Chapter 1

Introduction

1.1 General:

The application of quantum theory to condensed matter physics has revolutionised our understanding of materials and played a pivotal role in the information revolution during the last few decades (O’Reilly, 2005). At the most basic level, quantum theory enables us to understand why some solids are metals, some are insulators and some are semiconductors. It also allows us to understand the trends in the properties of different materials and to engineer materials to the properties we desire. The exact features of the electronic band structure of semiconductor materials, for instance, play a key role in determining their electronic and optoelectronic properties, and their usefulness for devices such as lasers, detectors and electronic integrated circuits. Details of the exchange interaction between electrons on neighbouring atoms determine the differences between ferromagnets, antiferromagnets, ferrimagnets and their applicability for data storage or transformer applications. The understanding and development of the functional solids which form the basis of modern technology has been achieved through a synergy between physicists, material scientists and engineers.

From the very onset, the interplay between quantum theory and experiments has revealed the importance of condensed matter physics. With the development of more powerful experimental techniques, such significance is attracting a wider scientific community. In the last few decades being fuelled by
the rapid development of sophisticated mathematical techniques, condensed matter physics has received considerable attention. On the other hand, theoretical approaches are also pushed towards their intrinsic limit, in order to provide reliable answers to the hitherto unresolved questions in complex situations. In recent years, a formulation of quantum mechanics in terms of algebraic structures has emerged as a viable alternative to the solution of Schrödinger like equations. Mathematicians are generally more interested in the abstract theory of groups, but the representation theory of groups of direct use in a large variety of physical problems is more useful to physicists. To keep up with the vast production of experimental observations, theoretical physics is constantly being tested to provide a collection of satisfactory models that can account for the observations. However, it should be clear that condensed matter physics is undergoing a radical change not simply as a result of technical advancements, one should also realize that as a consequence of new (and quite often unexpected) experimental results, an unprecedented effort toward constructing alternative theoretical models/methods and formulating novel ideas has taken place in recent years. Group theory is an elegant mathematical way of describing situations ranging from sub-nuclear to solid-state physics. In general, though numerous theoretical and experimental advances were made in condensed matter physics, still many fundamental questions remain unanswered. Symmetry is an extremely important concept in the development of scientific knowledge. The use of symmetry in physics, chemistry and related areas is widely recognized from both purely theoretical and computational view points. Group theory is the natural tool for dealing with symmetry arguments.

However, an algebraic formulation of energy band problem would be a powerful addition to the field of theoretical condensed matter physics as in the case of vibrational spectroscopy. A comprehensive theoretical treatment for most aspects of energy band determination of condensed matter physics necessarily has to rely on a Hamiltonian formulation. As a matter of fact, the typical theoretical procedure used to study a given problem consists of solving the Schrödinger equation for a periodic potential. If the situation is larger than a diatomic molecule,
the potential energy surface is a very complex function, composed of a
discouragingly large number of coordinates. A standard approach to this problem
involves approximating the potential energy surface by convenient analytical
functions. A widely used procedure of this type is the force field method, in which
one considers small displacements of coordinates from their equilibrium values,
thus obtaining a harmonic limit for the potential surface. This kind of approach, of
course, encounters difficulties as soon as one considers highly excited levels, and
once more, a large number of parameters are needed to achieve meaningful results.
Therefore new theoretical methods are required to introduce and apply.

In this Chapter, a brief account of the energy band and energy band
structure of solids are discussed. In addition, the definition of Groups, Lie groups,
Review of literature, Role of algebraic methods, representations of Lie groups, Lie
algebras, Casimir operator and the properties of Lie algebras are discussed.

1.2 Electronic Band Structure:

In condensed matter physics, the electronic band structure (or simply band
structure) of a solid describes ranges of energy that an electron is "forbidden" or
"allowed" to have. It is due to the diffraction of the quantum mechanical electron
waves in the periodic crystal lattice. The band structure of a material determines
several characteristics, in particular its electronic and optical properties.

As per the Bohr’s theory, the electrons cannot occupy arbitrary positions in
the atomic space surrounding the nucleus but only exist in predefined discrete
levels. Now consider what happens when two or more atoms come closer and each
has their discrete energy levels. Since the electromagnetic forces will come into
play as the distance between the atoms decreases, the energy levels will get
affected by this mutual interaction. As the inter atomic distance goes on
decreasing, the influence of these forces increases and the net result is that instead
of discrete energy levels, we now have a narrow range of energy band
corresponding to each energy level and these bands are known as energy bands (Ashcroft and Mermin, 1975; Dekker, 1957; Elliot and Gibson, 1974).

The electrons of a single free-standing atom occupy atomic orbitals forming a discrete set of energy levels. If several atoms are brought together into a molecule, their atomic orbitals split, as in a coupled oscillation. This produces a number of molecular orbitals proportional to the number of atoms. When a large number of atoms (of order $10^{20}$ or more) are brought together to form a solid, the number of orbitals becomes exceedingly large, and the difference in energy between them becomes very small, so the levels may be considered to form continuous bands of energy rather than the discrete energy levels of the atoms in isolation. However, some intervals of energy contain no orbitals, no matter how many atoms are aggregated, forming band gaps. Within an energy band, energy levels are so numerous as to be a near continuum. First, the separation between energy levels in a solid is comparable with the energy that electrons constantly exchange with phonons (atomic vibrations). Second, it is comparable with the energy uncertainty due to the Heisenberg uncertainty principle, for reasonably long intervals of time. As a result, the separation between energy levels is of no consequence.

Any solid has a large number of bands. Theoretically, it can be said to have infinitely many bands just as an atom has infinitely many energy levels. However, all but a few lie at energies so high that any electron that reaches those energies escapes from the solid. These bands are usually disregarded. Bands have different widths based upon the properties of the atomic orbitals from which they arise. Also, allowed bands may overlap, producing (for practical purposes) a single large band.

A useful way to visualize the difference between conductors, insulators and semiconductors is to plot the available energies for electrons in the materials. Instead of having discrete energies as in the case of free atoms, the available energy states form bands. Crucial to the conduction process is whether or not these
electrons are separated by a large gap from the conduction band, and in semiconductors there is a small gap between the valence band and conduction band so that thermal or other excitations can bridge the gap. With such a small gap, the presence of a small percentage of a doping material can increase conductivity dramatically.

Figure 1.1 shows a simplified picture of the bands in a solid that allows the three major types of materials to be identified: metals, semiconductors and insulators.

