THE ENERGY AND SEIDEL ENERGY OF CAYLEY GRAPHS ASSOCIATED TO DIHEDRAL, ALTERNATING AND SYMMETRIC GROUPS

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DEDICATION

This thesis is dedicated to my beloved supervisors, families and friends.

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ABSTRACT

The energy of a simple graph is defined as the summation of the absolute value of the eigenvalues of the adjacency matrix of the graph. It was motivated by the Hückel Molecular Orbital theory. The theory was used by chemists to estimate the energy associated with π-electron orbitals of molecules which is called as conjugated hydrocarbons. Meanwhile, the Seidel energy is defined as the summation of the absolute value of the eigenvalues of the Seidel matrix of the graph. Besides, a Cayley graph associated to a finite group is defined as a graph where its vertices are the elements of a group and two vertices g and h are joined with an edge if and only if h is equal to the product of x and g for some elements x in the subset X of the group. This research combines the topics in graph theory with group theory, namely on the energy and Seidel energy for Cayley graphs, with some finite groups, namely dihedral groups, alternating groups, and symmetric groups. The results are obtained by finding the isomorphism of the Cayley graphs with respect to the subsets of order one and two, and the generating set associated to the groups. The respected Cayley graphs are found and represented as the union of complete graphs, cycle graphs, and complete bipartite graphs. The obtained graphs are then mapped onto their adjacency matrix and Seidel matrix respectively to obtain the eigenvalues and Seidel eigenvalues of the graphs. Some group theory concepts and properties of special graphs are also used to find the generalizations of the eigenvalues of the Cayley graphs. Finally, the energy and the Seidel energy for the Cayley graphs associated to the dihedral groups, alternating groups, and symmetric groups are obtained by using the eigenvalues and the Seidel eigenvalues of the graphs, respectively. The results show that the Seidel energy of Cayley graphs with respect to subsets of order one associated to the groups are equal to their energy. It is also found that the Seidel energy of Cayley graphs with respect to some subsets of order two and the generating sets associated to the groups are larger than their energy.

ABSTRAK

Tenaga bagi suatu graf ringkas ditakrifkan sebagai hasil tambah nilai mutlak bagi nilai eigen matriks bersebelahan bagi graf tersebut. Ia telah diinspirasikan oleh teori orbital molekul Hückel. Teori ini telah digunakan oleh ahli kimia untuk menganggarkan tenaga berkaitan dengan orbital molekul π-elektron yang dipanggil sebagai hidrokarbon konjugasi. Sementara itu, tenaga Seidel ditakrifkan sebagai hasil tambah nilai mutlak bagi nilai eigen matriks Seidel bagi suatu graf. Selain itu, graf Cayley yang dikaitkan dengan kumpulan terhingga ditakrifkan sebagai graf dengan bucunya adalah unsur-unsur kumpulan tersebut dan dua bucu g dan h adalah terkait jika dan hanya jika h adalah sama dengan hasil darab x dan g untuk beberapa unsur x dalam subset X bagi kumpulan tersebut. Kajian ini menggabungkan topik dalam teori graf dengan teori kumpulan, iaitu pada tenaga dan tenaga Seidel bagi graf Cayley, dengan beberapa kumpulan terhingga iaitu kumpulan dihedral, kumpulan berselang-seli, dan kumpulan simetri. Keputusan diperolehi dengan mencari isomorfisma bagi graf Cayley berkaitan dengan subset berperingkat satu dan dua, dan subset penjana bagi kumpulan tersebut. Graf Cayley berkenaan diperolehi dan diwakili sebagai gabungan graf lengkap, graf kitar, dan graf bipartit lengkap. Graf-graf tersebut kemudiannya dipetakan ke matriks bersebelahan dan matriks Seidel, masing-masing untuk mendapatkan nilai eigen dan nilai eigen Seidel bagi setiap graf tersebut. Beberapa konsep teori kumpulan dan sifat bagi graf khusus juga telah digunakan untuk mencari generalisasi bagi nilai eigen dan nilai eigen Seidel bagi graf Cayley tersebut. Akhirnya, tenaga dan tenaga Seidel bagi graf Cayley bagi kumpulan dihedral, kumpulan berselang-seli, dan kumpulan simetri telah diperolehi, masing-masing dengan menggunakan nilai eigen dan nilai eigen Seidel bagi graf tersebut. Keputusan menunjukkan bahawa tenaga Seidel bagi graf Cayley berkaitan subset berperingkat satu bagi kumpulan tersebut adalah sama dengan tenaga mereka. Ia juga didapati bahawa tenaga Seidel bagi graf Cayley bagi beberapa subset berperingkat dua dan set penjana bagi kumpulan tersebut adalah lebih besar daripada tenaga mereka.

