$ of a graph G is the smallest number k for which G is k-colourable. Thus

$$\chi(G) = \min\{k : G \text{ is } k\text{-colourable.}\}$$

Definition 4.6. A graph G is *k-chromatic* if $\chi(G) = k$.

Definition 4.7. The *greedy colouring* relative to a vertex ordering v_1, v_2, \dots, v_n of $V(G)$ is obtained by colouring the vertices in the order v_1, v_2, \dots, v_n , assigning to v_i the smallest-indexed colour not already used on its lower-indexed neighborhood.

4.2.2 Lower bounds of the chromatic number

Proposition 4.1. Let H be a subgraph of a graph G . Then $\chi(H) \leq \chi(G)$.

Proof. We suppose that $\chi(G) = k$, then there exists a k-colouring ϕ of G . The colouring ϕ assigns distinct colours to every two adjacent vertices of H , since ϕ assigns distinct colours to every two adjacent vertices of G . Therefore, H is k-colourable, so that $k = \chi(G) \geq \chi(H)$ i.e $\chi(H) \leq \chi(G)$. □

Proposition 4.2. Let $\omega(G)$ be the clique number of a graph G , then $\omega(G) \leq \chi(G)$.

Proof. Recall that the clique number, $\omega(G)$, of a graph G is the maximal number of vertices in complete subgraph of G .

Obviously, by Proposition 4.1 above, we have $\omega(G) \leq \chi(G)$. □

Proposition 4.3. If G is a graph of order n , then

$$\frac{n}{\alpha(G)} \leq \chi(G)$$

where $\alpha(G)$ is the independence number of G .

Proof. Suppose that $\chi(G) = k$ and let there be given a k -colouring of G , the vertices being coloured with the same colour form an independent set. Let G be a graph with n vertices and ϕ a k -colouring of G . We define

$$V_i = \{v : \phi(v) = i\}$$

for $i = 1, 2, \dots, k$. Each V_i is an independent set. We have

$$|V_i| \leq \alpha(G).$$

Since

$$n = |V(G)| = |V_1| + |V_2| + \dots + |V_k| \leq k \cdot \alpha(G) = \chi(G)\alpha(G)$$

we have

$$\frac{n}{\alpha(G)} \leq \chi(G) \quad \square$$

4.2.3 Upper bounds of the chromatic number

Most upper bounds on the chromatic number come from algorithms that produce colourings. The most widespread one is the greedy algorithm.

Propositin 4.4. For any graph G , let $\Delta(G) = \max\{d(v) : v \in V(G)\}$. Then

$$\chi(G) \leq \Delta(G) + 1.$$

Proof. In a vertex-ordering, each vertex has at most $\Delta(G)$ earlier neighbours, so the greedy colouring cannot be forced to use more than $\Delta(G) + 1$ colours.

This proves that $\chi(G) \leq \Delta(G) + 1$. □

Proposition 4.5. Suppose that in every subgraph H of G there is a vertex with degree at most δ in H . Then

$$\chi(G) \leq \delta + 1.$$

Proof. There is a vertex with degree at most δ in G . We label that vertex v_n . There is a vertex with degree at most δ in $G - v_n$ that we label v_{n-1} . Label the vertex with degree at most δ in $G - \{v_n, v_{n-1}\}$ by v_{n-2} . Continuing to label all the vertices in G as v_1, v_2, \dots, v_n . Apply the greedy algorithm according to this labeling. At each step, the vertex we are going to colour is adjacent to at most δ vertices that are already coloured. Therefore, $\delta + 1$ colours will be enough. □

Proposition 4.6. Let G be any graph of order n . Then

$$\chi(G) \leq n - \alpha(G) + 1$$

Proof. Let X be a maximum independent set of G and assign the colour 1 to each vertex of X . Assigning distinct colours different from 1 to each vertex of $V(G) - X$ produces a proper colouring of G . Hence

$$\chi(G) \leq |V(G) - X| + 1 = n - \alpha(G) + 1$$

as well.

4.2.4 Chromatic Numbers of Generated Graphs

Two operations on graphs that are often encountered are the union and join.

Proposition 4.7. (See Zhang and Chartarand [59])

For any k graphs G_1, G_2, \dots, G_k ,

$$\chi(G_1 \cup G_2 \cup \dots \cup G_k) = \max\{\chi(G_i) : 1 \leq i \leq k\}.$$

So that, for any two graphs G_1 and G_2 ,

$$\chi(G_1 \cup G_2) = \max\{\chi(G_1), \chi(G_2)\}.$$

The following is then an immediate consequence of Proposition 4.7.

Corollary 4.1 If G is a graph with components G_1, G_2, \dots, G_k , then

$$\chi(G) = \max\{\chi(G_i) : 1 \leq i \leq k\}.$$

Proposition 4.8. If G is a nontrivial connected graph with blocks B_1, B_2, \dots, B_k , then

$$\chi(G) = \max\{\chi(B_i) : 1 \leq i \leq k\}.$$

Proof. This is a result analogous to Corollary 4.1 that expresses the chromatic number of a graph in term of the chromatic number of the blocks.

Proposition 4.9. (See Zhang and Chartarand [59])

Let G_1, G_2, \dots, G_k be graphs, then the chromatic number of the join of G_1, G_2, \dots, G_k is

$$\chi(G_1 \oplus G_2 \oplus \dots \oplus G_k) = \chi(G_1) + \chi(G_2) + \dots + \chi(G_k).$$

So that, for any two graphs G_1 and G_2 , the chromatic number of the join of G_1 and G_2 is

$$\chi(G_1 \oplus G_2) = \chi(G_1) + \chi(G_2).$$

Proof. Corollary 4.1 and Proposition 4.8 tell us that we can restrict our attention to 2-connected graphs when studying the chromatic number of graphs. In the case of joins, we have the above result.

In the join $G_1 \oplus G_2$ of G_1 and G_2 , no colour used on the subgraph G_1 can be the as a colour used on the subgraph G_2 , since every vertices of G_1 is adjacent to every vertices of G_2 . Since $\chi(G_1)$ colours are required for the subgraph G_1 and $\chi(G_2)$ colours are required for the subgraph G_2 , then

$$\chi(G_1 \oplus G_2) \geq \chi(G_1) + \chi(G_2);$$

Using any $\chi(G_1)$ colours to properly colour the subgraph G_1 of $G_1 \oplus G_2$ and using $\chi(G_2)$ different colours to colour the subgraph G_2 , we have

$$\chi(G_1 \oplus G_2) \leq \chi(G_1) + \chi(G_2).$$

□

4.3 Chromatic Numbers of classes of Graphs

4.3.1 Chromatic number of the Complete graphs

Proposition 4.10. Let K_n be the complete graph on n vertices. The chromatic number of K_n is

$$\chi(K_n) = n.$$

Proof. The complete graph on n vertices is clearly n -colourable, but not $(n-1)$ colourable. Thus $\chi(K_n) = n$. \square

4.3.2 Chromatic number of the k -partite graphs

Proposition 4.11.

- (1) The chromatic number of a k -partite graph is k .
- (2) Let G be a graph. If G is bipartite, then its chromatic number is $\chi(G) = 2$.

Proof.

We Give each vertex in a single partition one colour. Let i^{th} partition P_i with colour C_i . Since there are k -partitions, we will have k colours. This gives result (1) of Proposition 4.11.

A 2-colouring is obtained by assigning one colour to every vertex in one of the bipartition parts and another colour to every vertex in the other part. \square

4.3.3 Chromatic number of the Complete bipartite graphs

Let $K_{m,n}$ be the complete bipartite graph on $(m+n)$ vertices, with partition (V_1, V_2) , where $|V_1| = m$ and $|V_2| = n$.

Proposition 4.12. The chromatic number of $K_{m,n}$ is

$$\chi(K_{m,n}) = 2.$$

Proof. Since the complete bipartite graphs are bipartite. \square

4.3.4 Chromatic number of the Path graphs

Proposition 4.13. The path graphs P_n have the the chromatic number

$$\chi(P_n) = 2$$

Proof. Because, the path graphs are bipartite. \square

4.3.5 Chromatic number of the Cycle graphs

Proposition 4.14. Let C_n be a cycle graph on n vertices, with n even i.e. $n = 2k$. Then

$$\chi(C_{2k}) = 2.$$

Proof. A cycle graph C_n , $n = 2k$, is bipartite. So that, from Proposition 4.11, $\chi(C_{2k}) = 2$. □

Proposition 4.15. The cycle graphs C_n on n vertices, with n odd i.e. $n = 2k + 1$, have the chromatic number

$$\chi(C_{2k+1}) = 3.$$

Proof. Let v_1, \dots, v_{2k+1} be the vertices of cycle graph C_{2k+1} . If two colours were to suffice, then they would have to alternate around the cycle. Thus, the odd-subscripted vertices would have to be one colour and the even-subscripted ones the other. But vertex v_{2k+1} is adjacent to v_1 , which means that the odd-cycle graph C_{2k+1} is not 2-colourable. □

4.3.6 Chromatic number of the Wheel graphs

Let W_n be a wheel graph on n vertices, and $n - 1$ spokes, with $n \geq 4$.

Proposition 4.16. The chromatic number of the wheel graph W_n , on n vertices is given by

$$\chi(W_n) = \begin{cases} 3 & \text{if } n \text{ is odd,} \\ 4 & \text{if } n \text{ is even.} \end{cases}$$

Proof. For the wheel graphs W_n ,

- (1) if n odd i.e. $n = 2k + 1$, We use the fact that the wheel graph W_{2k+1} is the join of an even-cycle graph C_{2k} and complete graph K_1 , by the Proposition 4.9 above, we have

$$\begin{aligned} W_n &= W_{2k+1} = C_{2k} \oplus K_1 \\ \Rightarrow \chi(W_{2k+1}) &= \chi(C_{2k} \oplus K_1) \\ &= \chi(C_{2k}) + \chi(K_1) \\ &= 2 + 1 \\ &= 3; \end{aligned}$$

- (2) if n even i.e. $n = 2k$, The wheel graph W_{2k} is the join of an odd-cycle graph C_{2k+1} and complete graph K_1 . Then by the Proposition 4.9, we have

$$\begin{aligned} W_n &= W_{2k} = C_{2k+1} \oplus K_1 \\ \Rightarrow \chi(W_{2k}) &= \chi(C_{2k+1} \oplus K_1) \\ &= \chi(C_{2k+1}) + \chi(K_1) \\ &= 3 + 1 \\ &= 4. \end{aligned} \quad \square$$

4.3.7 Chromatic number of the Star graphs of length 1

Let $S_{n-1,1}$ be the star graph on n vertices, and with $n - 1$ rays of length 1, $n \geq 2$.