Figure 1.1: Simplified diagram of the electronic band structure of metals, semiconductors and insulators.

It is the width of these bands and their proximity to existing electrons that determines how mobile those electrons will be when exposed to an electric field. In metallic substances, empty bands overlap with bands containing electrons, meaning that electrons may move to what would normally be (in the case of a single atom) a higher-level state with little or no additional energy imparted. Thus,
the outer electrons are said to be "free," and ready to move at the beckoning of an electric field.

Band overlap will not occur in all substances, no matter how many atoms are in close proximity to each other. In some substances, a substantial gap remains between the highest band containing electrons (called valence band) and the next band, which is empty (called conduction band). As a result, valence electrons are "bound" to their constituent atoms and cannot become mobile within the substance without a significant amount of imparted energy. These substances are electrical insulators.

Materials that fall within the category of semiconductors have a narrow gap between the valence and conduction bands. Thus, the amount of energy required to motivate a valence electron into the conduction band where it becomes mobile is quite modest. At low temperatures, there is little thermal energy available to push valence electrons across this gap, and the semiconducting material acts as an insulator. At higher temperatures, though, the ambient thermal energy becomes sufficient to force electrons across the gap, and the material will conduct electricity.

Although electronic band structures are usually associated with crystalline materials; quasi-crystalline and amorphous solids may also exhibit band structures. However, the periodic nature and symmetrical properties of crystalline materials makes it much easier to examine the band structures of these materials theoretically. In addition, the well-defined symmetry axes of crystalline materials make it possible to determine the dispersion relationship between the momentum and energy of a material. As a result, virtually all of the existing theoretical work on the electronic band structure of solids has focussed on crystalline materials.

Although the number of states in all of the bands is effectively infinite, in an uncharged material the number of electrons is equal only to the number of protons in the atoms of the material. Therefore all of the states are not occupied by
electrons ("filled") at any time. The likelihood of any particular state being filled at any temperature is given by Fermi-Dirac statistics (Reif, 1965; Kittel, 1971). The probability is given by the following expression

\[
f(E) = \frac{1}{1 + e^{\frac{E-\mu}{k_B T}}}
\]

\(k_B\) is Boltzmann's constant, \(T\) is the temperature, \(\mu\) is the chemical potential (in semiconductor physics, this quantity is more often called the "Fermi level" and denoted \(E_F\)). The Fermi level naturally is the level at which the electrons and protons are balanced.

At \(T = 0\), the distribution is a simple step function (Kittel, 1971):

\[
f(E) = \begin{cases} 
1 & \text{if } 0 < E \leq E_F \\
0 & \text{if } E_F < E
\end{cases}
\]

At nonzero temperatures, the step "smooths out", so that an appreciable number of states below the Fermi level are empty and some states above the Fermi level are filled.

### 1.3 Concept of a Group:

The concept of groups had its origin more than 150 years ago. The development of the theory of groups was mainly due to the famous mathematicians like Gauss, Cauchy, Abel, Hamilton, Cayley. After the advent of modern quantum mechanics in 1925, it did not find much use in physics for time being. The applications of group theory in physics were soon recognized and the new tool was put to use in the calculation of atomic structures and spectra by H. A. Bethe, E. P. Wigner and others. Group theory has now become indispensable in most branches of physics and chemical physics (Cornwell, 1997; Kim, 2004; Joshi, 2005). It may be pointed out here that although a mathematician is
interested in the formal development of abstract group theory, a physicist finds its use in quantum physics and other branches of physics.

Let us consider a set $G$ of elements $G_1, G_2, G_3, \ldots$ is said to form a group if a law of multiplication of the elements satisfies the following conditions (Elliot and Dawber, 1979).

1. The product $G_a G_b$ of any two elements is itself an element in the set, i.e.

$$G_a G_b = G_d \text{ for some } G_d \text{ in } G \tag{1.01}$$

2. In multiplying three elements $G_a, G_b$ and $G_c$ together, it does not matter which product is made first. In other words,

$$G_a (G_b G_c) = (G_a G_b) G_c \tag{1.02}$$

where the products inside the bracket is carried out first.

3. One element of the set denoted by $E$ and is called identity must have properties

$$EG_a = G_a \text{ and } G_a E = G_a \text{ for any } G_a \text{ in the set } G \tag{1.03}$$

4. To each element $G_a$ in the set, there corresponds another element in the set, denoted by $G_a^{-1}$ and is called the inverse of $G_a$ which has the properties

$$G_a G_a^{-1} = E \text{ and } G_a^{-1} G_a = E \tag{1.04}$$

It may be noticed that four properties satisfied by sets are very much similar in nature. In connection with a group, we may note the following terms:

a. The number of elements in a group is called its order.

b. A group containing a finite number of elements is called a finite group.
c. A group containing an infinite number of elements is called an infinite group. An infinite group may be either discrete or continuous; if the number of the elements in a group is denumerably infinite (such as the number of all integers), the group is discrete; if the number of elements in a group is nondenumerably infinite (such as the number of all real numbers), and the group is continuous (Cornwell, 1997; Kim, 2004; Joshi, 2005).

1.4 Review of Literature:

For addressing quantum mechanical problems embedded in a group theoretical framework, a particularly powerful mathematical technique is that of continuous Lie groups and algebras. The matrix or algebraic formulation of quantum mechanics started to show its greater stability compared with the differential or wave formulation, at least in regard to matters inherent in symmetry problems. Lie algebraic methods have been very useful in the study of problems in physics ever since it was being introduced by Marius Sophus Lie at the end of 19th century. The importance of the concept of angular momentum in quantum mechanics, in contrast to classical mechanics (Wigner, 1964) was soon recognized and the necessary formalism was developed principally by Wigner, Weyl and Racah (Weyl, 1931; Wigner, 1931, 1964; Racah, 1942, 1949, 1950). The algebraic treatment of the angular momentum can be found nowadays in almost every textbook on quantum mechanics, often in parallel with the differential equation approach. In contrast, this cannot be said about another basic quantum mechanical system, namely the hydrogen atom, which is almost universally treated by the latter approach only. Yet, both the algebraic approach to the hydrogen atom by Pauli (1926) and the differential equation approach due to Schrödinger (1926b) originated almost at the same time. Since this latter approach was more accessible to physicists, and the significance of the symmetry concepts in the microscopic world was not fully appreciated at the time, the algebraic approach for the determination of the hydrogen atom energy spectrum was largely forgotten and the algebraic techniques in general were in abeyance for three decades. The revival of
these techniques came with the development of quantum mechanics of elementary particles, since for these systems the explicit form of the Hamiltonian is unknown and one can only make certain more or less plausible assumptions about its symmetry. In the midst of various attempts to solve this difficult problem, the elementary particle physicists examined several non-compact Lie algebras in the mid-1950s, hoping that they would provide a clue to the classification of elementary particles. Although this hope did not materialize, and in fact these were Lie algebras of compact Lie groups which enabled such a classification (Gell-Mann and Ne’eman, 1964), the non-compact groups turned out to be relevant as the so-called dynamical groups for atomic physics. We note at this occasion that various compact groups particularly their “prototype,” the unitary group or rather their Lie algebras are also extensively used in both nuclear (Moshinsky, 1968) and atomic and molecular many body problems (Paldus, 1974, 1976, 1981, 1986).

