ENERGY AND LAPLACIAN ENERGY OF GRAPHS RELATED TO A FAMILY OF FINITE GROUPS

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To my beloved family

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ABSTRACT

The energy of a graph is the sum of the absolute value of the eigenvalues of the adjacency matrix of the graph. This quantity is studied in the context of spectral graph theory. The energy of graph was first defined by Gutman in 1978. However, the motivation for the study of the energy comes from chemistry, dating back to the work by Hukel in the 1930s, where it is used to approximate the total π-electron energy of molecules. Recently, the energy of the graph has become an area of interest to many mathematicians and several variations have been introduced. In this research, new theoretical results on the energy and the Laplacian energy of some graphs associated to three types of finite groups, which are dihedral groups, generalized quaternion groups and quasidihedral groups are presented. The main aim of this research is to find the energy and Laplacian energy of these graphs by using the eigenvalues and the Laplacian eigenvalues of the graphs respectively. The results in this research revealed more properties and classifications of dihedral groups, generalized quaternion groups and quasidihedral groups in terms of conjugacy classes of the elements of the groups. The general formulas for the energy and Laplacian energy of the conjugacy class graph of dihedral groups, generalized quaternion groups and quasidihedral groups are introduced by using the properties of conjugacy classes of finite groups and the concepts of a complete graph. Moreover, the general formula for the energy of the non-commuting graph of these three types of groups are introduced by using some group theory concepts and the properties of the complete multipartite graph. Furthermore, the formulas for the Laplacian spectrum of the non-commuting graph of dihedral groups, generalized quaternion groups and quasidihedral groups are also introduced, where the proof of the formulas comes from the concepts of an AC-group and the complement of the graph. Graphs associated to the relative commutativity degree of subgroups of some dihedral groups are found as the complete multipartite graphs. Some formulas for the characteristic polynomials of the adjacency matrices of the graph associated to the relative commutativity degree of subgroups of some dihedral groups and its generalization for some cases depending on the divisors are presented. Finally, the energy and the Laplacian energy of these graphs for some dihedral groups are computed.

ABSTRAK

Tenaga bagi suatu graf adalah hasil tambah bagi nilai mutlak nilai eigen bagi matriks bersebelahan graf tersebut. Kuantiti ini dipelajari dalam konteks teori graf spektrum. Tenaga bagi graf pertama kali ditakrifkan oleh Gutman pada tahun 1978. Walau bagaimanapun, motivasi untuk kajian tentang tenaga ini berasal daripada kimia, bermula dengan kerja oleh Hukel pada tahun 1930-an, di mana ia digunakan untuk menganggarkan jumlah tenaga elektron-π bagi molekul. Baru-baru ini, tenaga bagi graf telah menjadi bidang yang menarik bagi banyak ahli matematik dan beberapa variasi telah diperkenalkan. Dalam kajian ini, hasil teori baharu bagi tenaga, dan tenaga Laplacian beberapa graf yang dikaitkan dengan tiga jenis kumpulan terhingga, iaitu kumpulan dihedral, kumpulan kuaternion teritlak dan kumpulan kuasidihedral telah ditunjukkan. Tujuan utama penyelidikan ini adalah untuk mencari tenaga dan tenaga Laplacian graf-graf tersebut masing-masing dengan menggunakan nilai eigen dan nilai eigen Laplacian bagi setiap graf. Hasil kajian ini memperlihatkan lagi sifat-sifat dan klasifikasi kumpulan dihedral, kumpulan kuaternion teritlak dan kumpulan kuasidihedral dari segi kelas kekonjugatan unsur kumpulan tersebut. Rumus umum untuk tenaga dan tenaga Laplacian bagi graf kelas kekonjugatan kumpulan dihedral, kumpulan kuaternion teritlak dan kumpulan kuasidihedral diperkenalkan dengan menggunakan sifat kelas kekonjugatan kumpulan terhingga dan konsep graf lengkap. Selain itu, rumus umum bagi tenaga untuk graf tak berulang dari ketiga-tiga jenis kumpulan ini diperkenalkan dengan menggunakan beberapa konsep teori kumpulan dan sifat-sifat graf multipartit. Tambahan pula, rumus bagi spektrum Laplacian bagi graf tak berulang, kumpulan dihedral, kumpulan kuaternion teritlak dan kumpulan kuasidihedral juga diperkenalkan, di mana bukti bagi rumus ini berasal daripada konsep AC-group dan pelengkap graf. Graf yang dikaitkan dengan darjah kekalisan tukar tertib relatif subkumpulan bagi sesetengah kumpulan dihedral dijumpai sebagai graf multipartit yang lengkap. Beberapa rumus bagi polinomial ciri matriks bersebelahan graf yang berkaitan dengan darjah kekalisan tukar tertib relatif subkumpulan sesetengah kumpulan dihedral dan pengitlakan untuk beberapa kes yang bergantung kepada pembahagi dibentangkan. Akhirnya, tenaga dan tenaga Laplacian bagi graf tersebut untuk beberapa kumpulan dihedral dikira.