Proposition 4.17. The chromatic number of the star graph $S_{n-1,1}$ is

$$\chi(S_{n-1,1}) = 2.$$

Proof. By considering $S_{n-1,1}$ as the join of the complement of complete graph $\overline{K_{n-1}}$ and K_1 . That is $S_{n-1,1} = \overline{K_{n-1}} \oplus K_1$. Note that $\chi(\overline{K_{n-1}}) = 1$. Hence

$$\begin{aligned} \chi(S_{n-1,1}) &= \chi(\overline{K_{n-1}} \oplus K_1) \\ &= \chi(\overline{K_{n-1}}) + \chi(K_1), \text{ by Proposition 4.9,} \\ &= 1 + 1 \\ &= 2. \quad \square \end{aligned}$$

4.3.8 Chromatic number of the Star graphs of length 2

Let $S_{\frac{n-1}{2},2}$ be the star graph on n vertices, with $\frac{n-1}{2}$ rays of length 2, $n \geq 3$.

Proposition 4.18. The chromatic number of the star graph $S_{\frac{n-1}{2},2}$ is

$$\chi(S_{\frac{n-1}{2},2}) = 2.$$

Proof. The star graph $S_{\frac{n-1}{2},2}$ is a bipartite graph. □

4.3.9 Chromatic number of the Lollipop Graphs

Let LP_n be the lollipop graph on n vertices, $n > 2$, consisting of the complete graph K_{n-1} on $(n - 1)$ vertices, appended by edge x_1x_2 to a single end vertex x_2 from K_{n-1} .

Proposition 4.19. The chromatic number of the lollipop graph LP_n , with base the complete graph on $(n - 1)$ vertices, is:

$$\chi(LP_n) = n - 1$$

Proof. From 4.3.1 we colour K_{n-1} , the subgraph of LP_n , with $n - 1$ colours. Let $x_2 \in V(K_{n-1})$ be coloured with colour 1. Then x_1 cannot be coloured with colour 1 because x_1x_2 is an edge of LP_n . However, x_1 can have any of the other colours for vertices in $V(K_{n-1} \setminus \{x_2\})$. Hence $\chi(LP_n) = n - 1$. □

4.3.10 Chromatic number of The Complete Split-bipartite Graph

Let $K_{\frac{n}{2}, \frac{n}{2}}$ be the complete split-bipartite graph on n vertices, and with $\frac{n^2}{4}$ edges.

Proposition 4.20. The chromatic number of the complete split-bipartite Graphs is

$$\chi(K_{\frac{n}{2}, \frac{n}{2}}) = 2.$$

Proof. Since they are bipartite. □

4.3.11 Chromatic number of the Friendship graph

Proposition 4.21. The chromatic number of the Friendship Graphs F_p on n vertices, where $p = \frac{n-1}{2}$, is

$$\chi(F_p) = 3.$$

Proof. Since they are constructed by p copies of the odd-cycle graph C_3 which has chromatic number $\chi(C_3) = 3$. □

4.4 Chromatic number of generalized Sun graph

4.4.1 Chromatic number of the Caterpillar graphs

Let $CT(k, l)$ be the caterpillar graph where k and l denote the number of vertices on the path and the number of pendant edges respectively. This graph has $n = k(l + 1)$ vertices. The chromatic number of the caterpillar graph $L(CT(k, l))$ is

$$\chi(L(CT(k, l))) = 2.$$

See Winter [46]

4.4.2 Chromatic number of the Complete Sun Graph

Let $CompSun(h, p)$ be the complete sun graph which consists of the complete graph K_p , with h end vertices appended to each of the p vertices in K_p . This graph has $n = (h + 1)p$ vertices.

Proposition 4.22. The chromatic number of the Complete sun Graphs is

$$\chi(CompSun(h, p)) = p.$$

Proof. Since they are constructed from the complete graph K_p which has chromatic number $\chi(K_p) = p$. See section 4.3.1. □

4.4.3 Chromatic number of the Complete Split-bipartite Sun Graph

Let $BipSun(h, p)$ be the complete split-bipartite sun graph which consists of the complete split-bipartite graph $K_{\frac{p}{2}, \frac{p}{2}}$, with h end vertices appended to each of the p vertices in $K_{\frac{p}{2}, \frac{p}{2}}$. This graph has $n = (h + 1)p$ vertices.

Proposition 4.23. The chromatic number of the Complete split-bipartite sun Graphs is

$$\chi(BipSun(h, p)) = 2.$$

Proof. Since they are constructed from the complete split-bipartite graph $K_{\frac{p}{2}, \frac{p}{2}}$ which has chromatic number $\chi(K_{\frac{p}{2}, \frac{p}{2}}) = 2$. See section 4.3.10.

4.4.4 Chromatic number of the Cycle Sun Graph

Let $CycleSun(h,p)$ be the cycle sun graph which consists of the cycle graph C_p , with h end vertices appended to each of the p vertices in C_p . This graph has $n = (h + 1)p$ vertices.

Proposition 4.24. The chromatic number of the Cycle sun Graphs is

$$\chi(CycleSun(h,p)) = \begin{cases} 2 & \text{if } p \text{ is even,} \\ 3 & \text{if } p \text{ is odd.} \end{cases}$$

Proof. Since they are constructed from the cycle graph C_p which has chromatic number

$$\chi(C_p) = 2 \text{ if } p \text{ is even and } \chi(C_p) = 3 \text{ if } p \text{ is odd. See section 4.3.5.} \quad \square$$

4.4.5 Chromatic number of the Wheel Sun Graph

Let $WheelSun(h,p)$ be the wheel sun graph which consists of the Wheel graph W_p , with h end vertices appended to each of the p vertices in W_p . This graph has $n = (h + 1)p$ vertices.

Proposition 4.25. The chromatic number of the Wheel sun Graphs is

$$\chi(WheelSun(h,p)) = \begin{cases} 4 & \text{if } p \text{ is even,} \\ 3 & \text{if } p \text{ is odd.} \end{cases}$$

Proof. Since they are constructed from the Wheel graph W_p which has chromatic number

$$\chi(W_p) = 4 \text{ if } p \text{ is even and } \chi(W_p) = 3 \text{ if } p \text{ is odd. See section 4.3.6.} \quad \square$$

4.4.6 Chromatic number of the Star Sun Graph

Let $StarSun(h,p)$ be the star sun graph which consists of the star graph $S_{p-1,1}$, with h end vertices appended to each of the p vertices in $S_{p-1,1}$. This graph has $n = (h + 1)p$ vertices.

Proposition 4.26. The chromatic number of the star sun Graphs is

$$\chi(StarSun(h,p)) = 2.$$

Proof. Since they are constructed from the star graph $S_{p-1,1}$ which has chromatic number $\chi(S_{p-1,1}) = 2$. See section 4.3.7. □

4.5 Chromatic number of the complement of the Cycle graph

Proposition 4.27. The chromatic number of the complement of the Cycle graph on n vertices, $n \geq 3$, is

$$\chi(\overline{C}_n) = \begin{cases} n - 2 & \text{for } n \text{ even} \\ n - 3 & \text{for } n \text{ odd} \end{cases}$$

Proof. We know that the complete graph, K_n , on n vertices is the join of the cycle graph, C_n and the complement of the cycle graph, \overline{C}_n . So, we write

$$K_n = C_n \oplus \overline{C}_n.$$

K_n is k -regular; C_n is 2-regular, and \overline{C}_n is $(k - 2)$ -regular, with $k = n - 1$.

And

$$\chi(K_n) = \chi(C_n \oplus \overline{C}_n) = \chi(C_n) + \chi(\overline{C}_n)$$

$$\Rightarrow \chi(\overline{C}_n) = \chi(K_n) - \chi(C_n) = n - a, \quad (a = 2 \text{ if } n \text{ is even, and } a = 3 \text{ if } n \text{ is odd}). \quad \square$$

4.6 Conclusion

In this chapter, we have determined the chromatic number of all the classes of graphs we had defined and of which we have analyzed the energy in the previous chapter. The chromatic number of a graph G is denoted by $\chi(G)$. So We found the chromatic number of the complete graph K_n , on n vertices is $\chi(K_n) = n$, while the chromatic number of the k -partite graphs G is $\chi(G) = k$.

Chapter 5

THE EIGEN-CHROMATIC RATIO OF CLASSES OF GRAPHS WITH ITS ASYMPTOTIC AND AREA ASPECTS

This chapter is original and based on publication (see P. A. Winter, R. M. Mayala and P. Namayanja [56]).

5.1 Ratios and Areas

Ratios have always been an important aspect of graph theoretical definitions. The following are examples of various ratios which have been studied which provide motivation for the new ratios which we discuss here: expanders (see Alon and Spencer [2]), the central ratio of graph (see Buckley [13]), Eigen-pair ratio of classes of graphs (see Winter and Jessop [49]), independence and Hall ratios (see Gábor [20]), tree-cover ratio of graphs (see Winter and Adewusi [48]), the eigen-energy formation ratio of graphs (see Winter and Sarvate [55]), the chromatic-cover ratio of graphs (see Winter [46]), the eigen-complete difference ratio (see Winter and Ojako [54]). These ratios provided the motivation for our definition of the eigen-chromatic ratio which we discuss below.