A close relationship of the angular momentum and the so(3) algebra dates certainly to the prequantum mechanics era, while the realization that SO(4) is the symmetry group of the Kepler problem was first demonstrated by Fock (1935). Following the developments in the late 1950’s and early 1960’s mentioned above, the original algebraic approach of Pauli was considerably simplified and systematized using the language and concepts of Lie algebras. A completely new aspect was the introduction of dynamical groups in field theory and particle physics (Barut and Bohm, 1965; Dothan et al., 1965). In particular the non-compact groups O(2,1) and O(4,2) (Barut, 1971) enabled a simple and elegant treatment of the hydrogen atom and other simple quantum mechanical systems. We wish to recall at this point that group theoretical methods, although greatly developed by pioneers of quantum mechanics (Wigner, 1931; Weyl, 1931) were subsequently in abeyance for a long time as mentioned earlier. In fact, a number of physicists expressed a certain proudness when claiming that they can “get along without it” (Condon and Shortley, 1935), and the approach was even referred to as a “group pest” by some. It is interesting to observe a rather dramatic change in this attitude during the last few decades which is perhaps best documented by comparing the old and new editions of Condon and Shortley’s atomic structure
theory (Condon and Odabasi, 1980). Nevertheless, the above-mentioned elegant and simple treatments of the hydrogen atom and similar problems have yet to make their way into more elementary texts on quantum mechanics. One of the reasons for the slow acceptance of these techniques, as well as for the original overlook of the group theoretical and algebraic methods, is undoubtedly related to their abstract character and inherent complexity. Indeed, a proper understanding of Lie group structure requires an intimate knowledge of not only the standard theory of finite groups, but also of topology and manifold theory. Nevertheless, the basic concepts are quite simple, particularly when presented in the context of physical applications, and at the much simpler Lie algebra level, since the group structure is unnecessary for many useful applications.

However the use of Lie algebras as a tool to systematically investigate physical systems (the so called spectrum generating algebra) did not develop fully until the 1970’s when it was introduced in a systematic fashion by F. Iachello and A. Arima in the study of spectra of atomic nuclei (Interacting Boson Model) (Arima and Iachello, 1975, 1976, 1978, 1979; Iachello and Arima, 1987; Iachello and Isacker, 1991). The highest expression of group theoretical methods in nuclear physics is definitely offered by this interacting boson model. This approach, introduced for even-even nuclei in 1975 (Arima and Iachello, 1975, 1976; Iachello and Arima, 1987) and extended to more complex nuclear systems in the following years (Arima and Iachello, 1978, 1979; Iachello and Isacker, 1991), is important for its unprecedented power in describing virtually any kind of experimental situation in nuclear physics. More significantly, the interacting boson model is the first example of a comprehensive theoretical model based on a dynamical symmetry environment.

This kind of strategy was then exported to the world of molecules (Iachello and Levine, 1982, 1995; Iachello, 1981; Roosmalen et al., 1982, 1983a, 1983b, 1984; Frank and Isacker, 1994; Iachello et al., 1995; Frank et al., 1996; Lemus and Frank, 1991, 1994; Child and Lawton, 1982; Benjamin and Levine, 1983; Kellman, 1985; Child and Zhu, 1998; Iachello et al., 1991; Iachello and Oss, 1996;
C. E. Wulfman played a great role in the introduction of the algebraic approach to molecular Spectroscopy. He was the pioneer to publish the first paper on the algebraic approach to molecular Spectroscopy in 1979 (Wulfman, 1979; Levine and Wulfman, 1979). As a matter of fact, the only difference between nuclei and molecules from the viewpoint of the building blocks used is that when dealing with molecules, one has to start with a diatomic unit. This is equivalent to considering boson operators related to the dipole character of the diatom. Consequently, a different dynamical symmetry (of smaller dimension than that used in nuclear physics) is adopted in the description of molecular systems. It is perhaps worthwhile to comment here that algebraic models, after an initial introductory period during which they were considered to be elegant for the known physical facts, are now used in practical problems of current interest. As in the case of nuclear systems, it was realized that the dynamical symmetry framework was far from simply being just a different language used to address a problem. For molecular spectroscopy as well, algebraic techniques were able to demonstrate their suitability to address successfully even quite difficult situations.

In connection with molecular spectroscopy, however, it is important to mention that dynamical symmetries constitute a big step forward over a conventional use of symmetry arguments, especially those concerning the description and classification of energy spectra denoting specific degeneracy patterns. One could state, in a rather restrictive parallel, that the amount of information gained in going from a degeneracy symmetry to a dynamical one is similar to that obtained in going from a static to a dynamical study of forces acting in a conventional mechanical system. As a matter of fact, dynamical symmetries contain within themselves both the degeneracy aspects of a physical system and the complete machinery for describing transitions among different states (i.e., the dynamical behaviour of the physical object at issue). All these tasks can be carried out in the extremely compact and convenient framework of Lie groups and algebras. It is not just a matter of language; however, the use of group theoretical tools very often allows one to address situations inaccessible by means of
conventional methods of quantum mechanics. A comprehensive and up-to-date review of mathematical concepts, physical aspects, practical applications and numerical implementation of algebraic models in molecular spectroscopy was presented by S. Oss in 1996 (Oss, 1996). The brief review work of F. Iachello and S. Oss (2002) reflects the scenario of the field upto 2002 alongwith the perspectives for the algebraic method in the first decade of the 21st century.