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LIST OF ABBREVIATIONS

UTM	-	Universiti Teknologi Malaysia
HMO	-	Hückel Molecular Orbital
AD	-	Alzheimer Disease
GAP	-	Groups, Algorithms, and Programming

LIST OF SYMBOLS

a_{ij}	-	(i, j)-entry of a matrix
$A(\Gamma)$	-	Adjacency matrix of a graph Γ
$Cay(G, X)$	-	Cayley graph of a group G with respect to a subset X
$f(\Gamma, x)$	-	Characteristic polynomial of a graph Γ
K_r	-	Complete graph on r vertices
$\overline{\Gamma}$	-	Complement of a graph
$d(v_i)$	-	Degree of a vertex v_i
$E(\Gamma)$	-	Edge-set of a graph Γ
λ_n	-	The n^{th} eigenvalues
Γ	-	Graph
$\varepsilon(\Gamma_G)$	-	Energy of a graph Γ of a group G
G	-	Group
e or 1	-	Identity
N_n	-	Null graph
$\|G\|$	-	Order of a group G
θ_n	-	Seidel eigenvalues
$SE(\Gamma_G)$	-	Seidel energy of a graph Γ of a group G
S	-	Subset of a group G
$X^{(i)}$	-	Subset X of order i
I_n	-	Unit matrix of order n
$V(\Gamma)$	-	Vertex-set of a graph Γ

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Cayley graphs have a wide real life application in many areas, especially in the field of biology and computer science. For instance, in the field of biology, Cayley graphs on symmetric groups appeared in molecular biology when permutations are used to represent the sequences of genes in chromosomes and genomes while some operations on the permutations represent evolutionary events. In the field of computer science, Cayley graphs are used in the representation of interconnection and networks. The vertices in the Cayley graphs represent the processing elements and the memory modules while the edges represent the communication lines.

In addition, the theory of Cayley graphs has developed into a branch in algebraic graph theory. This research is focused in constructing the Cayley graphs associated to some finite groups in group theory. The Cayley graph of a group is first defined by Arthur Cayley in 1878 as a graph with the elements of a group G as the vertices and there is an edge joining the vertices g_1 and g_2 in G if and only if there is $x \in X$, where X is a subset of G, such that the product of x and g_1 is equal to g_2. The subset X of G does not include the identity element of G and it holds the inverse-closed property where every element of the subset has an inverse under the operation that is also an element of the subset. The Cayley graph of G with respect to the subset X is often denoted as $Cay(G, X)$ [1].

Meanwhile, the energy of a graph Γ is defined as the summation of all positive values of the eigenvalues of the adjacency matrix of the graph. The set of all eigenvalues of the graph is referred to as the spectrum of the graph. Let Γ be a finite and undirected simple graph, with vertex set $V(\Gamma)$ and edge set $E(\Gamma)$. The number of vertices of Γ is n, and its vertices are labelled by $v_1, v_2, \ldots, v_n$. The adjacency matrix, $A(\Gamma)$, of the graph Γ is a square matrix of size $n \times n$, whose ij-entry is equal to 1 if the vertices v_i and v_j are adjacent and is equal to zero otherwise. The characteristic polynomial of the adjacency matrix, which is det$(\lambda I_n - A(\Gamma))$, where I_n is the unit matrix of order n is said to be the characteristic polynomial of the graph Γ and often denoted by $f(\Gamma, x)$. Since the eigenvalues of a graph Γ are defined as the eigenvalues of its adjacency matrix $A(\Gamma)$, so they are just the roots of the equation $f(\Gamma, x) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$.