We show that the complete graph is associated with the value $1/2$ when a large number of atoms are involved - this has allowed for the investigation of a molecular stability associated with the idea of hyper/hypo- energetic graphs, elaborated below.

By introducing the average degree of a graph together with the Riemann integral of each new ratio defined, we associated area with classes of graphs (see Winter and Adewusi [48], Winter and Jessop [50], Winter and Sarvate [55], Winter, Jessop and Adewusi [51], Winter and Ojako [54]).

5.2 Main definitions

In this section, we combine the two concepts of energy and chromatic number of graphs (defined and studied respectively in sections 3.2 and 4.3 above) to form a ratio. We introduce the idea of ratio, asymptotes and areas involving the energy and chromatic number of a graph G .

Let $G = (V, E)$ be a graph of order $|V| = n$ and of size $|E| = m$.

Definition 5.1.

The *eigen-chromatic ratio* of a graph G , of order n , is denoted by $eig_\chi(G)$ and defined as

$$eig_\chi(G) = \frac{\chi(G)}{E(G)}$$

where $\chi(G)$ is the chromatic number of G and $E(G)$ the energy of G .

Definition 5.2.

Let $eig_\chi(G) = f(n)$ for every graph $G \in \mathfrak{F}$, where \mathfrak{F} is a class of graphs. The asymptotic behaviour of $f(n)$ is called the *eigen-chromatic asymptote* of G and denoted by $Asyeig_\chi(G)$. That is,

$$Asyeig_\chi(G) = \lim_{n \rightarrow \infty} f(n).$$

This asymptote gives a measure of the *asymptotic effect* of the chromatic number on the energy of the original graph, and is referred to as the *eigen-chromatic asymptotic effect*. This idea translates to the effect in the molecular graph theory.

Eigen-Chromatic stability: The Hyper/Hypo Chromatic Stability Effect.

The *eigen-chromatic ratio* of a graph G is a form of energy distribution among the colour classes determined by $\chi(G)$. The *eigen-chromatic asymptote* gives an indication of this distribution when a large number of vertices are involved as in molecular graph theory. We show that the eigen-chromatic asymptote for the complete graph on n vertices is $\frac{1}{2}$, while most graphs have an asymptote of 0, which motivates for the following two definitions (see [24]):

1. A graph G is said to be *eigen-chromatically stable* if the eigen-chromatic asymptote is not zero i.e if

$$Asyeig_\chi(G) \neq 0;$$

otherwise it is *eigen-chromatically unstable*.

2. A graph G is said to be *hyper eigen-chromatically stable* if its eigen-chromatic asymptote is bigger or equal to $\frac{1}{2}$, i.e if

$$Asyeig_\chi(G) \geq \frac{1}{2}$$

and *hypo eigen-chromatically stable* if its eigen-chromatic asymptote is less than $\frac{1}{2}$ and positive, i.e if

$$0 < Asyeig_\chi(G) < \frac{1}{2}.$$

Definition 5.3.

Let \mathfrak{F} be a class of graphs and $G \in \mathfrak{F}$ be a graph with m edges. Then the *eigen-chromatic area* is defined as:

$$A_{\mathfrak{F}(n)}^\chi = \frac{2m}{n} \int f(n) dn$$

with $A_{\mathfrak{F}(k)}^\chi = 0$ where k is the smallest number of vertices for which $eig_\chi(G) = f(n)$ is defined.

Note that $\frac{2m}{n}$ is the average degree of $G \in \mathfrak{F}$, referred to as the *length* of G . The integral part is referred to as its *height*, which we always make positive.

Although the eigen-chromatic ratio $f(n)$ takes on discrete values, we assume it is continuous for the purpose of the definition of area (and asymptote above) so that we have a form of *comparative analysis* between classes of graphs (and molecules with a large amount of atoms).

This comparative analysis is relevant once we know the area (and asymptote) of the complete graph, allowing for the idea similar to that of hyper/hypo energetic graphs (see Stevanovic [41]).

5.3 Eigen-Chromatic Ratio and Area

Now we find the eigen-chromatic ratio for all the classes of graphs seen in previous chapters and the related eigen-chromatic area.

5.3.1 The Complete graphs

Let K_n be the complete graph on n vertices, of size $m = \frac{n(n-1)}{2}$ (see section 1.8.1). From Proposition 4.10, $\chi(K_n) = n$ and using results from section 3.4.1, we have

$$\begin{aligned} eig_\chi(K_n) &= \frac{\chi(K_n)}{E(K_n)} \\ &= \frac{n}{2(n-1)}. \end{aligned}$$

The *eigen-chromatic asymptote* of K_n , denoted by $Asyeig_\chi(K_n)$, is

$$\begin{aligned} Asyeig_\chi(K_n) &= \lim_{n \rightarrow \infty} \frac{n}{2n-2} \\ &= \frac{1}{2}; \end{aligned}$$

and the *eigen-chromatic area* of K_n is

$$\begin{aligned} A_{K_n}^\chi &= \frac{2m}{n} \int \frac{n}{2n-2} dn \\ &= n-1 \int \frac{n}{2n-2} dn \\ &= \frac{n-1}{2} \int \frac{n}{n-1} dn \\ &= \frac{n-1}{2} (n + \ln |n-1| + C). \end{aligned}$$

The function $f(n) = \frac{n}{2n-2}$ is defined if $2n-2 \neq 0$ i.e if $n \neq 1$, so that with smallest order of G for which $f(n)$ is defined is 2. Hence we have: $A_{K_2}^\chi = \frac{2-1}{2} (2 + \ln |2-1| + C) = 0 \Rightarrow C = -2$, so

$$A_{K_n}^\chi = \frac{n-1}{2} (n + \ln |n-1| - 2).$$

5.3.2 The Path, Cycle and Wheel graphs on an even number of vertices

We determine the eigen-chromatic ratio, and its associated aspects, of paths, cycles and wheels on an even number of vertices using the results found in chapter 3 and chapter 4.

The path graphs P_n on n vertices have the chromatic number

$$\chi(P_n) = 2 \text{ (see section 4.3.4)}$$

and the energy

$$E(P_n) = 2 \left[\operatorname{cosec} \left(\frac{\pi}{2(n+1)} \right) - 1 \right], \text{ for } n \text{ even (see section 3.2.1).}$$

The cycle graphs C_n on n vertices, with n even have the chromatic number

$$\chi(C_n) = 2 \text{ (see section 4.3.5)}$$

and the energy

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2 \cos \left(\frac{2\pi j}{n} \right) \right| = 4 \cot \left(\frac{\pi}{n} \right), \text{ with } n = 2t \text{ and } t \text{ even (see section 3.2.2).}$$

Let W_n be the wheel graph, on n vertices, and $n - 1$ spokes, with $n \geq 4$. The wheel graphs W_n , on n vertices, with n even have the chromatic number

$$\chi(W_n) = 4 \text{ (see section 4.3.6)}$$

and the energy

$$E(W_n) = 2\sqrt{n} - 2 + 2 \operatorname{cosec} \left(\frac{\pi}{2(n-1)} \right) \text{ (see section 3.2.3).}$$

Lemma 3.2.4 and Theorem 3.2.6 will simplify the eigen-chromatic ratio when a large number of vertices are involved.

The Path graph

The *eigen-chromatic ratio* of P_n with n even, is

$$\begin{aligned} \operatorname{eig}_\chi(P_n) &= \frac{\chi(P_n)}{E(P_n)} \\ &= \frac{2}{2 \left[\operatorname{cosec} \left(\frac{\pi}{2(n+1)} \right) - 1 \right]} \\ &= \frac{1}{\operatorname{cosec} \left(\frac{\pi}{2(n+1)} \right) - 1}; \end{aligned}$$

the *eigen-chromatic asymptote* of P_n is

$$\begin{aligned}
 Asyeig_{\chi}(P_n) &= \lim_{n \rightarrow \infty} \frac{1}{\operatorname{cosec}\left(\frac{\pi}{2(n+1)}\right) - 1} \\
 &= \lim_{n \rightarrow \infty} \frac{1}{\frac{2n}{\pi}} \\
 &= \lim_{n \rightarrow \infty} \frac{\pi}{2n} \\
 &= 0;
 \end{aligned}$$

the *eigen-chromatic area* of P_n is

$$\begin{aligned}
 A_{P_n}^{\chi} &= \frac{2m}{n} \int \frac{1}{\operatorname{cosec}\frac{\pi}{2(n+1)} - 1} dn \\
 &= \frac{2(n-2)}{n} \int \frac{1}{\operatorname{cosec}\frac{\pi}{2(n+1)} - 1} dn.
 \end{aligned}$$

The Cycle graph

The *eigen-chromatic ratio* of C_n , of order n , with n even, is

$$\begin{aligned}
 eig_{\chi}(C_n) &= \frac{\chi(C_n)}{E(C_n)} \\
 &= \frac{2}{4\cot\left(\frac{\pi}{n}\right)} \\
 &= \frac{1}{2\cot\left(\frac{\pi}{n}\right)};
 \end{aligned}$$

the *eigen-chromatic asymptote* of C_n denoted by $Asyeig_{\chi}(C_n)$ is

$$\begin{aligned}
 Asyeig_{\chi}(C_n) &= \lim_{n \rightarrow \infty} \frac{1}{2\cot\left(\frac{\pi}{n}\right)} \\
 &= 0;
 \end{aligned}$$

the *eigen-chromatic area* of C_n is

$$\begin{aligned}
 A_{C_n}^{\chi} &= \frac{2m}{n} \int \frac{1}{2\cot\left(\frac{\pi}{n}\right)} dn \\
 &= 2 \int \frac{1}{2\cot\left(\frac{\pi}{n}\right)} dn \\
 &= \int \frac{1}{\cot\left(\frac{\pi}{n}\right)} dn
 \end{aligned}$$

The Wheel graph

The *eigen-chromatic ratio* of W_n , of order n , with n even, is

$$\begin{aligned} eig_\chi(W_n) &= \frac{\chi(W_n)}{E(W_n)} \\ &= \frac{4}{2\sqrt{n} - 2 + 2\operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} \\ &= \frac{2}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} \end{aligned}$$

the *eigen-chromatic asymptote* of W_n denoted by $Asyeig_\chi(W_n)$ is

$$\begin{aligned} Asyeig_\chi(W_n) &= \lim_{n \rightarrow \infty} \frac{2}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} \\ &= 0; \end{aligned}$$

the *eigen-chromatic area* of W_n is

$$\begin{aligned} A_{W_n}^\chi &= \frac{2m}{n} \int \frac{2}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} dn \\ &= 2 \cdot \frac{2n-2}{n} \int \frac{2}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} dn \\ \Rightarrow A_{W_n}^\chi &= 8 \cdot \frac{n-1}{n} \int \frac{1}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} dn. \end{aligned}$$

In the same way, we can determine the eigen-chromatic ratio for paths, cycles and wheels on an odd number of vertices.