This algebraic method was also applied to treat various complex and non-rigid molecules by F. Iachello et al. (Iachello and Oss, 1993a; Iachello et al., 2003). This method has also been applied extensively to study various spectroscopic aspects of Benzene and its dimmers (Iachello and Oss, 1991, 1993a, 1993b, 1995; Halonen, 1982). A two-dimensional Lie algebraic technique has been recently introduced by F. Iachello and S. Oss (1996) and preliminarily applied to the vibrational analysis of pure bending modes of the acetylene molecule. In that work, it was shown that, besides U(2) (one dimensional) and U(4) (three-dimensional) dynamic symmetries, one can also consider U(3) as the proper Lie algebra for representing vibrations in the description of degenerate bending excitations in linear molecules. As widely discussed elsewhere (Iachello and Levine, 1995) U(4) methods are capable to account simultaneously for rotational and vibrational degrees of freedom. Later in 1998, the study of intensities of infrared transition in the two-dimensional algebraic model has been done by S. Oss and M. A. Temsamani (1998). In most of the works as mentioned above the vibrational spectra has been studied but molecular electronic spectra has been studied by A. Frank et al. (1986, 1989). In the last few years Lie algebras have been used extensively by Ramendu Bhattacharjee and co-workers to illustrate the spectra of various polyatomic molecules including various bio-molecules like metalloporphyrins and nano particles like C\textsubscript{60}, C\textsubscript{70}, C\textsubscript{80} (Choudhury et al., 2008a, 2008b, 2009a, 2009b, 2010; Das, 2010, 2011; Kalyan, 2011a, 2011b; Karumuri, 2008a, 2008b, 2009a, 2009b, 2009c, 2010a, 2010b; Sarkar, 2006, 2008, 2009; Sen, 2011a, 2011b).
In all these above applications, the groups used were compact, so that their unitary representations could reproduce the observed discrete and finite dimensional spectra. The algebras associated with the group were used to generate the spectra, while the representation matrices of the group were used to calculate time-dependent excitations of the bound levels (Alhassid et al., 1978; Alhassid and Koonin, 1981). However, many of these systems have both discrete and continuous spectra. For example, diatomic molecules may dissociate, above certain energy, in two parts or one may wish to study atom-atom scattering. Y. Alhassid, F. Gursey and F. Iachello provided the first steps towards the extension of algebraic techniques to the description of scattering processes, by connecting the scattering states of certain potentials to the representations of some groups (Alhassid et al., 1983a, 1983b, 1986; Frank and Wolf, 1984; Wu et al., 1987, 1989). Frank and Wolf (Frank and Wolf, 1984) suggested that the potential group was the most natural avenue for constructing algebraic theories of scattering and used it for determining the S-matrix associated with a class of potentials. The results of their investigation are that, for problems whose bound state solutions are describable by a compact group G, the scattering solutions are simply obtained by an analytic continuation into the complex plane of some of the quantum numbers characterizing the bound states in G. At the same time, the compact group G is analytically continued into a non-compact group G*. The scattering states are related to the unitary infinite-dimensional representations of G* (Wybourne, 1974). They showed that in case of one dimensional potentials the group structure of the corresponding bound state problem is that of SU(2) while the scattering states are obtained by a proper analytic continuation of SU(2) to SU(1, 1). They showed that the realization of SU(2) is connected with the Morse potential (Morse, 1929). This potential plays an important role in molecular physics and it has been the subject of several other group theoretical investigations (Levine and Wulfman, 1979; Berrondo and Palma, 1980) although always confined to the bound state part of the spectrum. They also showed that realization of SU(1,1) is connected with the Pöschl-Teller potential (Pöschl and Teller, 1933). This Pöschl Teller potential emerges in a variety of problems in physics, such as the soliton solutions to the Korteweg-de Vries equation (Lax, 1968), the Hartree mean field equation of a
many-body system with a δ-function two-body interaction (Calogero and Degasperis, 1975; Yoon and Negele, 1977) and in connection with completely integrable many-body one-dimensional systems (Calogero, 1975). Also how several potentials can be generated by SU(1,1) are described by C. V. Sukumar and G. Levai (Sukumar, 1986; Levai, 1994).

The Lie algebraic methods up to now have focussed essentially on the description of bound (Arima and Iachello, 1976, 1978; Iachello, 1981; Roosmalen et al., 1982; Iachello and Levine, 1982; Levine and Wulfman, 1979; Roy et al., 2010, 2011) and scattering states (Alhassid et al., 1983a, 1983b, 1986; Frank and Wolf, 1984; Alhassid and Wu, 1984; Alhassid et al., 1984) in a variety of fields. Schrödinger equation for some asymmetric double well potentials have also been studied by R. Koc and D. Haydargil using Lie algebra (Koc and Haydargil, 2004). J. Sadeghi and B. Pourhassan used su(1,1) algebra to explain Hall effect (Sadeghi and Pourhassan, 2009). By mapping the quantum mechanical problem onto an algebraic structure, representation theory immediately provides the excitation energies and eigen states.

However, there is one missing category in the group theoretical description of quantum systems, namely, hamiltonians with periodic potentials. In this case, the energy spectrum is characterized by energy bands and gaps. Therefore we extend the group theoretical framework by showing that Lie algebraic techniques can be applied to such problems where energy bands can be understood in the context of representation theory. This is precisely the standpoint taken in this paper, in which we shall attempt to present a very simple and hopefully pedagogical as well as motivated approach to this topic.

1.5 The Role of Lie Algebraic Methods:

The Lie algebraic formulation discussed above can be used to study problems of relevance in physics and chemistry. Particularly, in case of molecules, the formulation can be used to analyze vibrational and rotational spectra.
Electronic spectra also can be attacked with the algebraic model. However, the field in which the algebraic method has had most impact is that of vibrational spectroscopy. To deal with the physical problems, following are the important advantages of the algebraic method:

a. In the energy spectra, from the very beginning anharmonicities are put in.

b. The Lie algebraic methods allow us to calculate wave functions and thus observables such as energies, intensities of transitions (infrared, Raman, Franck-Condon) etc.

c. Lie algebraic methods can adequately explain different states of a potential such as bound states, scattering states and also transition matrices without solving the Schrödinger equation.

d. Only by choosing the correct algebra and their representation a set of potentials can be approached which indeed corresponds to different physical situations.