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LIST OF SYMBOLS

$A(\Gamma)$	-	Adjacency matrix of Γ
$Z(G)$	-	Center of a group G
$C_G(x)$	-	Centralizer of x in G
Γ_G^{com}	-	Commuting graph of G
K_n	-	Complete graph
$K_{n_1,n_2,\ldots,n_p}$	-	Complete multipartite graph
$\bar{\Gamma}$	-	Complement of a graph
$d(G)$	-	Commutativity degree of a group G
$cl(a)$	-	Conjugacy class of element a
Γ_G^{cl}	-	Conjugacy class graph of G
D_{2n}	-	Dihedral group of order $2n$
$E(\Gamma)$	-	Edge-set of Γ
λ_n	-	Eigenvalue
$\varepsilon(\Gamma)$	-	Energy of Γ
Q_{4n}	-	Generalized quaternion group
$\Gamma_{H,G}$	-	Graph associated to the relative commutativity degree of subgroup H of finite group G
$\langle x \rangle$	-	Group generated by the element x
$L(\Gamma)$	-	Laplacian matrix of Γ
$LE(\Gamma)$	-	Laplacian energy of Γ
$\tau(n)$	-	Number of the divisors of n
QD_{2^n}	-	Quasidihedral group of order 2^n
$d(H,G)$	-	Relative commutativity degree of H in G
$\mathfrak{D}(G)$	-	Set of the relative commutativity degree of H in G
$V(\Gamma)$	-	Vertex-set of Γ

CHAPTER 1

INTRODUCTION

1.1 Introduction

In graph theory, the energy of a graph is the sum of the absolute values of the eigenvalues of the adjacency matrix of the graph. This quantity is studied in the context of spectral graph theory. The energy of graph was first defined by Gutman in 1978 [1]. However, the motivation for the study of the energy comes from chemistry, where the research can be traced back to the 1930s. It is used to approximate the total π-electron energy of molecules [2]. On the other hand, the Laplacian energy of the graph was first defined by Gutman and Zhou in 2006 [3], which states that the Laplacian energy of a graph is the sum of the absolute deviations (i.e. distance from the mean) of the eigenvalues of its Laplacian matrix.

This research focuses on some graphs such as that associated to three types of groups,which are dihedral groups, generalized quaternion groups and quasidihedral groups, and the main aim of the study is to find the general formulas for the energy and the Laplacian energy of these graphs. As preliminary results for further studies, the adjacency matrices, the Laplacian matrices, spectrum and Laplacian spectrum of the graphs are given. Then, the energy and Laplacian energy of these graphs are computed and the general formulas for them are found.

According to Abdollahi [4], the non-commuting graph related to finite groups has been first considered by Erdos, with vertices are non-central elements of a group and two vertices are adjacent if they do not commute. In 1990, Bertram *et al.* [5] introduced a new graph which was related to conjugacy classes of finite groups. The vertices of this graph are non-central conjugacy classes in which two vertices are adjacent if their cardinalities are not co-prime. Many researches have been done using algebraic graph theory. In 2012, Erfanian and Tolue [6] introduced a new graph, called conjugate graph, in which the vertices are non-central elements of the group. Two vertices of this graph are adjacent if they are conjugate.