5.3.3 Star graphs with rays of length 1

Let $S_{n-1,1}$ be the star graph on n vertices, and with $n-1$ rays of length 1, $n \geq 2$. As seen in the preceding chapters, $S_{n-1,1}$ have the chromatic number

$$\chi(S_{n-1,1}) = 2$$

and the energy

$$E(S_{n-1,1}) = 2\sqrt{n-1};$$

The *eigen-chromatic ratio* of $S_{n-1,1}$, of order n is

$$\begin{aligned} eig_{\chi}(S_{n-1,1}) &= \frac{\chi(S_{n-1,1})}{E(S_{n-1,1})} \\ &= \frac{2}{2\sqrt{n-1}} \\ &= \frac{1}{\sqrt{n-1}}; \end{aligned}$$

the *eigen-chromatic asymptote* of $S_{n-1,1}$ denoted by $Asyeig_{\chi}(S_{n-1,1})$ is

$$\begin{aligned} Asyeig_{\chi}(S_{n-1,1}) &= \lim_{n \rightarrow \infty} \frac{1}{\sqrt{n-1}} \\ &= \lim_{n \rightarrow \infty} \frac{1}{\sqrt{n}} \\ &= 0; \end{aligned}$$

the *eigen-chromatic area* of $A_{S_{n-1,1}}$ is

$$\begin{aligned} A_{S_{n-1,1}}^{\chi} &= \frac{2m}{n} \int \frac{1}{\sqrt{n-1}} dn \\ &= \frac{2(n-1)}{n} \int \frac{1}{\sqrt{n-1}} dn \\ &= \frac{2(n-1)}{n} (2\sqrt{n-1} + C). \end{aligned}$$

The function $f(n) = \frac{1}{\sqrt{n-1}}$ is defined if $n-1 > 0$, so that the smallest order of G for which $f(n)$ is defined is 2. Thus

$$A_{S_{1,1}}^{\chi} = \frac{2(2-1)}{2} (2\sqrt{2-1} + C) = 0 \Rightarrow C = -2, \text{ so}$$

$$A_{S_{n-1,1}}^{\chi} = \frac{2(n-1)}{n} (2\sqrt{n-1} - 2) = \frac{4(n-1)}{n} (\sqrt{n-1} - 1).$$

5.3.4 Star graphs with rays of length 2

Let $S_{\frac{n-1}{2},2}$ be the star graph on n vertices, and with $\frac{n-1}{2}$ rays of length 2, $n \geq 3$. Since the chromatic number of the star graph $S_{\frac{n-1}{2},2}$ is

$$\chi(S_{\frac{n-1}{2},2}) = 2$$

and the energy of the star graph $S_{\frac{n-1}{2},2}$ is

$$E(S_{\frac{n-1}{2},2}) = n - 3 + \sqrt{2(n+1)};$$

$$eig_{\chi}(S_{\frac{n-1}{2},2}) = \frac{2}{n-3+\sqrt{2(n+1)}}.$$

$$\begin{aligned} Asyeig_{\chi}(S_{\frac{n-1}{2},2}) &= \lim_{n \rightarrow \infty} \frac{2}{n-3+\sqrt{2(n+1)}} \\ &= 0; \end{aligned}$$

$$\begin{aligned} A_{S_{\frac{n-1}{2},2}}^{\chi} &= \frac{2m}{n} \int \frac{2}{n-3+\sqrt{2(n+1)}} dn \\ &= \frac{2(n-1)}{n} \int \frac{2}{n-3+\sqrt{2(n+1)}} dn \\ \Rightarrow A_{S_{\frac{n-1}{2},2}}^{\chi} &= \frac{4(n-1)}{n} \int \frac{1}{n-3+\sqrt{2(n+1)}} dn. \end{aligned}$$

Let us compute $I = \int \frac{1}{n-3+\sqrt{2(n+1)}} dn$,

$$\sqrt{2(n+1)} = t \Rightarrow n = \frac{1}{2}(t^2 - 2) \Rightarrow dn = t dt$$

$$\Rightarrow I = \int \frac{t dt}{\frac{1}{2}(t^2 - 2) - 3 + t} = 2 \int \frac{t dt}{t^2 + 2t - 8}$$

$$\Rightarrow I = \frac{2}{3}(\ln[(t-2)(t+4)^2]) + C = \frac{2}{3}(\ln[(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) + C, \text{ so}$$

$$A_{S_{\frac{n-1}{2},2}}^{\chi} = \frac{4(n-1)}{n} \left(\frac{2}{3}(\ln[(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) + C \right)$$

With smallest order 3 we have:

$$\frac{4(3-1)}{3} \left(\frac{2}{3}(\ln[(\sqrt{2(3+1)}-2)(\sqrt{2(3+1)}+4)^2]) + C \right) = 0 \Rightarrow \frac{2}{3} \ln[16(1+\sqrt{2})] + C = 0$$

$$\Rightarrow C = -\frac{2}{3} \ln[16(1+\sqrt{2})];$$

So

$$\begin{aligned} A_{S_{\frac{n-1}{2},2}}^{\chi} &= \frac{8(n-1)}{3n} ((\ln[(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) - \ln[16(1+\sqrt{2})]) \\ \Rightarrow A_{S_{\frac{n-1}{2},2}}^{\chi} &= \frac{8(n-1)}{3n} \ln \frac{[(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]}{16(1+\sqrt{2})} \end{aligned}$$

5.3.5 The Lollipop Graphs

The chromatic number and the energy of the lollipop graph LP_n are respectively: $\chi(LP_n) = n - 1$ and $E(LP_n) = n - 3$, as seen previously.

The *eigen-chromatic ratio* of LP_n is

$$eig_{\chi}(LP_n) = \frac{\chi(LP_n)}{E(LP_n)} = \frac{n - 1}{n - 3}.$$

The *eigen-chromatic asymptote* of LP_n is

$$\begin{aligned} Asyeig_{\chi}(LP_n) &= \lim_{n \rightarrow \infty} eig_{\chi}(LP_n) \\ &= \lim_{n \rightarrow \infty} \frac{n - 1}{n - 3} = \lim_{n \rightarrow \infty} \frac{\frac{n-1}{n}}{\frac{n-3}{n}} = 1. \end{aligned}$$

So that

$$Asyeig_{\chi}(LP_n) = 1.$$

5.3.6 The Complete Split-bipartite Graph

Let $K_{\frac{n}{2}, \frac{n}{2}}$ be the complete split-bipartite graph on n vertices ($n \geq 6$, n is even), and with $\frac{n^2}{4}$ edges.

As seen previously, the chromatic number of the complete split-bipartite Graphs is

$$\chi(K_{\frac{n}{2}, \frac{n}{2}}) = 2;$$

and the energy is:

$$E(K_{\frac{n}{2}, \frac{n}{2}}) = n.$$

The *eigen-chromatic ratio* of $K_{\frac{n}{2}, \frac{n}{2}}$ is

$$eig_{\chi}(K_{\frac{n}{2}, \frac{n}{2}}) = \frac{2}{n}$$

with

$$\begin{aligned} Asyeig_{\chi}(K_{\frac{n}{2}, \frac{n}{2}}) &= \lim_{n \rightarrow \infty} \frac{2}{n} \\ &= 0. \end{aligned}$$

The *eigen-chromatic area* of $K_{\frac{n}{2}, \frac{n}{2}}$ is

$$\begin{aligned} A_{K_{\frac{n}{2}, \frac{n}{2}}}^{\chi} &= \frac{2m}{n} \int \frac{2}{n} dn \\ &= \frac{2n^2}{n} \int \frac{2}{n} dn \\ &= \frac{n}{2} \int \frac{2}{n} dn \\ &= n(\ln(n) + C). \end{aligned}$$

With smallest order 6 we have: $C = -\ln 6$, so

$$= n(\ln(n) - \ln 6)$$

$$= n \ln \left(\frac{n}{6} \right).$$

5.3.7 The Friendship graph

The chromatic number and the energy of the Friendship graphs are, respectively,

$$\chi(F_p) = 3 \text{ (Section 4.3.11)}$$

and

$$E(F_p) = (2p - 1) + \sqrt{1 + 8p} \text{ (Theorem 3.4.2).}$$

The *eigen-chromatic ratio* of F_p is

$$eig_\chi(F_p) = \frac{3}{(2p - 1) + \sqrt{1 + 8p}}.$$

$$\Rightarrow eig_\chi(F_{\frac{n-1}{2}}) = \frac{3}{(n - 2) + \sqrt{4n - 3}}.$$

The *eigen-chromatic asymptote* of $F_{\frac{n-1}{2}}$ is

$$Asyeig_\chi(F_{\frac{n-1}{2}}) = \lim_{n \rightarrow \infty} \frac{3}{(n - 2) + \sqrt{4n - 3}}$$

$$= 0;$$

The *eigen-chromatic area* of $F_{\frac{n-1}{2}}$ is

$$A_{F_{\frac{n-1}{2}}}^\chi = \frac{2m}{n} \int \frac{3}{(n - 2) + \sqrt{4n - 3}} dn$$

$$= \frac{3(n - 1)}{n} \int \frac{3}{(n - 2) + \sqrt{4n - 3}} dn \quad (m = \frac{3n - 3}{2})$$

$$= \frac{9(n - 1)}{n} \int \frac{1}{(n - 2) + \sqrt{4n - 3}} dn$$

$$\Rightarrow A_{F_{\frac{n-1}{2}}}^\chi = \frac{9(n - 1)}{n} \int \frac{1}{(n - 2) + \sqrt{4n - 3}} dn.$$

5.4 Sun graphs with their Asymptotic and Area aspects

In Section 1.8.12, we defined the generalized sun graph $SG(h,p)$ as a graph consisting of a base graph G on p vertices and h end vertices appended to each of the p vertices in G .