1.6 Lie groups:

A group in which the law of composition and the law of inversion are continuous in all the group elements, is called a topological group. The dependence of the elements \(x_1, x_2, \text{etc.}\), of a topological group \(G\) on its \(r\) continuous parameters can be written explicitly as \(x_i \equiv x_i(a_1, a_2, \ldots, a_r)\), \(x_2 \equiv x_2(b_1, b_2, \ldots, b_r)\) etc.

Let \(x_1 x_2 \equiv x_3(c_1, c_2, \ldots, c_r)\) and \(x_i^{-1} \equiv x_4(d_1, d_2, \ldots, d_r)\).

The parameters of \(x_3\) and \(x_4\) can be expressed as functions of the parameters of \(x_1\) and \(x_2\), that is,
A topological group is called an \( r \)-dimensional Lie group if there exists a neighbourhood \( N \) of the identity element \( e \) such that the continuous parameters of the product of two elements and those of the inverse of an element in \( N \) are continuous differentiable functions of the parameters of the elements, that is, if \( c_i \)'s and \( d_i \)'s of (1.05) are analytic functions of \( a_i \)'s and \( b_i \)'s for elements in \( N \) provided that \( x_3 \) and \( x_4 \) lie in \( N \) when \( x_1 \) and \( x_2 \) do. In addition, there will be laws for combining the other \( n - r \) discrete parameters.

We see that it is convenient to choose the continuous parameters of a Lie group such that the image of the identity element \( e \) is the origin of the parameter space, i.e., \( e \equiv x(0, 0, 0, \ldots, 0) \). Having this parameterization, due to the analytical properties of the Lie groups, an element near the identity may be written as

\[
x(0,0,\ldots,\varepsilon,\ldots,0) = x(0,0,\ldots,0) + i\varepsilon I_j(0,0,\ldots,0),
\]

(1.06)

to first order in \( \varepsilon_j \). The operator \( I_j \) can be obtained from (1.06) and is given by

\[
I_j = \lim \left[ \frac{1}{\varepsilon_j} \{ x(0,\ldots,\varepsilon_j,\ldots,0) - x(0,0,\ldots,0) \} \right]
\]

(1.07)

For a Lie group, all the properties can be derived from the \( r \) operators \( I_j(1 \leq j \leq r) \) which need to be defined only near the identity element of the group.

We can arrive at an element of the group at a finite distance apart from the identity by the successive application of the product rule. Thus, let us say that we wish to generate the element \( x(0,0,\ldots, a_j, \ldots,0) \). To do the same, let us first write \( a_j = N\varepsilon_j \), where \( N \) is a large positive integer so that \( \varepsilon_j \) is a small quantity.
Then, \[ x(0,0,\ldots, a_j, \ldots,0) = \left[ x(0,0,\ldots, \epsilon_j, \ldots,0) \right]^N \]
\[ = \left[ e + i \epsilon J_j \right]^N = \left[ e + i \left( \frac{a_j}{N} \right) J_j \right]^N \] (1.08)

Now, allowing N to tend to infinity and using the algebraic identity

\[ \lim_{N \to \infty} \left( 1 + \frac{x}{N} \right)^N = \exp(x) \]

We have from (1.08)

\[ x(0,0,\ldots, a_j, \ldots,0) = \exp(i a_j I_j) \] (1.09)

which is an exact result. We are to understand the exponential function on the right-hand side of (1.09) as being formally equivalent to its expansion in the powers of the operator \( I_j \). It may be noted that for a general element of the group, we can easily extend the above result to obtain

\[ x(a_1, a_2, \ldots, a_r) = \exp \left[ \sum_{j=1}^{r} i a_j I_j \right] \] (1.10)

Here we note that all the elements of the Lie group belonging to the subset containing the identity can be obtained by giving various values to the parameters \( a_j \) on the respective prescribed intervals. That is why the operators \( I_j \) are called the generators of the Lie group. Also we should note here that with \( r \) continuous parameters a Lie group has \( r \) generators.

### 1.7 Lie Algebras and Representations of Lie Groups:

Let us consider a Lie group with \( r \) continuous parameters \( a_k \) having the \( r \) generators \( I_1, I_2, \ldots, I_r \). It is seen that any element of the Lie group can be expressed in the form...
\[ x(a_1, a_2, \ldots, a_r) = \exp \left[ \sum_{k=1}^{r} i a_k I_k \right] \]  

(1.11)

For a finite group, it is seen that all the properties of the group can be obtained from the structure of its multiplication table. It can be shown that for a Lie group, the commutators of its generators determine the structure of the group.

Thus, let us consider two particular elements of the Lie group of the form

\[ x(0,0,\ldots, a, \ldots, 0) = \exp(i a_k I_k) \]

\[ x(0,0,\ldots, a, \ldots, 0) = \exp(i a_l I_l) \]

Here, the product of these two elements \( \exp(i a_k I_k)\exp(i a_l I_l) \), must belong to the group and hence must be expressible in the form (1.11) with some values of the parameters \( a_k \). Since the generators of a Lie group do not, in general commute with each other (they commute only when the Lie group under consideration is abelian), there is no simple way of writing this product element. However, we may use the fact that such a product involves the commutator of \( I_k \) and \( I_l \). Now, for the product \( \exp(i a_k I_k)\exp(i a_l I_l) \) to belong to the group, it therefore follows that the commutator \([I_k, I_l]\) must be a linear combination of the generators, i.e.

\[ [I_k, I_l] = \sum_{j=1}^{r} c_{kl}^j I_j, \quad l \leq k, \ l \leq r \]

(1.12)

where \( c_{kl}^j \) are certain coefficients. It is known that the commutators of pairs of generators of a Lie group determine the structure of the Lie group completely in analogy with the multiplication table for a finite group. Hence the coefficients \( c_{kl}^j \) are known as the structure constants of the Lie group. These structure constants are the characteristic property of the Lie group and do not depend on any particular representation of the generators. Since the generators of a Lie group themselves are not unique, hence these structure constants are also not unique.
Eq. (1.12) provides us with a law of composition between any two elements of the vector space such that the resulting vector is also an element of the vector space. In fact, the set of real linear combinations of the generators of a Lie group is a Lie algebra.

A Lie algebra is a real $r$-dimensional vector space $L$ with elements $(x, y, z, \ldots)$ endowed with a law of composition for any two elements of $L$ denoted by $[x, y]$ such that

$$[x, y] \in L$$
$$[x, y] = -[y, x]$$
$$[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0$$

for all $x, y, z \in L$. We refer the law of composition $[x, y]$ as the commutator of $x$ and $y$.