1.2 Research Background

The theory of groups of finite order is said to date back from the time of Cauchy as he has credited for the first attempt at classifications with a view to forming a theory from a number of isolated facts [7]. In mathematics, a group is an algebraic structure consisting of a set of elements equipped with an operation that combines any two elements to form a third element and that satisfies four conditions called the group axioms. A finite group is a group having a finite order. Dihedral groups, generalized quaternion groups and quasidihedral groups are examples of finite groups. In 2013 Barzgar *et al.* [8] have shown that a finite group G admits three relative commutativity degrees if and only if $G - Z(G)$ is a non-cyclic group of order pq, where p and q are primes and they also determined all the relative commutativity degrees of some known groups. Group theory has many important applications in physics, chemistry, material science and graph theory. There are many researches in constructing a graph by a group, for instance, the non-commuting graph Γ_G^{ncom} was first considered by Paul Erdos when he posted that a group whose non-commuting graph has no infinite complete subgraph and determine whether it is true that there is a finite bound on the cardinalites of complete subgraphs in 1975 [9]. In 2006 Abdollahi *et al.* [4] explored how the graph theoretical properties of the non-commuting graph can effect on the group theoretical properties of a group and they conjectured that if two non-abelian finite groups are such that their non-commuting graphs are isomorphic to one another, then the groups have the same order. In 2012 Erfanian and Tolue [6] introduced the conjugate graph Γ_G^c associated to a non-abelian group and showed that the conjugate graph of a finite group is isomorphic to non-abelian finite simple group. In addition, Tolue and Erfanian 2013 in [10] also generalized the non-commuting graph Γ_G^{ncom} to relative non-commuting graph $\Gamma_{H,G}^{ncom}$ for all non-abelian group G and subgroup H of G and they gave some results about $\Gamma_{H,G}^{ncom}$. They have also proved that if (H_1, G_1) and (H_2, G_2) are relative isoclinic then $\Gamma_{H_1,G_1}^{ncom} \cong \Gamma_{H_2,G_2}^{ncom}$ under special conditions.

Moreover, the energy of a graph Γ, often denoted by $\varepsilon(\Gamma)$, is defined to be the sum of the absolute value of the eigenvalues of its adjacency matrix. This graph invariant is very closely connected to a chemical quantity known as total π-electron energy of conjugated hydrocarbon molecules. Recently, the energy of a graph has become a quantity of interest to mathematicians, where several variations have been introduced. The energy of a graph was first defined by Gutman in 1978 [1]. However, the motivation for his definition appeared much earlier in the 1930s, when Erich Huckel proposed the famous Huckel Molecular Orbital Theory. Huckel method allows chemists to approximate energies associated with π-electron orbitals in a special class of molecules called conjugated hydrocarbons [11].

In [1], Gutman introduced his definition of the energy of a general simple graph. In the past decade, interest in the energy of a graph has increased and many different versions have been conceived. In 2006, Gutman and Zhou [3] defined the Laplacian energy of a graph as the sum of the absolute deviations (i.e. distance from the mean) of the eigenvalues of its Laplacian matrix. Similar variants of graph energy were devolved for the signless Laplacian [12], the distance matrix [13] and the incidence matrix [14]. In 2010, Cavers *et al.* [15] first studied the normalized Laplacian energy of a graph and the Laplacian spectrum has been studied by many researchers in [16–22]. The contribution on the energy of graphs associated to finite groups are not available in the existing literature.

In this research, the energy and Laplacian energy of the conjugacy class graphs, non-commuting graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups are computed. Furthermore, the graphs associated to the relative commutativity degree of some dihedral groups are found and the characteristic polynomials of the adjacency matrices of these graphs are determined and used to find the energy of the graphs associated to the relative commutativity degrees of some dihedral groups.