According to Woods in [2], the study on the energy of general simple graphs was first defined by Gutman [3] inspired from the Hückel Molecular Orbital (HMO) Theory proposed in 1930s by Hückel. The HMO Theory has been used by chemists in approximating the energies related with π-electron orbitals in conjugated hydrocarbon molecules.

In 2009, Li *et al.* [4] explained that in the early days, when computers were not widely accessible, the calculation of the HMO total π-electron energy was a huge problem. In order to overcome the difficulty, various approaches have been offered to calculate the approximate calculation of the π-electron energy. Within the approximation, the total energy of the π-electrons, denoted by ε, is then obtained, which is by summing up the individual electron energies. In conjugated hydrocarbons, the total number of π-electrons is equal to the number of vertices of the associated molecular graph. After a few considerations, they finalized the definition of the energy of the graph by the summation of the absolute values of the eigenvalues of the molecular graph.

This research aims to determine the Cayley graphs associated to some finite groups, and further to compute the energy of the Cayley graphs associated to the groups. The procedures are consisted of generating the elements, vertices and edges for the Cayley graphs of the groups being studied, finding the isomorphisms and generalizations of the Cayley graphs, building the adjacency matrix for each Cayley graph, calculating the eigenvalues of the adjacency matrices and finally computing the energy of the Cayley graphs. Besides the ordinary energy of graph, this research is also interested in finding the Seidel energy of the Cayley graphs. The general form of the results are determined and presented at the end of the study.

1.2 Research Background

The study on Cayley graphs was initiated by Arthur Cayley in 1878 and since then, they have been many researchers presenting their interest on the topics. The theory has been advanced into a significant branch in algebraic graph theory. There are many problems regarding Cayley graphs that have been studied by many researchers. For instance, Babai and Seress [5], Lakshmivarahan *et al.* [6], Friedman [7], Adiga and Ariamanesh [8] and many more have specifically studied on the Cayley graphs related to permutations groups. In addition, Konstantinova in [9] has presented the historical changes of the problems related to families of Cayley graphs and included various applications of Cayley graphs in solving combinatorial, graph-theoretical, and applied problems.

Meanwhile, studies on the spectrum of the Cayley graphs by using algebraic graph theory was first considered by Babai in [10]. In the following years, many researchers (see [11] - [14]) have extended or applied the concept to find the eigenvalues of Cayley graphs. There are also researchers that use other method besides using Babai's. For instance, Diaconis and Shahshahani [15] and Ghorbani and Nowroozi-Larki [16] have used a different method which is via the character table of the related groups to arrive to the spectrum.

Furthermore, there are also a few researchers who studied specifically on the eigenvalues and the energy of unitary Cayley graphs. For instance, Balakrishnan [17] has determined the energy of unitary Cayley graphs where his works was later extended by Ramaswamy and Veena in [18]. In [19], Foster-Greenwood and Kriloff and in [20], Liu and Li have also applied the concept to study on the unitary Cayley graphs and their energy.

Over the years, there has been considerable attention in the literature associated to the studies on Cayley graphs related to groups especially on the properties of the graphs. Although the literatures are growing, the topic related to Cayley graphs can be explored more. Therefore in this research, the Cayley graphs associated to some finite groups, namely the dihedral groups, alternating groups and symmetric groups are constructed and the applications of the findings are extended to the computations of the spectrum of the said graphs and further the ordinary energy and Seidel energy of the graphs.