The commutators of the generators of a Lie group defined in Eq. (1.12) satisfy the above properties, hence we obtain the following relations among the structure constants:

$$C_{jl}^j = -C_{lk}^j$$
$$\sum_{m=1}^r \left[ C_{kl}^m C_{jm} + C_{lj}^m C_{km} + C_{jk}^m C_{lm} \right] = 0$$

(1.14)

Since the generators $I_k$ are Hermitian, Eq. (1.12) shows that the structure constants $C_{kl}^j$ are purely imaginary.

It may be noted here that the importance of the Lie algebra lies in the fact that we may generate a representation of the Lie group by considering a matrix representation of the Lie algebra. Now, if we are able to find a set of $r$ square matrices all of order $p$ (let us say), such that they satisfy the commutation relations (1.12) with the given structure constants, then using these for the $I_k$'s in Eq. (1.11), we would generate a $p$-dimensional representation of the Lie group.
Thus, we can take it as a general rule that a representation of a Lie algebra can be used to generate a representation of the associated Lie group.

Let us now apply the above discussion to SU(2), as an example. The three generators of SU(2) can be chosen to be the Pauli spin matrices

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(1.15)

which are a set of three independent traceless hermitian matrices of order 2. For the generators of SU(2) we can then choose the set \( \{ E, \sigma_x, \sigma_y, \sigma_z \} \), where \( E \) is the unit matrix of order 2.

The generators of SU(2) given in (1.15) satisfy the commutation relations

\[
[\sigma_j, \sigma_k] = 2i \sum_l \epsilon_{jkl} \sigma_l
\]

(1.16)

where \( \epsilon_{jkl} \) is the fully antisymmetric tensor of rank 3 whose only nonvanishing elements are

\[
\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = -\epsilon_{213} = -\epsilon_{132} = -\epsilon_{321} = 1
\]

(1.17)

Here the indices \( j, k, l \) stand for any of \( x, y, z \) or for 1, 2, 3. It should be noted here that the six equations in (1.17) is generally abbreviated into a single equation and is written as \( \epsilon_{123} = 1 \) and all permutations with proper signs. One can see here that the components of the tensor \( \epsilon_{jkl} \) multiplied by \( 2i \) are evidently the structure constants of SU(2). Thus, the Lie algebra of SU(2) is the set of all real linear combinations of \( \sigma_x, \sigma_y \) and \( \sigma_z \).

To make the conception more clear let us now look at the following three matrices:
\[ \lambda_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \lambda_2 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \lambda_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \] (1.18)

We can easily verify that all these three matrices satisfy the same commutation relations as the generators \( \sigma^i \)'s, i.e.

\[ \left[ \lambda_j, \lambda_k \right] = 2i \sum_i \epsilon_{jkl} \lambda_l. \] (1.19)

Thus we see that the \( \lambda \)'s generate a representation of the Lie algebra of SU(2) and can therefore be used to generate a three-dimensional representation of SU(2) itself.

For a Lie group, the maximum number of mutually commuting generators is called its rank. Thus, the rank of SO(3) is 1 because no two of its generators \( L_x, L_y \) and \( L_z \) commute with each other. On the same reasoning, the rank of SU(2) is also 1.

1.8 Casimir Operator:

For a Lie group, Casimir operator is the operator which commutes with all the generators of the Lie group. These operators play a very important role since they are associated with constants of the motion. They can also be defined as those operators which commute with all the elements of the Lie algebra. The number of independent Casimir operators of a Lie group is equal to its rank. They are constructed from powers of the operators of the algebra or generators of the group.

Thus, the one and only Casimir operator of SO(3) is \( \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \), which commutes with each of \( \hat{L}_x, \hat{L}_y \) and \( \hat{L}_z \). Similarly, the only Casimir operator of SU(2) is \( \hat{\sigma}^2 = \hat{\sigma}_x^2 + \hat{\sigma}_y^2 + \hat{\sigma}_z^2 \).

The Casimir operators of a Lie group can be diagonalized simultaneously with its generators. Hence the eigenvalues of the Casimir operators may be used to
label the irreducible representation of the Lie group. The Casimir operator $\hat{L}$ of $\text{SO}(3)$ thus has the eigenvalues $l(l+1)$, where $l$ takes on all non-negative integral values and hence the irreducible representation of $\text{SO}(3)$ may be labeled by the index $l$. The Casimir operator $\sigma^2$ of $\text{SU}(2)$ has, in general, the eigenvalues $j(j+1)$, where $j$ takes all non-negative integral and half-odd-integral values.

On the basis of the brief discussion on Lie groups and Lie algebras made in this section now we are in a position to summarize the properties of the Lie algebras which are given in the following section.

1.9 Properties of Lie Algebras:

A. Definition:

Let us consider a set of operators as $\hat{X}_a \ (a = 1, \ldots, r)$. If this set of operators satisfying the commutation relations

$$\left[ \hat{X}_a, \hat{X}_b \right] = \sum_c C^c_{ab} \hat{X}_c$$

(1.20)

where

$$C^c_{ab} = -C^c_{ba} \quad \text{and} \quad \left[ \hat{X}_a, \hat{X}_a \right] = 0$$

(1.21)

together with the Jacobi identity

$$\left[ \left[ \hat{X}_a, \hat{X}_b \right], \hat{X}_c \right] + \left[ \left[ \hat{X}_b, \hat{X}_c \right], \hat{X}_a \right] + \left[ \left[ \hat{X}_c, \hat{X}_a \right], \hat{X}_b \right] = 0$$

(1.22)

it is said to form a Lie algebra $G$

$$x_a \in G$$

(1.23)

In a similar way, a subalgebra $G'$ of $G$ also can be defined.

Let us consider a subset $Y_i$ of the $x_a$'s. Now, if
Chapter 1

\[
[\hat{Y}_i, \hat{Y}_j] = \sum_k C^k_{ij} \hat{Y}_k
\]  

(1.24)

the subset \( \hat{Y}_i \) of the \( \hat{X}_a \)'s is said to form a subalgebra \( G' \) of \( G \).