1.3 Problem Statements

Many researches have been carried out on graphs related to finite groups and likewise graphs related to finite groups are introduced. These include the conjugacy class graph, conjugate graph, commuting graph and non-commuting graph. Some research discussed on certain properties of the commuting graph of dihedral groups and they obtained the chromatic number and clique number of these commuting graphs [23]. Also, many researches have been carried out on the energy of the graph not associated with groups with its adjacency matrix and eigenvalues [1, 8, 12, 19]. In addition, a research on Laplacian energy related to Laplacian matrix and its eigenvalues had been done [3]. Some work gave the bound to the energy of k-regular graph on n vertices. There are works on energy and some Hamiltonian properties of graphs, which presented sufficient conditions for some Hamiltonian properties of graphs. Furthermore, there had been previous work on maximum degree energy of graph, and from a study on the concept of maximum degree matrix of a simple graph, a bound for eigenvalues of this matrix had been obtained. Also the maximum degree energy of the graph and a bound for the energy had been obtained while other research had shown that if the maximum degree of the energy of a graph is rational, then it must be an even integer. However, this shows the need of a link between the energy of graphs and graphs associated to finite groups. Thus, this gives a motivation to this research. Hence, in this research, the following questions are addressed and answered.

1. What is the energy of the graphs related to finite groups?
2. What are the conjugacy class graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups? How can the graphs be constructed to develop the general formulas for their energy and Laplacian energy?
3. What are the relation between the energy and the Laplacian energy of the conjugacy class graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups?
4. What are the non-commuting graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups and how can they be constructed from their complement graphs?
5. How can the general formulas of the energy and the Laplacian eigenvalues of the graphs in 4 be formulated?
6. What are the graphs associated to the relative commutativity degree of subgroups of some dihedral groups? How can these graphs be constructed to develop formulas of their energy and Laplacian energy?

Table 1.1 gives a summary of the previous study on the energy of graph and graphs associated to finite group which include the approach, finding and limitation.

Table 1.1: Previous study on the energy of a graph and graphs associated to finite groups

Author	**Approach**	**Finding**	**Limitation**
Gutman 1978	Adjacency matrix and eigenvalues of a graph.	Define the energy of a graph	Simple graphs
Bapat and Pati in 2004	Concept of the additive compound.	Proved that energy of a graph is never an odd integer.	Simple undirected graphs of order *n*.
Gutman and Zhou in 2006	Laplacian and Laplacian eigenvalues of a graph.	Laplacian energy of a graph.	Simple graphs.
Pirzad and Gutman in 2008	Product of two specified graphs and their eigenvalues properties.	Proved that energy of graph is never square root of an odd integer.	Simple finite graphs.
Covers *et al*. in 2010	Concept of the general randic index of a graph.	Provided upper and lower bounds for normalized Laplacian energy.	Simple graphs.
Kinkear *et al*. in 2017	Adjacency matrix and eigenvalues of a graph are extended.	Energy of extended adjacency matrix of a graph.	Connected graphs of order *n*.
Bertram et al. in 1990	Concepts of the conjugacy classes of a finite group.	introduced Conjugacy class graph related to finite group.	Non-abelian finite groups, non-central conjugacy classes of a group.
Abdollahi in 2006	Definition of the non-commuting graph and its properties.	Some studies in non-commuting graph which is considered by Erdos in 1975.	Non-abelian finite groups, non-commuting elements of a group.
Erfanian and Tolue in 2012	Properties of the conjugates elements in a group.	Define the conjugate graph related to finite group.	Non-abelian finite groups, conjugate elements in a finite group.
Tolue and Erfanian in 1012	Concepts and properties of the non-commuting graph and the relative commutativity degree of subgroup of finite group.	Non-commuting graph generalized to the relative non-commuting graph of finite group.	Relative commutativity degree of subgroups of a finite non-abelian group.
Erfanian and Tolue in 2013	Concepts of the relative commutativity degree of subgroup of finite group.	Define the relative *n*-th non-commuting graph.	Relative commutativity degree of subgroups of a finite non-abelian group

1.4 Objectives of the Research

The main objectives of this research are:

1. To formulate the general formulas for the energy of the conjugacy class graphs and the non-commuting graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups.
2. To develop formulas for the Laplacian energy of the conjugacy class graphs and the Laplacian spectrum of non-commuting graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups.
3. To develop the graphs associated to the relative commutativity degrees of some dihedral groups and determined the characteristic polynomials of the adjacency matrices of these graphs.
4. To construct the formulas of the energy and the Laplacian energy of the graphs associated to the relative commutativity degrees of some dihedral groups.