1.3 Problem Statements

The study on Cayley graphs was initiated a long time ago by Arthur Cayley in 1878 while the study on the energy of graphs have just started in 1978 motivated by Hückel Molecular Orbital Theory in 1930s. Although many previous studies have been done on Cayley graphs associated to groups, there are lack of studies describing the structure of the Cayley graphs of finite groups specifically for the dihedral groups, alternating groups and symmetric groups in general. Therefore, part of the aim of this study is to construct and determine the general formula of the Cayley graphs of some finite groups. The studies combining a few fields in mathematics such as group theory, graph theory and linear algebra are very interesting to be explored yet not many researchers focused on the energy of graphs related to groups. Therefore, this research intended to study the energy of the Cayley graphs associated to some finite groups by applying the knowledge from linear algebra. Besides there are lack of studies on the other types of energy of graphs associated to groups. Thus, this research extends the studies to compute the Seidel energy of Cayley graphs associated to some finite groups.

1.4 Research Objectives

The objectives of this study are:

1. To determine the Cayley graphs with respect to subsets of order one and two associated to the dihedral groups, alternating groups, and symmetric groups.
2. To establish the energy of the Cayley graphs with respect to subsets of order one and two associated to the dihedral groups, alternating groups, and symmetric groups.
3. To develop the Seidel energy of the Cayley graphs with respect to subsets of order one and two associated to the dihedral groups, alternating groups, and symmetric groups and their general form.

1.5 Scope of the Study

This research combines three area of studies, namely group theory, graph theory and some knowledge in linear algebra. The first part of the research focused on the construction of the Cayley graphs associated to the dihedral groups, alternating groups and symmetric groups. The Cayley graphs are with respect to subsets of order one and two of the groups, including some generating set of the groups.

Meanwhile, the second part of this research focused on computing the ordinary energy and the Seidel energy of the Cayley graphs associated to the dihedral groups, alternating groups and symmetric groups.

1.6 Significance of Findings

This research is meant to add up as new findings on the topics of the energy of graphs related to finite groups. The major contributions of this work which are the computation of the energy of the graphs can actually be corresponded to the molecular structures in chemical graph theory where the bonding of atoms are presented as simple graphs in mathematics. Therefore, this research is keen to increase the works on the energy of graphs and would also help chemists all around the world to calculate the energy of molecular structures in much simpler way in future, plus it is more time and costs saving.

Besides, the procedure can also be applied to other field of sciences. For instances in medical, the methodology of the energy of graph was used in the search for the genetic causes of Alzheimer Disease (AD) and for modeling of the spread of epidemics. The application of the energy helped explains the understanding of network breakdown in AD using advanced mathematical descriptors. The concept of spectral graph theory were applied to provide novel metrics of structural connectivity based on 3-Tesla diffusion weighted images in AD patients and healthy controls. The connectivity networks were reconstructed using whole-brain tractography and the cortical disconnection were examined based on the energy of the graph and its spectrum. It has been found that the number of disconnected cortical regions rised with the number of copies of the risk gene in AD patients. Each additional copy of the risk gene have lead to more dysfunctional networks with weakened or abnormal connections, providing evidence for the disconnection syndrome.

Based on the examples given, it is no doubt that the study of energy of graph is of great significance. Many practical problems in real life can be represented in graphs or networks and the concept of the energy of graph can be applied. Interestingly, the analysis of the graphs can be made accordingly, to the increment or decrement of the energy values.

1.7 Research Methodology

The research started by constructing the Cayley graphs associated to the dihedral groups, alternating groups, and symmetric groups. The adjacency of the vertices of the Cayley graphs are computed by using the definition of Cayley graph. Groups, Algorithms and Programming (GAP) software is used to assist in some computations that involve large groups in which the manual computations is almost impossible. By using the software, the connectivities of the vertices of the Cayley graphs associated to some finite groups are computed using the for-loop function provided. The procedure includes the generation of the vertices of the Cayley graph which consists of the elements of the related groups. Since the Cayley graph considered are with respect to a certain subset, then the Cayley graphs are constructed according to certain cases of subset of order starting from order one, followed by subset of order two.

The second part of this thesis is the computations of the spectrum of the Cayley graphs followed by the computations of the energy and Seidel energy of the Cayley graphs. By using the definition of the energy of graph, which is to sum all the positive values of the eigenvalues of the graph, the first step to calculate the energy is to build the adjacency matrix for each Cayley graphs and find their eigenvalues respectively. Maple software is then used to assist in the formation of large adjacency matrices especially for the groups of higher order. The pattern of the adjacency matrices are observed and the general form of the spectrum are determined. Finally, the energy of the Cayley graphs are computed by applying the definition and the general form is found. The procedure for the computations of Seidel energy is similar to the ordinary energy except that the eigenvalues for the Seidel energy are obtained from the Seidel matrix of the Cayley graphs. Figure 1.1 illustrates the research methodology for this research.