We denote this situation by

\[
\hat{X}_a \in G, \, \hat{Y}_i \in G', \, G \supseteq G'
\]

(1.25)

We say an algebra (or subalgebra) as Abelian if all its elements commute

\[
\left[ \hat{X}_a, \hat{X}_b \right] = 0, \, \forall \hat{X}_a \in G
\]

(1.26)

B. Physical Realization of Lie Algebra:

Associated with each Lie algebra there is a group of transformation where the operators of the algebra are the generators of the group. So for the purpose of the definition of Lie algebra it is not necessary to specify any explicit form of the operators. Once Lie algebra has been defined in the abstract sense via the defining commutation relations Eq. (1.20 & 1.22), it is of practical interest to find physical realizations of the generators in terms of position and momentum operators, which also satisfy these defining commutation relations. We shall call such a set of concrete operators a realization of the Lie algebra. In practice, as we shall see, we often work backwards by starting with a set of concrete operators which do not close under commutation and adding to our set any new operators which are necessary to close out the commutation relations. In this manner we obtain a realization of some Lie algebra. This is also a standard procedure for combining or merging two realizations of two different Lie algebras into a realization of a bigger Lie algebra.

As an example consider the important three-dimensional Lie algebra often denoted as so(3) or su(2), whose defining commutation relations can be cast in the form
Well-known realizations of the generators of this Lie algebra are given by the three components of the orbital angular momentum vector \( \vec{L} = \vec{r} \times \vec{p} \), the three components of the spin \( \vec{S} = \frac{1}{2} \vec{\sigma} \) realized in terms of the Pauli spin matrices or the total one-electron angular momentum \( \vec{J} = \vec{L} + \vec{S} \). The components of each of these vector operators satisfy the defining commutation relations Eq. (1.27) if we use atomic units. We should also note that the vector cross-product example mentioned earlier also satisfies Eq. (1.27) if we define \( E_j = i e_j \); \( j = 1, 2, 3 \).

Associated with each operator realization of a Lie algebra we generally have a vector space on which these operators act. For the realization given by \( \vec{L} \) this might be either an abstract space of angular momentum states \( |lm\rangle \), \( l = 0, 1, 2, \ldots; m = -l, -l+1, \ldots, l \) or a concrete realization of them as spherical harmonic functions \( Y_{lm}(\theta, \phi) \). We can then consider the matrix elements of the operators with respect to this vector space of states and this leads to the important concept of a matrix representation of a Lie algebra.

C. Matrix Representation of Lie Algebra:

Given a Lie algebra with defining commutation relations Eq. (1.20 & 1.22), we can consider the generators \( \hat{E}_i \) as operators acting on some \( n \)-dimensional vector space \( \mathbf{W} \). If \( \{|i\rangle : i = 1, 2, \ldots, n\} \) is a basis set for \( \mathbf{W} \), then

\[
\hat{E}_k |j\rangle = \sum_i |i\rangle \langle i | \hat{E}_k |j\rangle; \quad i, j = 1, 2, \ldots, n
\]  

(1.28)

where \( \langle i | \hat{E}_k |j\rangle \) is a matrix element of \( E_k \). Denoting by \( E_k \) the matrix representing \( \hat{E}_k \) it is easily shown that

\[
[\hat{E}_1, \hat{E}_2] = i\hat{E}_3, \quad [\hat{E}_2, \hat{E}_3] = i\hat{E}_1, \quad [\hat{E}_3, \hat{E}_1] = i\hat{E}_2 \tag{1.27}
\]
\[ [E_i, E_j] = \sum_k C_{ijk} E_k \] (1.29)

and we say that the matrices \( E_i \), generate a matrix representation of the Lie algebra since they have the same defining commutation relations.

The problem of classifying all matrix representations of a given Lie algebra is an important but difficult one. The first step is to classify all the irreducible representations. Once the irreducible representations are obtained, then any matrix representation can be constructed using the irreducible representations as building blocks. Thus, given any matrix representation of a Lie algebra we can always obtain an equivalent one by applying a similarity transformation to all the matrices representing the generators. If we can do this in such a way that all the matrices have an identical block diagonal structure then we say that the representation is reducible since the block matrices will form smaller dimensional matrix representations of the Lie algebra. For example, if each \( E_i \) has the form

\[
E_i = \begin{pmatrix} A_i & 0 \\ 0 & B_i \end{pmatrix}
\]

where \( A_i \) and \( B_i \) are \( l \times l \) and \( m \times m \) matrices, respectively, then it is easily verified that the \( A_i \) form a matrix representation and so do the \( B_i \). If we cannot obtain such a reduction by any similarity transformation then we say that the representation is irreducible.

The algebras should be written by lower case letters and their associated groups of transformations by capital letters. Thus, \( \text{so}(3) \) denotes the algebra of special (s) orthogonal (o) transformations in three (3) dimensions, while \( \text{SO}(3) \) denotes the associated group. It has become customary, however, to denote both groups and algebras by capital letters. The letter \( \text{S} \) denotes special transformations, that is, transformations with determinant +1. Both orthogonal and special orthogonal algebras have the same number of operators.
D. Number of Operators in the Lie Algebra

For any admissible Lie algebra, one knows the number of operators in the algebra, denoted by \( r \) (called the order of the algebra) and is given in Table 1.1

**Table 1.1** Number of the operators in Lie algebras (Iachello and Levine, 1995)

<table>
<thead>
<tr>
<th>Algebra</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>( U(n) )</td>
<td>( n^2 )</td>
</tr>
<tr>
<td>( SU(n) )</td>
<td>( n^2 - 1 )</td>
</tr>
<tr>
<td>( SO(n) )</td>
<td>( \frac{1}{2} n(n-1) )</td>
</tr>
<tr>
<td>( Sp(n) )</td>
<td>( \frac{1}{2} n(n+1) )</td>
</tr>
<tr>
<td>( G_2 )</td>
<td>14</td>
</tr>
<tr>
<td>( F_4 )</td>
<td>52</td>
</tr>
<tr>
<td>( E_6 )</td>
<td>78</td>
</tr>
<tr>
<td>( E_7 )</td>
<td>133</td>
</tr>
<tr>
<td>( E_8 )</td>
<td>248</td>
</tr>
</tbody>
</table>
E. General Representation of su(2) and su(1,1) Lie Algebra:

The defining commutation relations for the su(2) and su(1,1) Lie algebra are

\[
\begin{align*}
[\hat{J}_x, \hat{J}_y] &= i\gamma \hat{J}_z \\
[\hat{J}_y, \hat{J}_z] &= i\hat{J}_x \\
[\hat{J}_z, \hat{J}_x] &= i\hat{J}_y
\end{align*}
\]  \hspace{1cm} (1.30)