5.4.1 The Caterpillar Graph

The chromatic number of $L(CT(k,l))$ is $\chi(L(CT(k,l))) = 2$ (see section 4.3.2). The energy of $L(CT(k,l))$ is (see section 3.3.2):

$$E(L(CT(k,l))) = k(l-1) + \sum_{j=2}^k \left| \frac{1}{2} \left(l-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right|$$

$$+ \sum_{j=2}^k \left| \frac{1}{2} \left(l-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(l+1)\sigma_j + (l^2 + 6l + 1)} \right) \right|$$

$$\text{where } \sigma_j = 2\cos\left(\frac{(k+1-j)\pi}{k}\right), \text{ for } j = 1, \dots, k.$$

If we take $l = 2$, then $n = 3k$, so that

$$E(L(CT(\frac{n}{3}, 2))) = \frac{n}{3}(2-1) + \sum_{j=2}^{\frac{n}{3}} \left| \frac{1}{2} \left(2-1 + \sigma_j - \sqrt{\sigma_j^2 + 2(2+1)\sigma_j + (4+12+1)} \right) \right|$$

$$+ \sum_{j=2}^{\frac{n}{3}} \left| \frac{1}{2} \left(2-1 + \sigma_j + \sqrt{\sigma_j^2 + 2(2+1)\sigma_j + (4+12+1)} \right) \right|$$

$$\text{where } \sigma_j = 2\cos\left(\frac{(\frac{n}{3}+1-j)\pi}{\frac{n}{3}}\right), \text{ for } j = 1, \dots, \frac{n}{3};$$

$$= \frac{n}{3} + \sum_{j=2}^{\frac{n}{3}} \left| \frac{1}{2} \left(1 + \sigma_j - \sqrt{\sigma_j^2 + 6\sigma_j + 17} \right) \right|$$

$$+ \sum_{j=2}^{\frac{n}{3}} \left| \frac{1}{2} \left(1 + \sigma_j + \sqrt{\sigma_j^2 + 6\sigma_j + 17} \right) \right|$$

$$\text{where } \sigma_j = 2\cos\left(\frac{(\frac{n}{3}+1-j)\pi}{\frac{n}{3}}\right), \text{ for } j = 1, \dots, \frac{n}{3}.$$

For large $n = n'$ and

$$\sigma_j = 2\cos\left(\frac{(\frac{n}{3}+1-j)\pi}{\frac{n}{3}}\right) \leq 2.$$

To simplify notation, we consider dominant terms in the energy function and note that

$$\begin{aligned}
E(L(CT(\frac{n}{3}, 2))) &\approx \frac{n'}{3} + \sum_{j=2}^{\frac{n'}{3}} \left| \frac{1}{2} (1 + \sigma_j - \sqrt{\sigma_j^2}) \right| \\
&+ \sum_{j=2}^{\frac{n'}{3}} \left| \frac{1}{2} (1 + \sigma_j + \sqrt{\sigma_j^2}) \right| \\
&= \frac{n'}{3} + \frac{1}{2} \left(\frac{n'}{3} - 1 \right) + \frac{1}{2} \left(\frac{n'}{3} + 4 \right) \approx \frac{2n'}{3}.
\end{aligned}$$

Thus for n large, we have:

$$\begin{aligned}
eig_{\chi}(L(CT(\frac{n}{3}, l))) &= \frac{2}{\frac{2n}{3}} \\
&= \frac{3}{n}.
\end{aligned}$$

$$\begin{aligned}
Asyeig_{\chi}(L(CT(\frac{n}{3}, l))) &= \lim_{n \rightarrow \infty} \frac{3}{n} \\
&= 0;
\end{aligned}$$

$$\begin{aligned}
A_{L(CT(\frac{n}{3}, l))}^{\chi} &= \frac{2(n-1)}{n} \int \frac{3}{n} dn \\
&= \frac{6(n-1)}{n} \int \frac{1}{n} dn \\
&= \frac{6(n-1)}{n} (\ln(n) + C).
\end{aligned}$$

With smallest order 3 we have: $C = -\ln 3$, so

$$\begin{aligned}
A_{L(CT(\frac{n}{3}, l))}^{\chi} &= \frac{6(n-1)}{n} (\ln(n) - \ln 3) \\
&= \frac{6(n-1)}{n} \ln \frac{n}{3}.
\end{aligned}$$

5.4.2 The Complete Sun Graph

The energy of the complete sun graph $CompSun(h, p)$ is

$$E(CompSun(h, p)) = (p-1)\sqrt{1+4h} + \sqrt{(p-1)^2+4h} \text{ (see section 3.3.2);}$$

The chromatic number of the Complete sun Graphs is

$$\chi(CompSun(h, p)) = p \text{ (see section 4.4.2).}$$

The *eigen-chromatic ratio* of $CompSun(h,p)$ is

$$eig_{\chi}(CompSun(h,p)) = \frac{\chi(CompSun(h,p))}{E(CompSun(h,p))} = \frac{p}{(p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}}.$$

The *eigen-chromatic asymptote* of $CompSun(h,p)$ is

$$\begin{aligned} Asyeig_{\chi}(CompSun(h,p)) &= \lim_{n \rightarrow \infty} \frac{p}{(p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}} \\ &= \lim_{(h+1)p \rightarrow \infty} \frac{p}{(p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}} \\ &= \lim_{p \rightarrow \infty} \frac{p}{(p-1)\sqrt{1+4h} + \sqrt{(p-1)^2 + 4h}} = \frac{1}{\sqrt{1+4h} + 1}. \end{aligned}$$

So, for

$$h = 1, Asyeig_{\chi}(CompSun(1,p)) = \frac{1}{\sqrt{5} + 1} \cong 0.309$$

$$h = 2, Asyeig_{\chi}(CompSun(2,p)) = \frac{1}{\sqrt{9} + 1} \cong 0.25$$

$$h = 3, Asyeig_{\chi}(CompSun(3,p)) = \frac{1}{\sqrt{13} + 1} \cong 0.217$$

⋮

$$h = 100, Asyeig_{\chi}(CompSun(100,p)) = \frac{1}{\sqrt{401} + 1} \cong 0.047$$

⋮

$$h = 245, Asyeig_{\chi}(CompSun(245,p)) = \frac{1}{\sqrt{981} + 1} \cong 0.0309$$

⋮

This implies that $0 < Asyeig_{\chi}(CompSun(h,p)) < \frac{1}{2}$.

Remark: The asymptote of the complete sun graph with $h = 1$ is 0.309 which is $\frac{1}{2}$ golden ratio of 0.618; for $h = 245$ the asymptote is 0.0309 (to 4 decimal places) which is $\frac{1}{20}$ of golden ratio.

We get the golden ratio for $h = 1$, then $p = \frac{n}{2}$, so

$$\begin{aligned} eig_{\chi}(CompSun(1, \frac{n}{2})) &= \frac{n}{\frac{\sqrt{5}}{2}(n-2) + \frac{1}{2}\sqrt{(n-2)^2 + 16}} \\ &= \frac{2n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2 + 16}}; \end{aligned}$$

$$\begin{aligned}
Asyeig_{\chi}(CompSun(1, \frac{n}{2})) &= \lim_{n \rightarrow \infty} \frac{2n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2 + 16}} \\
&= \frac{2}{2\sqrt{5} + 1} \\
&\cong 0.365.
\end{aligned}$$

And the *eigen-chromatic area* of $CompSun(1, \frac{n}{2})$ is

$$\begin{aligned}
A_{CompSun(1, \frac{n}{2})}^{\chi} &= \frac{n+2}{4} \int \frac{n}{\frac{\sqrt{5}}{2}(n-2) + \frac{1}{2}\sqrt{(n-2)^2 + 16}} dn \\
&= \frac{n+2}{2} \int \frac{n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2 + 16}} dn.
\end{aligned}$$

5.4.3 The Complete Split-bipartite Sun Graph

The energy of the complete split-bipartite sun graph is

$$E(BipSun(h,p)) = \sqrt{p^2 + 16h} + 2(p-2)\sqrt{h} \text{ (see section 3.3.3)}$$

The chromatic number of the Complete split-bipartite sun Graphs is

$$\chi(BipSun(h,p)) = 2 \text{ (see section 4.4.3).}$$

The *eigen-chromatic ratio* of $BipSun(h,p)$ is

$$\begin{aligned}
eig_{\chi}(BipSun(h,p)) &= \frac{\chi(BipSun(h,p))}{E(BipSun(h,p))} \\
&= \frac{2}{\sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}}.
\end{aligned}$$

The *eigen-chromatic asymptote* of $BipSun(h,p)$ is

$$\begin{aligned}
Asyeig_{\chi}(BipSun(h,p)) &= \lim_{n \rightarrow \infty} \frac{2}{\sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}} \\
&= \lim_{(h+1)p \rightarrow \infty} \frac{2}{\sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}} \\
&= \lim_{p \rightarrow \infty} \frac{2}{\sqrt{p^2 + 16h} + 2(p-2)\sqrt{h}} = 0.
\end{aligned}$$