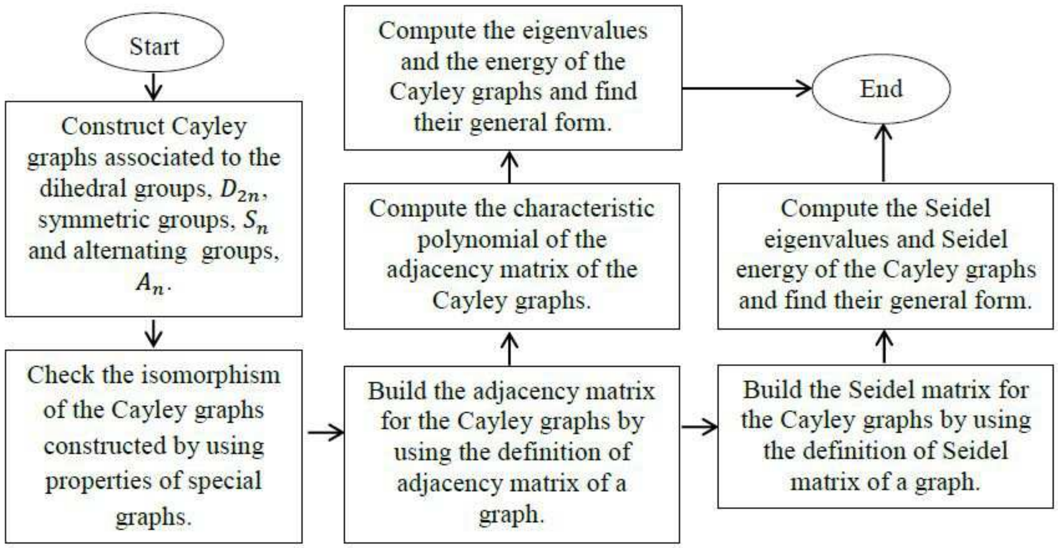

Figure 1.1 Research methodology flowchart

1.8 Thesis Organization

This thesis is organized into six chapters. First, Chapter 1 gives a brief overview and introduction to the thesis. The statement of the problem is stated and the research questions are pointed out. The objectives, the scope, the significance and the methodology of the study are also specified in this chapter.

In the next chapter which is Chapter 2, firstly some basic concepts and properties from group theory and graph theory are introduced followed by some knowledge from linear algebra. Some properties, definitions and theorems found by other researchers are also included and explained. The chapter is followed by the elaborations of previous works done by other researchers which relate to the scope of the research.

Next, Chapter 3 presents the constructions of the Cayley graphs associated to the dihedral groups, D_{2n}, the alternating groups, A_n, and the symmetric groups, S_n. The Cayley graphs presented are with respect to a subset of the groups where the subsets are of order one and two. The general form of the Cayley graphs associated to the groups are presented in the form of theorems followed by some examples to illustrate the results.

In Chapter 4, the energy of the Cayley graphs associated to D_{2n}, A_n, and S_n with respect to subsets of order one and two are presented. The computations of the energy of the Cayley graphs are conducted by summing up the positive values of the eigenvalues of the graphs which were obtained from their adjacency matrices. The results are then presented in the form of lemmas and theorems.

In Chapter 5, another type of energy of the Cayley graphs is presented, namely the Seidel energy. The computations of the Seidel energy of the Cayley graphs are conducted by summing up the positive values of the Seidel eigenvalues of the graphs which are obtained by first determining the Seidel matrices. The results are also presented in the form of lemmas and theorems.

Lastly, Chapter 6 provides the summary and conclusion of the overall findings in this thesis. This chapter also encloses the suggestions for future research on the energy of graphs associated to groups. Figure 1.2 illustrates the content of the whole thesis.