1.5 Scope of the Research

This research focuses on some graphs related to finite groups, in particular finite non-abelian groups, which are dihedral groups, generalized quaternion groups and quasidihedral groups. These groups have the same properties but different structures and by using the size of the conjugacy classes of these groups, the conjugacy class graphs with less isolated vertices can be obtained, which is necessary to compute the energy of the graph. Moreover the non-commuting graph is the complement of the commuting graph and the commuting graphs related to these groups are the union of complete graphs. Hence, their complements are complete multipartite graphs with no isolated vertices. Similarly, the graphs associated to subgroups of dihedral groups are complete multipartite graphs. In this research, the energy and the Laplacian energy of some graphs associated to the mentioned finite groups are the main objectives. The conjugacy class graphs, the non-commuting graphs associated to the dihedral groups, generalized quaternion groups, and quasidihedral groups are used to find their energy and Laplacian energy. This research has provided new theoretical results on the energy and Laplacian energy of some graphs that can be used in chemistry to find the energy of a molecular structure theoretically.

1.6 Significance of the Research

The major contribution of this research is to provide new theoretical results on the energy and Laplacian energy of some graphs associated to dihedral groups generalized quaternion groups and quasidihedral groups and the formulas for the energy and the Laplacian energy of these graphs has been successfully generalized. In chemistry, in case of graphs representing conjugated molecules, the energy of the graph $\varepsilon(\Gamma)$ is closely related to their total π-electron energy E_π, as calculated within Huckel molecular orbital approximation. In most case $E_\pi = \varepsilon(\Gamma)$ which can be used to calculate the energy of molecular structures in a much simpler way. The results in this research revealed more properties and classifications of groups in the scope of the research in terms of conjugacy classes of the elements of the groups.

1.7 Research Methodology

This research begins by studying the fundamental concepts of the adjacency matrices and the eigenvalues of the conjugacy class graphs and non-commuting graphs related to the dihedral groups, generalized quaternion groups and quasidihedral groups. Firstly, the conjugacy class graphs of dihedral groups, generalized quaternion groups and quasidihedral groups are obtained as the complete graphs or union of complete graphs depending on parity of n, by using the definition of the conjugacy class and the conjugacy class graph of a finite group. Next, by using the definition of the energy of the graph and the properties of the eigenvalues of the complete graph, the energy of conjugacy class graphs of dihedral groups, generalized quaternion groups and quasidihedral groups are found. By using the characteristic polynomial formula of a complete multipartite graph $K_{n_1,n_2,\ldots,n_p}$ and the concepts of the complement of a graph, the eigenvalues and the energy of the non-commuting graph of dihedral groups, generalized quaternion groups and quasidihedral groups are obtained.

There are different versions of the energy of the graph that have been conceived, one is Laplacian energy related to the Laplacian matrix of the graph which is also considered in this research. In the first step of this part, the Laplacian matrices of the conjugacy class graphs of the dihedral groups, generalized quaternion groups and quasidihedral groups and the properties of the eigenvalues of the complete graph K_n are studied. Then, the Laplacian energy of the conjugacy class graphs of dihedral groups, generalized quaternion groups and quasidihedral groups are found. Furthermore, some concepts of an AC-group, the commuting graph and the eigenvalues of the complement of the graph are studied. Based on these studies the general formulas for the Laplacian eigenvalues of the non-commuting graphs of the dihedral groups, generalized quaternion groups and quasidihedral groups are found.

The concepts of the relative commutativity degree of subgroups of some dihedral groups are studied. Then, graphs associated to the relative commutativity degree of subgroups of dihedral groups are found by using these concepts with properties of the number of the divisors of n and the sum of these divisors. These results are used to find the energy and the Laplacian energy of the graphs associated to the relative commutativity degree of subgroups of dihedral groups D_{2n}, when n is an odd prime integer. Maple software is used for complex computations, such as the Cayley table for the groups, the characteristics polynomials and the eigenvalues of the adjacency matrices of the graphs and also in visualizing graphs.

Figure 1.1 illustrates the research methodology of this thesis.