If $h = 1$ then $p = \frac{n}{2}$, so

$$\begin{aligned}
A_{BipSun(1, \frac{n}{2})}^{\chi} &= \frac{2\frac{n}{16}(n+8)}{n} \int \frac{2}{\sqrt{(\frac{n}{2})^2 + 16} + 2(\frac{n}{2} - 2)} dn \\
&= \frac{n+8}{4} \int \frac{1}{\sqrt{(\frac{n}{2})^2 + 16} + 2(\frac{n}{2} - 2)} dn \\
\Rightarrow A_{BipSun(1, \frac{n}{2})}^{\chi} &= \frac{n+8}{2} \int \frac{dn}{\sqrt{n^2 + 64} + 2n - 8}.
\end{aligned}$$

5.4.4 The Star Sun Graph

The energy of the Star sun graph is

$$E(StarSun(h,p)) = 2\sqrt{p-1+4h} + 2(p-2)\sqrt{h} \text{ (see section 3.3.5).}$$

The chromatic number of the star sun Graphs is

$$\chi(StarSun(h,p)) = 2 \text{ (see section 4.4.6).}$$

The *eigen-chromatic ratio* of $StarSun(h,p)$ is

$$\begin{aligned} eig_{\chi}(StarSun(h,p)) &= \frac{\chi(StarSun(h,p))}{E(StarSun(h,p))} \\ &= \frac{2}{2\sqrt{p-1+4h} + 2(p-2)\sqrt{h}} \\ &= \frac{1}{\sqrt{p-1+4h} + (p-2)\sqrt{h}} \end{aligned}$$

The *eigen-chromatic asymptote* of $StarSun(h,p)$ is

$$\begin{aligned} Asyeig_{\chi}(StarSun(h,p)) &= \lim_{(h+1)p \rightarrow \infty} \frac{1}{\sqrt{p-1+4h} + (p-2)\sqrt{h}} \\ &= \lim_{p \rightarrow \infty} \frac{1}{\sqrt{p-1+4h} + (p-2)\sqrt{h}} \\ &= 0. \end{aligned}$$

If $h = 1$ then $p = \frac{n}{2}$, so

$$\begin{aligned} A_{StarSun(1, \frac{n}{2})}^{\chi} &= \frac{2(n-1)}{n} \int \frac{dn}{\sqrt{\frac{n}{2}-1+4} + (\frac{n}{2}-2)\sqrt{1}} \\ &= \frac{2(n-1)}{n} \int \frac{dn}{\sqrt{\frac{n}{2}+3} + (\frac{n}{2}-2)}. \end{aligned}$$

5.4.5 The Cycle Sun Graph

The energy of the cycle sun graph is

$$E(CycleSun(h,p)) = 2 \sum_{k=0}^{p-1} \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h} \text{ (see section 3.3.6).}$$

The chromatic number of the Cycle sun Graphs is

$$\chi(CycleSun(h,p)) = 2 \text{ if } p \text{ is even.}$$

and

$$\chi(CycleSun(h,p)) = 3 \text{ if } p \text{ is odd (see section 4.4.4).}$$

The *eigen-chromatic ratio* of $CycleSun(h,p)$ is

$$\begin{aligned} eig_{\chi}(CycleSun(h,p)) &= \frac{\chi(CycleSun(h,p))}{E(CycleSun(h,p))} \\ &= \frac{2}{2 \sum_{k=0}^{p-1} \sqrt{\cos^2 \left(\frac{2\pi k}{p} \right) + h}} \end{aligned}$$

if p is even ;

$$eig_{\chi}(CycleSun(h,p)) = \frac{3}{2 \sum_{k=0}^{p-1} \sqrt{\cos^2 \left(\frac{2\pi k}{p} \right) + h}}$$

if p is odd .

The *eigen-chromatic asymptote* of $CycleSun(h,p)$ is, ($a = 3$ if p is odd, or $a = 2$ if p is even)

$$\begin{aligned} Asyeig_{\chi}(CycleSun(h,p)) &= \lim_{(h+1)p \rightarrow \infty} \frac{a}{2 \sum_{k=0}^{p-1} \sqrt{\cos^2 \left(\frac{2\pi k}{p} \right) + h}} \\ &= \lim_{p \rightarrow \infty} \frac{a}{2 \sum_{k=0}^{p-1} \sqrt{\cos^2 \left(\frac{2\pi k}{p} \right) + h}} \\ &= \lim_{p \rightarrow \infty} \frac{a}{2p\sqrt{1+h}} = 0. \end{aligned}$$

If $h = 1$ then $n = (h + 1)p = (1 + 1)p = 2p \Rightarrow p = \frac{n}{2}$, so

$$\begin{aligned} E(CycleSun(1, \frac{n}{2})) &= 2 \sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}} \right) + 1} \\ &= 2 \sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1} \end{aligned}$$

$$A_{CycleSun(1, \frac{n}{2})}^{\chi} = \frac{2m}{n} \int \frac{2}{2 \sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}} dn$$

(if p is even), and

$$A_{CycleSun(1, \frac{n}{2})}^X = \frac{2m}{n} \int \frac{3}{2 \sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}} dn$$

(if p is odd).

$$A_{CycleSun(1, \frac{n}{2})}^X = \frac{2n}{n} \int \frac{1}{\sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}} dn$$

(if p is even), and

$$A_{CycleSun(1, \frac{n}{2})}^X = \frac{2n}{n} \int \frac{3}{2 \sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}} dn$$

(if p is odd).

$$A_{CycleSun(1, \frac{n}{2})}^X = 2 \int \frac{dn}{\sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}}$$

(if p is even), and

$$A_{CycleSun(1, \frac{n}{2})}^X = 3 \int \frac{dn}{\sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2 \left(\frac{4\pi k}{n} \right) + 1}}$$

(if p is odd).

5.4.6 The Wheel Sun Graph

The energy of the wheel sun graph is (see section 3.3.4)

$$E(WheelSun(h,p)) = 2 \sum_{k=1}^{p-2} \sqrt{\cos^2 \left(\frac{2\pi k}{p-1} \right) + h} + \sqrt{(1 + \sqrt{p})^2 + 4h} + \sqrt{(1 - \sqrt{p})^2 + 4h}.$$

The chromatic number of the Wheel sun Graphs is

$$\chi(WheelSun(h,p)) = 4 \text{ if } p \text{ is even.}$$

and

$$\chi(WheelSun(h,p)) = 3 \text{ if } p \text{ is odd (see section 4.4.5).}$$

The *eigen-chromatic ratio* of $WheelSun(h,p)$ is

$$\begin{aligned} eig_{\chi}(WheelSun(h,p)) &= \frac{\chi(WheelSun(h,p))}{E(WheelSun(h,p))} \\ &= \frac{4}{2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}} \end{aligned}$$

if p is even ;

$$eig_{\chi}(WheelSun(h,p)) = \frac{3}{2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}}$$

if p is odd .

The *eigen-chromatic asymptote* of $WheelSun(h,p)$ is, ($a = 3$ if p is odd, or $a = 4$ if p is even)
 $Asyeig_{\chi}(WheelSun(h,p))$

$$\begin{aligned} &= \lim_{(h+1)p \rightarrow \infty} \frac{a}{2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}} \\ &= \lim_{p \rightarrow \infty} \frac{a}{2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + h + \sqrt{(1+\sqrt{p})^2 + 4h} + \sqrt{(1-\sqrt{p})^2 + 4h}}} \\ &= 0. \end{aligned}$$

If $h = 1$ then $n = (h + 1)p = (1 + 1)p = 2p \Rightarrow p = \frac{n}{2}$, so

$$\begin{aligned} E(WheelSun(1,p)) &= 2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + 1 + \sqrt{(1+\sqrt{p})^2 + 4} + \sqrt{(1-\sqrt{p})^2 + 4}} \\ &= 2 \sum_{k=1}^{p-2} \sqrt{\cos^2\left(\frac{2\pi k}{p-1}\right) + 1 + \sqrt{p + 2\sqrt{p} + 5} + \sqrt{p - 2\sqrt{p} + 5}} \end{aligned}$$

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{2m}{n} \int \frac{4}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}} dn$$

(if p is even), and

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{2m}{n} \int \frac{3}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}} dn$$

(if p is odd).

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{2^{\frac{3(n-2)+2}{2}}}{n} \int \frac{4}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}} dn$$

(if p is even), and

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{2^{\frac{3(n-2)+2}{2}}}{n} \int \frac{3}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}} dn$$

(if p is odd).

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{12(n-2) + 8}{n} \int \frac{dn}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}}$$

(if p is even), and

$$A_{WheelSun(1, \frac{n}{2})}^x = \frac{9(n-2) + 6}{n} \int \frac{dn}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2 \left(\frac{2\pi k}{\frac{n}{2}-1} \right) + 1 + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2} + 5}} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2} + 5}}}$$

(if p is odd).

Conjecture 1. The eigen-chromatic asymptote of all the classes of graphs lies on the interval $[0, \frac{1}{2}]$, except that of Lollipop graph which is equal to 1.

Theorem 5.1. The eigen-chromatic ratio and asymptote for all the classes \mathfrak{F} of graphs studied in this chapter are summarized in the following table.

\mathfrak{F}	$\underline{eig_\chi(\mathfrak{F})}$	$\underline{Asyeig_\chi(\mathfrak{F})}$
1) K_n :	$\frac{n}{2n-2}$	$\frac{1}{2}$
2) P_n :	$\frac{1}{\operatorname{cosec}\frac{\pi}{2(n+1)} - 1}$	0
3) C_n :	$\frac{1}{2\cot(\frac{\pi}{n})}$	0
4) W_n :	$\frac{2}{\sqrt{n} - 1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)}$	0
5) $S_{n-1,1}$:	$\frac{1}{\sqrt{n-1}}$	0
6) $S_{\frac{n-1}{2},2}$:	$\frac{2}{n-3 + \sqrt{2(n+1)}}$	0
7) LP_n :	$\frac{n-1}{n-3}$	1
8) $K_{\frac{n}{2}, \frac{n}{2}}$:	$\frac{2}{n}$	0
9) $F_{\frac{n-1}{2}}$:	$\frac{3}{(n-2) + \sqrt{4n-3}}$	0

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<u>\mathfrak{F}</u>	<u>$eig_\chi(\mathfrak{F})$</u>	<u>$Asyeig_\chi(\mathfrak{F})$</u>
10) $L(CT(k,l)):$	$\frac{3}{n}$	0
11) $CompSun(h,p):$	$\frac{p}{(p-1)\sqrt{1+4h} + \sqrt{(p-1)^2+4h}}$	$(0, \frac{1}{2})$
12) $BipSun(h,p):$	$\frac{2}{\sqrt{p^2+16h} + 2(p-2)\sqrt{h}}$	0
13) $StarSun(h,p):$	$\frac{1}{\sqrt{p-1+4h} + (p-2)\sqrt{h}}$	0
14) $CycleSun(h,p):$	$\frac{2}{2\sum_{k=0}^{p-1} \sqrt{\cos^2\left(\frac{2\pi k}{p}\right) + h}}$	0
15) $WheelSun(h,p):$	-	0

Theorem 5.2. The eigen-chromatic area for all the classes \mathfrak{F} of graphs studied in this chapter are summarized in the following table.