Where \( \gamma = 1 \) refers to su(2) and \( \gamma = -1 \) refers to su(1, 1). The Casimir operator, which commutes with all generators, is given by

\[
\hat{J}^2 = \gamma (\hat{J}_x^2 + \hat{J}_y^2) + \hat{J}_z^2
\]  \hspace{1cm} (1.31)

For \( \gamma = 1 \), this is just the familiar square of the angular momentum vector \( J^2 = (\hat{J} \cdot \hat{J}) \). For the study of spectral properties of these operators it is convenient to use the ladder operators \( \hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \). Then, the defining relations Eq. (1.30) can be expressed in terms of \( \hat{J}_\pm \) and \( \hat{J}_z \)

\[
\begin{align*}
[\hat{J}_+, \hat{J}_-] &= 2\gamma \hat{J}_z \\
[\hat{J}_z, \hat{J}_\pm] &= \pm \hat{J}_\pm
\end{align*}
\]  \hspace{1cm} (1.32, 1.33)

and the Casimir operator can be written in the form

\[
\hat{J}^2 = \gamma \hat{J}_+ \hat{J}_- + \hat{J}_z^2 - \hat{J}_z
\]  \hspace{1cm} (1.34)

It is well known that a set of mutually commuting operators can be simultaneously diagonalized (Messiah, 1970). For su(1,1) and su(2) the maximum number of such operators is two. For su(2) \( \gamma = 1 \), we could choose any of the pairs
\{ \hat{J}_i^2, \hat{J}_i \}, \ i = 1, 2, 3 \) and the representation theory would be the same in each case. However, for \( \text{su}(1,1) \) \( \gamma = -1 \), each such choice of a pair of mutually commuting operators leads to a different set of nonequivalent representations.

### 1.10 Present Work:

Lie groups and their associated Lie algebras play a central role in quantum mechanics (Barut, 1971; Wybourne, 1974; Hamermesh, 1962; Gilmore, 1974; Bohm, 1979). Their areas of application include fundamental quantum field theories, elementary particle symmetry and conservation laws, special function theory (Miller, 1968), angular momentum theory (Biedenharn and Louck, 1981a, 1982b) and, more recently, the practical development of the unitary group approach to configuration interaction (Paldus, 1974, 1976, 1981) and the systematic study of large-order perturbation theory via the Lie algebra \( \text{SO}(4,2) \) (Cizek and Vrscay, 1982). As mentioned in the literature, the Lie algebraic methods up to now have focussed essentially on the description of bound states (Arima and Iachello, 1976, 1978; Iachello, 1981; Roosmalen et al., 1982; Iachello and Levine, 1982; Levine and Wulfman, 1979; Roy et al., 2010, 2011), scattering states (Alhassid et al., 1983a, 1983b, 1986; Frank and Wolf, 1984; Alhassid and Wu, 1984; Alhassid et al., 1984) and in the description of vibrational spectra of various polyatomic molecules including various bio-molecules like metalloporphyrins and nano particles like \( C_{60}, C_{70}, C_{80} \) (Choudhury et al., 2008a, 2008b, 2009a, 2009b, 2010; Das, 2010, 2011; Kalyan, 2011a, 2011b; Karumuri, 2008a, 2008b, 2009a, 2009b, 2009c, 2010a, 2010b; Sarkar, 2006, 2008, 2009; Sen, 2011a, 2011b) by Ramendu Bhattacharjee and co-workers, yet no works has been reported in the use of Lie algebra for the determination of energy bands and their structures in solids. However, there is one missing category in the group theoretical description of quantum systems, namely, hamiltonians with periodic potentials. In this case, the energy spectrum is characterized by energy bands and gaps. Therefore we extend the group theoretical framework to such problems where energy bands can be understood in the context of representation theory. This is
precisely the standpoint taken in this paper. It is noteworthy that other conventional theoretical methods such as Wigner-Seitz Cellular Method, Nearly Free Electron Theory, Tight Binding Approximation, Kronig-Penney Model, Green Function Method, Density Functional Theory, Muffin-tin approximation etc. (all these mentioned methods are described more elaborately in Chapter 2) are being used by several theoretical scientists for analysis of energy band structures, but our main intention in use of Lie algebra is to evaluate its usefulness in energy band computation so that a single methodology can be used in a wider range of spectral region, thereby decreasing the extent of approximation. Our main interest is in Lie algebras, rather than their corresponding Lie groups, as they arise more naturally as a practical tool for the systematic calculation of matrix elements of various quantum mechanical operators.

It should be emphasized that a detailed knowledge of Lie algebras is not essential to the understanding of the applications we shall consider, since all of our results will be presented in a simple pedagogical manner using only the familiar concepts of operators, matrices, commutators and representation theories.

1.11 Different Chapters of the Thesis:

In this work we aim to explore condensed matter physics with the help of group theoretical approach; in particular using Lie algebra. Our research findings are written in the thesis containing following chapters:

Chapter-1: Introduction.

As already discussed, the first chapter contains an overview of solid state physics and electronic energy bands in general. In this chapter, the review of literature, the basic definitions & properties of groups, The role of Lie algebraic methods, Lie groups, Lie algebras, properties of Lie algebras, Casimir operator, General representation of su(2) and su(1,1) Lie algebra are also discussed. Moreover, a brief description of matrix representations of Lie algebras are discussed.
The second chapter will contain description of various theoretical methods which are being exercised to determine the energy bands of solids.

The third chapter will contain the description of how Schrödinger equation can be arrived at by applying Lie algebraic method. Also in this chapter different states of Pöschl-Teller potential which is a periodic potential is illustrated with the aid of su(2) & su(1,1) Lie algebraic method.

Chapter-4: An su(1,1) Algebraic Approach to Periodic Potential.
The fourth chapter will contain the description of how Schrödinger equation for Scraf potential can be explained with the help of su(1,1) Lie algebraic method.

Chapter-5: Unitary Representation of su(1,1) Lie Algebra and the Determination of Energy Bands.
The fifth chapter will contain the description of unitary representation of su(1,1) Lie algebra and its convenience in determining the energy bands and gaps. Also in this chapter, energy band structure obtained by Lie algebraic method is explained.

Chapter-6: Conclusion and Prologue to the Future
The sixth chapter will contain the whole findings of the research work. In addition to this, the major conclusions are given.