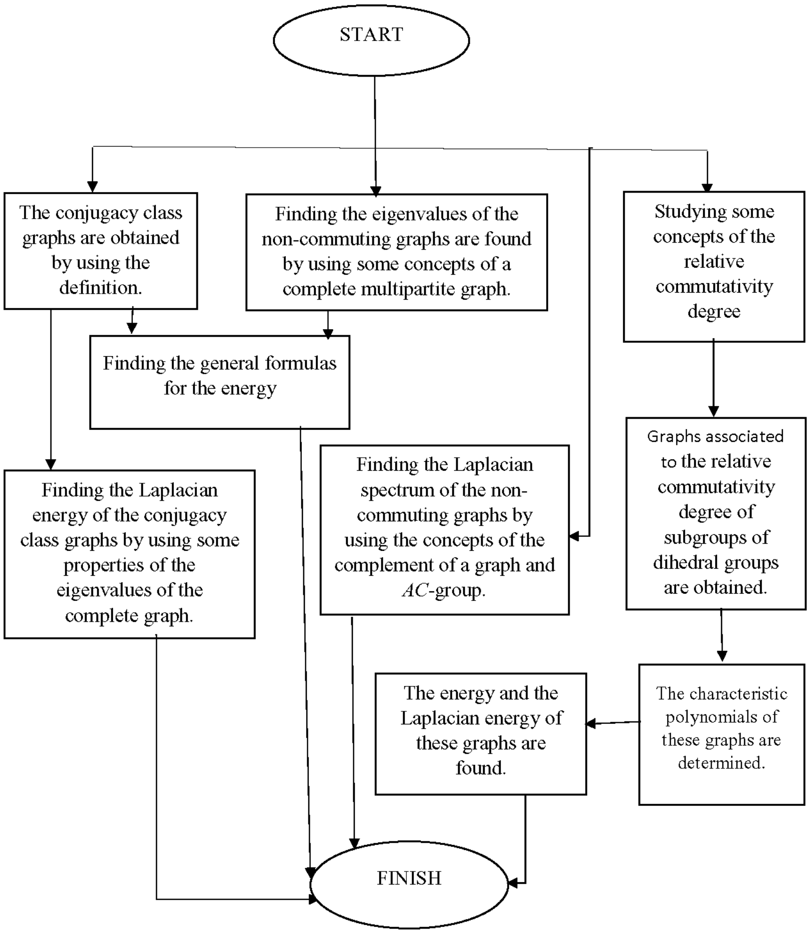

Figure 1.1: Research methodology

1.8 Thesis Organization

This research seeks to understand the structure of the energy, the Laplacian energy, the spectrum and the Laplacian spectrum of some graphs related to some finite groups. This thesis is organized as follows:

Chapter 1 provides the introduction to the whole thesis, including research background, problem statement, research objectives, scope, significance of findings, research methodology and thesis organization.

Chapter 2 deals with the preliminary results of this research. Some basic definitions and concepts on group theory and graph theory related to this research are presented. Various works and results by different researchers concerning some graphs related to finite groups, the energy of a graph and the Laplacian energy of a graph are also included.

In Chapter 3, the conjugacy class graphs of dihedral groups, generalized quaternion groups and quasidihedral groups are considered and the general formulas for the energy of these graphs are presented. Furthermore, the eigenvalues of the adjacency matrices of the non-commuting graph of dihedral groups, generalized quaternion groups and quasidihedral groups are presented and the general formulas for the energy of these graphs are found.

Chapter 4 presents the Laplacian energy of some graphs associated to some finite groups.The number of edges and vertices of the conjugacy class graphs of the Dihedral groups, generalized quaternion groups and quasidihedral groups are determined, and the eigenvalues of the adjacency matrices of these graphs are considered. These results are used to introduce the general formulas for the Laplacian energy of the conjugacy class graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups. Moreover, the Laplacian spectrum of the non-commuting graphs related to dihedral groups, generalized quaternion groups and quasidihedral groups are found.

In Chapter 5, the graphs associated to the relative commutativity degree of subgroups of some dihedral groups are found as the complete multipartite graphs. Then, the characteristic polynomials of the adjacency matrices of these graphs are determined. Furthermore, the energy and the Laplacian energy of this graph related to dihedral groups are computed for some cases depending on the divisors of n.