<u>\mathfrak{F}</u>	<u>$A_{\mathfrak{F}(n)}^\chi$</u>
1) $K_n:$	$\frac{n-1}{2}(n + \ln n-1 - 2)$
2) $P_n:$	$\frac{2(n-2)}{n} \int \frac{1}{\operatorname{cosec} \frac{\pi}{2(n+1)} - 1} dn$
3) $C_n:$	$\int \frac{1}{\cot(\frac{\pi}{n})} dn$

$$\begin{aligned}
4) W_n: & \quad \frac{8(n-1)}{n} \int \frac{1}{\sqrt{n}-1 + \operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)} dn \\
5) S_{n-1,1}: & \quad \frac{4(n-1)}{n} (\sqrt{n-1} - 1) \\
6) S_{\frac{n-1}{2},2}: & \quad \frac{8(n-1)}{3n} \ln \frac{[(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]}{16(1+\sqrt{2})} \\
7) K_{\frac{n}{2}, \frac{n}{2}}: & \quad n \ln \left(\frac{n}{2}\right) \\
8) F_{\frac{n-1}{2}}: & \quad \frac{9(n-1)}{n} \int \frac{1}{(n-2) + \sqrt{4n-3}} dn \\
9) L(CT(k,l)): & \quad \frac{6(n-1)}{n} \ln \frac{n}{3} \\
10) \operatorname{CompSun}(1, \frac{n}{2}): & \quad \frac{n+2}{2} \int \frac{n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2 + 16}} dn. \\
11) \operatorname{BipSun}(1, \frac{n}{2}): & \quad \frac{n+8}{2} \int \frac{dn}{\sqrt{n^2 + 64 + 2n - 8}} \\
12) \operatorname{StarSun}(1, \frac{n}{2}): & \quad \frac{2(n-1)}{n} \int \frac{dn}{\sqrt{\frac{n}{2} + 3} + (\frac{n}{2} - 2)} \\
13) \operatorname{CycleSun}(1, \frac{n}{2}): & \quad 3 \int \frac{dn}{\sum_{k=0}^{\frac{n}{2}-1} \sqrt{\cos^2\left(\frac{4\pi k}{n}\right) + 1}} \\
14) \operatorname{WheelSun}(1, \frac{n}{2}): & \quad \frac{9(n-2)+6}{n} \int \frac{dn}{2 \sum_{k=1}^{\frac{n}{2}-2} \sqrt{\cos^2\left(\frac{2\pi k}{\frac{n}{2}-1}\right) + 1} + \sqrt{\frac{n}{2} + 2\sqrt{\frac{n}{2}} + 5} + \sqrt{\frac{n}{2} - 2\sqrt{\frac{n}{2}} + 5}}
\end{aligned}$$

Hypothesis 5.1. The eigen-chromatic area of the complete graph is the largest of all classes of graphs for large n .

Theorem 5.3. The eigen-chromatic stability for all the classes \mathfrak{F} of graphs studied in this chapter are determined in the following table.

<u>\mathfrak{F}</u>	<u>eigen-chromatic stability</u>
1) The complete graph K_n , on n vertices	is <i>hyper eigen-chromatically stable</i>
2) The path graphs P_n on n vertices	is <i>eigen-chromatically unstable</i>
3) The cycle graphs C_n on n vertices	is <i>eigen-chromatically unstable</i>
4) The wheel graphs W_n on n vertices	is <i>eigen-chromatically unstable</i>
5) The star graph $S_{n-1,1}$, on n vertices, with $n - 1$ rays of length 1	is <i>eigen-chromatically unstable</i>
6) The star graph $S_{\frac{n-1}{2},2}$, on n vertices, with $\frac{n-1}{2}$ rays of length 2	is <i>eigen-chromatically unstable</i>
7) The lollipop graph LP_n on n vertices	is <i>hyper eigen-chromatically stable</i>
8) The complete split-bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$, on n vertices	is <i>eigen-chromatically unstable</i>
9) The Friendship graph F_n on $2n + 1$ vertices	is <i>eigen-chromatically unstable</i>
10) The Caterpillar Graph $L(CT(k,l))$	is <i>eigen-chromatically unstable</i>
11) The Complete Sun Graph $CompSun(h,p)$	is <i>hypo eigen-chromatically stable</i>
12) The Complete Split-bipartite Sun Graph $BipSun(h,p)$	is <i>eigen-chromatically unstable</i>
13) The Star Sun Graph $StarSun(h,p)$	is <i>eigen-chromatically unstable</i>
14) The Cycle Sun Graph $CycleSun(h,p)$	is <i>eigen-chromatically unstable</i>
15) The Wheel Sun Graph $WheelSun(h,p)$	is <i>eigen-chromatically unstable</i>

Corollary 5.1. The complete, the lollipop and the complete sun graph are the only eigen-chromatically stable classes of graphs in the collection of classes discussed above.

5.5 Second Order Differential Equation Associated With The Eigen-Chromatic Ratio of The Complete Graph: Paired Solutions

We notice that if f and g are two solutions of an ordinary differential equation, then so is the sum; in fact, so is any linear combination $\alpha f + \beta g$ where α and β are constants. And such two solutions f and g satisfying the same differential equation are called *paired solutions*. For example, \cos and \sin are paired for the ordinary differential equation $y'' + y = 0$; \cosh and \sinh are paired, for the ordinary differential equation $y'' - y = 0$ (See Winter, Mayala and Namayanja [56], Zill [61], Zill and Wright [62]).

The eigen-chromatic ratio of the complete graph on n vertices is $\frac{n}{2n-2}$.

setting

$$y = \frac{n}{2n-2},$$

now

$$y' = \frac{dy}{dn} = \frac{d}{dn} \left[\frac{n}{2n-2} \right] = \frac{-2}{(2n-2)^2} = \frac{d}{dn} \left[\frac{1}{2n-2} \right].$$

Also:

$$y'' = \frac{dy'}{dn} = -2 \frac{d}{dn} \left[\frac{1}{(2n-2)^2} \right] = \frac{8}{(2n-2)^3}.$$

Thus:

$$2y' + (n-1)y'' = \frac{-4}{(2n-2)^2} + (n-1) \frac{8}{(2n-2)^3} = 0.$$

So that:

$$y'' + \frac{2}{n-1}y' = 0.$$

Put $P = y' \Rightarrow P' = y''$, so

$$P' + \frac{2}{n-1}P = 0.$$

Integrating factor is $e^{2 \int \frac{dn}{n-1}} = (n-1)^2$, so that $(n-1)^2 P = C$. Hence $P = \frac{C}{(n-1)^2}$. So that

$$y' = \frac{C}{(n-1)^2}.$$

We thus have:

$$y = \frac{-C}{n-1} + C' \Rightarrow y = \frac{K}{n-1} + K' \text{ (with } K, K' \in \mathbb{R}\text{)}.$$

Thus the two distinct functions $y_1 = \frac{n}{2n-2}$ and $y_2 = \frac{K}{n-1} + K'$ satisfy the same differential equation:

$$2y' + (n-1)y'' = 0$$

called paired solutions.

5.6 The Eigen-chromatic Ratio of Complements of some Graphs with its Asymptotic and Area aspects

We remind that the complement, \overline{G} , of a graph G , has the same vertex set as G and v_i and v_j are adjacent in \overline{G} if and only if they are not adjacent in G .

5.6.1 The Complete Split-bipartite Graphs

Let $K_{\frac{n}{2}, \frac{n}{2}}$ be the complete split-bipartite graph on n vertices ($n \geq 6$, n is even), with $\frac{n^2}{4}$ edges, and $\overline{K}_{\frac{n}{2}, \frac{n}{2}}$ be the complement of $K_{\frac{n}{2}, \frac{n}{2}}$. We denote that $\overline{K}_{\frac{n}{2}, \frac{n}{2}}$ consists of two disjoint copies of $K_{\frac{n}{2}}$, and It has $\frac{n-2}{4}$ edges. Its energy is therefore (see Winter and Ojako [54])

$$E(\overline{K}_{\frac{n}{2}, \frac{n}{2}}) = 2n - 4$$

and Its chromatic number is

$$\chi(\overline{K}_{\frac{n}{2}, \frac{n}{2}}) = \frac{n}{2}.$$

So that, the Eigen-chromatic ratio of $\overline{K}_{\frac{n}{2}, \frac{n}{2}}$ is

$$\begin{aligned} eig_{\chi}(\overline{K}_{\frac{n}{2}, \frac{n}{2}}) &= \frac{\chi(\overline{K}_{\frac{n}{2}, \frac{n}{2}})}{E(\overline{K}_{\frac{n}{2}, \frac{n}{2}})} \\ &= \frac{\frac{n}{2}}{2n-4} \\ &= \frac{n}{4(n-2)}; \end{aligned}$$

the *eigen-chromatic asymptote* of $\overline{K}_{\frac{n}{2}, \frac{n}{2}}$ denoted by $Asyeig_{\chi}(\overline{K}_{\frac{n}{2}, \frac{n}{2}})$ is

$$\begin{aligned} Asyeig_{\chi}(\overline{K}_{\frac{n}{2}, \frac{n}{2}}) &= \lim_{n \rightarrow \infty} \frac{n}{4(n-2)} \\ &= \frac{1}{4}; \end{aligned}$$

the *eigen-chromatic area* of $\overline{K}_{\frac{n}{2}, \frac{n}{2}}$ is

$$\begin{aligned} A_{\overline{K}_{\frac{n}{2}, \frac{n}{2}}}^{\chi} &= \frac{2m}{n} \int \frac{n}{4(n-2)} dn \\ &= \frac{n-2}{2n} \int \frac{n}{4(n-2)} dn \\ &= \frac{n-2}{4n} \int \frac{n}{n-2} dn \\ &= \frac{n-2}{4n} (n + 2 \ln |n-2| + C). \end{aligned}$$