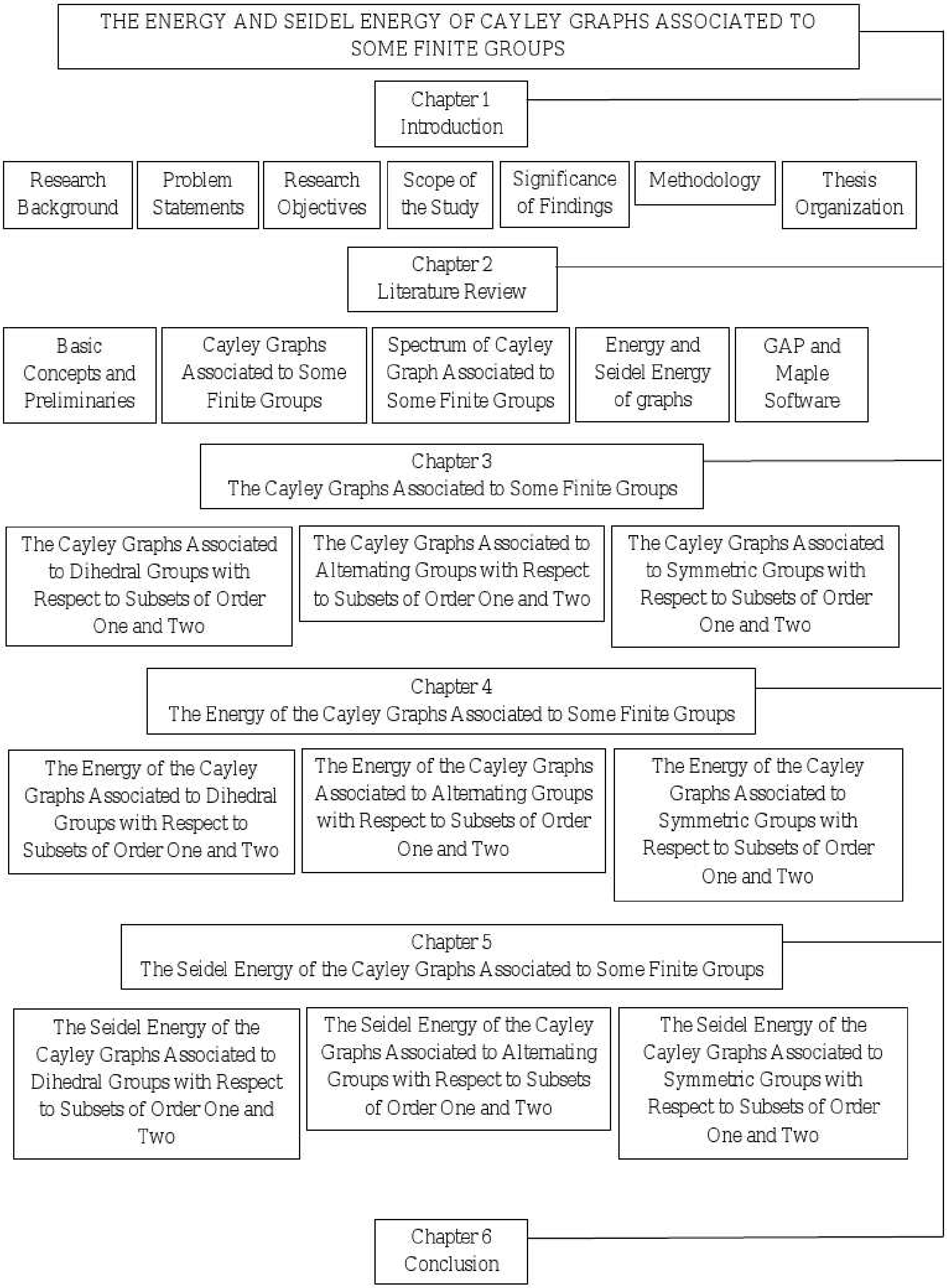

Figure 1.2 Thesis organization chart

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