Finally, the summary and conclusion of the whole thesis are given in Chapter 6. Possible directions for further research are proposed.

The thesis organization is illustrated in Figure 1.2.

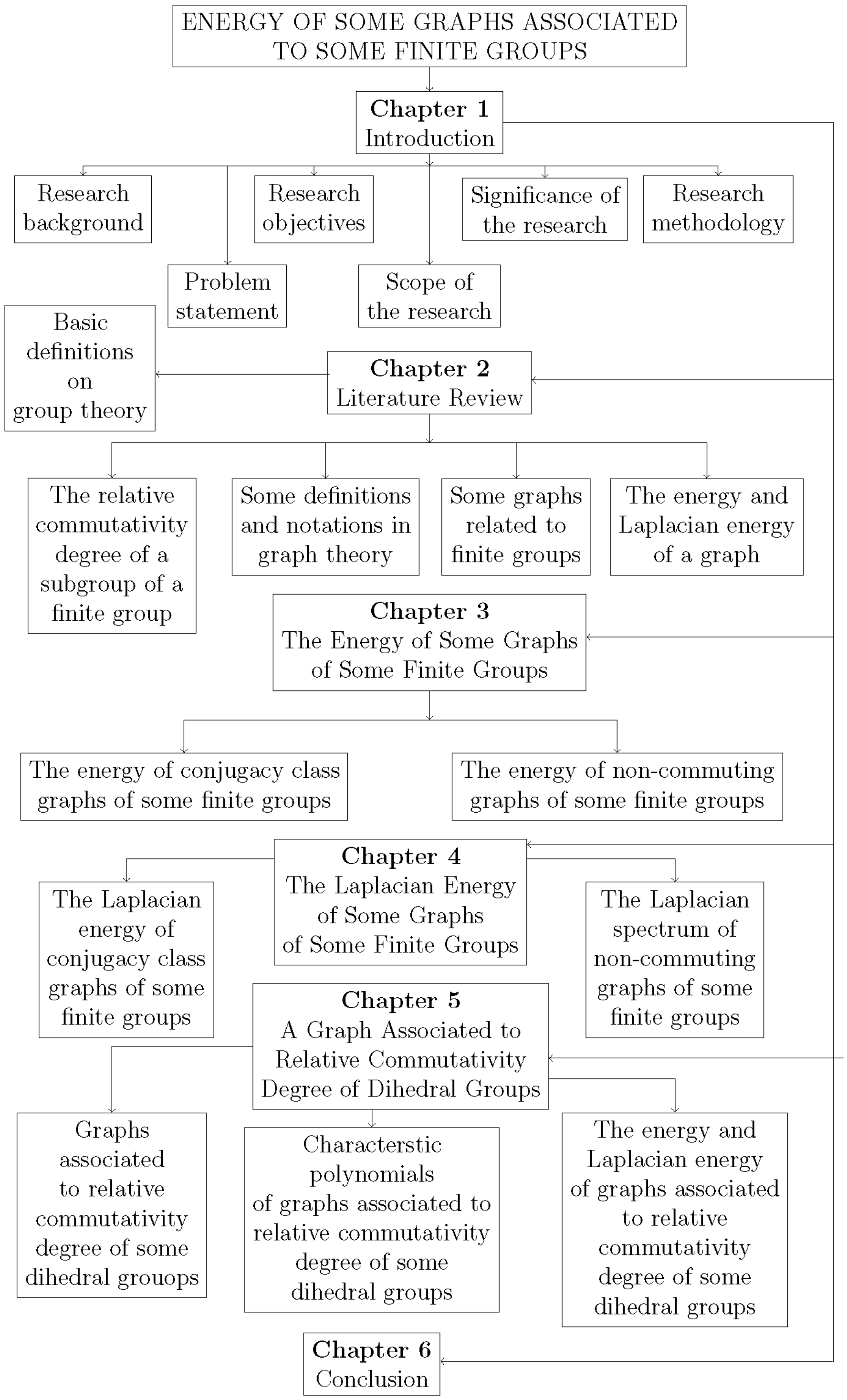

Figure 1.2: Thesis organization

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