The function $f(n) = \frac{n}{4(n-2)}$ is defined if $4n-8 \neq 0$ i.e if $n \neq 2$, so that with smallest order 6 we have: $A_{\overline{K}_{\frac{6}{2}, \frac{6}{2}}}^{\chi} = \frac{6-2}{24} (6 + 2 \ln |6-2| + C) = 0 \Rightarrow C = -2(3 + 2 \ln 2)$, so

$$A_{\overline{K}_{\frac{n}{2}, \frac{n}{2}}}^{\chi} = \frac{n-2}{4n} (n + 2 \ln |n-2| - 2(3 + 2 \ln 2)).$$

The eigen-chromatic ratio for the complement of the complete split-bipartite graph is

$$f(n) = \frac{n}{4(n-2)}.$$

And the eigen-chromatic ratio of the original graph, $K_{\frac{n}{2}, \frac{n}{2}}$ is

$$g(n) = eig_{\chi}(K_{\frac{n}{2}, \frac{n}{2}}) = \frac{2}{n}.$$

5.6.2 The Lollipop Graphs

Let LP_n be the lollipop graph on n vertices, $n > 2$. The complement of LP_n , denoted by \overline{LP}_n , consists of a star graph on $n-1$ vertices and an isolated vertex. Its energy is (see Winter and Ojako [54])

$$E(\overline{LP}_n) = 2\sqrt{n-2}$$

and Its chromatic number is

$$\chi(\overline{LP}_n) = 2.$$

The *eigen-chromatic ratio* of \overline{LP}_n is

$$\begin{aligned} eig_\chi(\overline{LP}_n) &= \frac{\chi(\overline{LP}_n)}{E(\overline{LP}_n)} \\ &= \frac{1}{\sqrt{n-2}} \end{aligned}$$

The *eigen-chromatic asymptote* of \overline{LP}_n is

$$\begin{aligned} Asyeig_\chi(\overline{LP}_n) &= \lim_{n \rightarrow \infty} \frac{1}{\sqrt{n-2}} \\ &= 0; \end{aligned}$$

The *eigen-chromatic area* of \overline{LP}_n is

$$\begin{aligned} A_{LP_n}^\chi &= \frac{2m}{n} \int \frac{1}{\sqrt{n-2}} dn \\ &= \frac{2m}{n} (2\sqrt{n-2}) \\ &= \frac{4m}{n} (\sqrt{n-2} + C). \end{aligned}$$

With smallest order 3 we have: $C = -1$, so

$$A_{LP_n}^\chi = \frac{4m}{n} (\sqrt{n-2} - 1);$$

where m is the size of \overline{LP}_n .

5.6.3 The Star Graphs with rays of length 1

Let $S_{n-1,1}$ be the star graph on n vertices, and with $n-1$ rays of length 1, $n \geq 2$. The complement of $S_{n-1,1}$ denoted by $\overline{S}_{n-1,1}$, is a complete graph on $n-1$ vertices together with an isolated vertex. Its energy is

$$E(\overline{S}_{n-1,1}) = 2n - 4 \text{ (see Winter and Ojako [54]);}$$

and Its chromatic number is

$$\chi(\overline{S}_{n-1,1}) = n - 1.$$

The *eigen-chromatic ratio* of $\overline{S}_{n-1,1}$ is

$$\begin{aligned} eig_\chi(\overline{S}_{n-1,1}) &= \frac{\chi(\overline{S}_{n-1,1})}{E(\overline{S}_{n-1,1})} \\ &= \frac{n-1}{2n-4}; \end{aligned}$$

the *eigen-chromatic asymptote* of $\overline{S}_{n-1,1}$ denoted by $Asyeig_{\chi}(\overline{S}_{n-1,1})$ is

$$\begin{aligned} Asyeig_{\chi}(\overline{S}_{n-1,1}) &= \lim_{n \rightarrow \infty} \frac{n-1}{2n-4} \\ &= \frac{1}{2}; \end{aligned}$$

the *eigen-chromatic area* of $A_{\overline{S}_{n-1,1}}$ is

$$\begin{aligned} A_{\overline{S}_{n-1,1}}^{\chi} &= \frac{2m}{n} \int \frac{n-1}{2n-4} dn \\ &= \frac{m}{n} \int \frac{n-1}{n-2} dn \\ &= \frac{m}{n} (n + \ln(n-2) + C). \end{aligned}$$

With smallest order 3 we have: $C = -3$, so

$$A_{\overline{S}_{n-1,1}}^{\chi} = \frac{m}{n} (n + \ln(n-2) - 3);$$

where m is the size of $\overline{S}_{n-1,1}$.

Conjecture 5.6.1. The eigen-chromatic asymptote of complements of graphs discussed above lies on the interval $[0, \frac{1}{2}]$.

Theorem 5.6.1. The complement of the complete split-bipartite graphs and the complement of the star graphs with length 1 are eigen-chromatically stable.

5.7 Conclusion

In this chapter, we have defined the eigen-chromatic ratio and asymptote of classes of graph. We attached the average degree of a class of graph to the Riemann integral for the eigen-chromatic ratio (as a function of the number of vertices n involved) to get the eigen-chromatic area.

After having determined the eigen-chromatic ratio, the eigen-chromatic asymptote and the eigen-chromatic area for all the classes of graphs, we have noticed the following:

- The lower bound on eigen-chromatic asymptote is 0
- The upper bound on eigen-chromatic asymptote is 1
- The eigen-chromatic asymptote for the Complete graph K_n and the Lollipop graph LP_n , on n vertices, is $\frac{1}{2}$ and 1, respectively. So that, they are hyper eigen-chromatically stable.
- The eigen-chromatic asymptote of the complete sun graph $CompSun(h,p)$ lies on the interval $(0, \frac{1}{2})$. So that, it is hypo eigen-chromatically stable.
- All the other classes of graphs are not eigen-chromatically stable. This is the case, for example, of the path, cycle, wheel and star graphs.

We also found the paired solutions of the second order differential equation associated with the eigen-chromatic ratio for the Complete Graph.

Chapter 6

CONCLUSION

6.1 Summary

In this thesis, We have presented a new ratio associated with classes of graphs, called the *eigen-chromatic ratio*, by combining the two graph theoretical concepts of *energy* and *chromatic number*. The motivation for combining the energy, and chromatic number of a graph, into a ratio, arose from the need to understand, in molecular graph theory, the energy distribution among the atoms of a molecule, where only different atoms are bonded (for example, covalent bonding). In molecules where a large number of atoms are involved, classes of graphs involving the complete graph appears to give the most stable of such an energy distribution.

We began this dissertation with the presentation of the graph theoretical definitions used, together with the different classes of graphs.

In chapter 2, We presented different techniques used to find the eigenvalues of adjacency matrices associated with certain classes of graphs. We also showed that we can use the idea of complements to find the eigenvalues of some regular graphs such as a complete graph.

In chapter 3, We used the analytical methods for determining the energy of some classes of graphs, We analyzed the energies of the path graph, cycle graph and wheel graph on n vertices. We expressed the energy of cycles, paths and wheels in terms of simplified expressions using the cotangent or cosecant.

In chapter 4, We have determined the chromatic number of all the classes of graphs of which we have analyzed the energy. For example, We found the chromatic number of the complete graph K_n , on n vertices is $\chi(K_n) = n$, while the chromatic number of the k -partite graphs G is $\chi(G) = k$.

In chapter 5, After having determined the eigen-chromatic ratio, the eigen-chromatic asymptote and the eigen-chromatic area for all the classes of graphs, we have noticed the following:

- The eigen-chromatic ratio of the complete graph on n vertices, as a function of n , to be paired with another function, as solutions of a second order ordinary differential equation.
- The lower bound on eigen-chromatic asymptote is 0
- The upper bound on eigen-chromatic asymptote is 1
- The eigen-chromatic asymptote for the Complete graph K_n , on n vertices, is $\frac{1}{2}$. So that, the Complete graph is hyper eigen-chromatically stable; The Lollipop graph as well.

- The eigen-chromatic asymptote of the complete sun graph $CompSun(h,p)$ lies on the interval $(0, \frac{1}{2})$. So that, It is hypo eigen-chromatically stable.
- All the other classes of graphs are not eigen-chromatically stable. This is the case, for example, of the path, cycle, wheel and star graphs.

We propose that the eigen-chromatic area of the complete graph is the largest of all such areas of all classes of graphs.

6.2 Future research

During the preparation of this thesis, the following preoccupations have been posed:

- 1) We can use variations of the chromatic number, for example the circular chromatic number (see G. Fan [65] and X. Zhu [66]).
- 2) Need to solve our conjectures in thesis:
 - (a) is the area of complete graph the largest among all classes?
 - (b) does there exist a class of graphs with asymptote bigger than 1?
- 3) Replace energy with two forms of Laplacian energy. And to combine the concepts of two types of *Laplacian energy* and *chromatic number* of graphs to form two ratios each referred to as the Laplacian eigen-chromatic ratio, associated with a connected graph G .

The research required to answer these preoccupations could form the basis for additional research on topics covered in this thesis.

Chapter 7

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