EXPLORATION OF QUASI EXACTLY SOLVABLE MATRIX MODELS FOR JAHN TELLER SYSTEMS

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Supervisor
Assoc.Prof.Dr. Ramazan KOÇ
Co-supervisor:Assoc.Prof.Dr. Hayriye TÜTÜNCÜLER

By
Eser ÖZKEKLİKÇİ (KÖRCÜK)
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Approval of the Graduate School of Natural and Applied Sciences.

Prof. Dr. Sadettin ÖZYAZICI
Director

I certify that this thesis satisfies all the requirements as a thesis for the degree of Doctor of Philosophy.

Prof. Dr. Zihni ÖZTÜRK
Head of Department

This is to certify that we have read this thesis and that in our opinion it is fully adequate, in scope and quality, as a thesis for the degree of Doctor of Philosophy.

Assoc.Prof.Dr. Ramazan KOÇ
Co-supervisor:Assoc.Prof.Dr. Hayriye TÜTÜNCÜLER
Major Supervisor

Examining Committee Members:

Prof.Dr. Zihni ÖZTÜRK

Prof.Dr.İhsan ÜNVER

Prof.Dr. Ali Ulvi YILMAZER

ABSTRACT

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ÖZKEKLİKÇİ (KÖRCÜK), Eser
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Co-supervisor:Assoc.Prof.Dr. Hayriye TÜTÜNCÜLER
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Lie algebras play important role for solving the quantum mechanical problems. Exactly and quasi exactly solvable (QES) systems can be classified using algebraic approachs in which the Hamiltonians are expressed in terms of the generators of the Lie algebra. In this thesis, quasi exact solvability of some Jahn Teller (JT) Hamiltonians and quantum mechanical potentials have been discussed in the framework of the Lie algebra.

This work includes two main parts. In the first part, QES quantum mechanical potentials whose eigenstates and eigenfunctions have been obtained in terms of the orthogonal polynomials and these potentials have been obtained from each other by a proper transformation.

The second part covers the solutions of the $E \otimes \epsilon$ and $T \otimes t$ JT Hamiltonians. It is well known that JT effect (electron vibron coupling) is important phenomenon in high symmetry systems for understanding the structure and dynamics of molecules and solids. The quasi exact solution of the $E \otimes \epsilon$ JT Hamiltonian has been obtained in the context of the osp(2,2) Lie super algebra.This Hamiltonian has been reduced in the form of one variable differential equations by introducing a similarity transformation technique. The $T \otimes t$ JT Hamiltonian has been solved using the rotating wave approximation method which is based on Lie type transformation and simplifies the mathematical complexity of the JT problems. Its eigenvalues and associated eigenfunctions have been obtained in a closed form when the coupling constant is smaller than the natural frequency of the oscillator. The applicability of this method is firstly demostrated for a simple system known as Jaynes Cumming (JC) Hamiltonian in the literature.

These methods can also be extended to solve the other JT Hamiltonians which includes multi boson or multi boson-fermion systems.

Key words: Jahn Teller Effect, Lie (super)algebra, Quasi-exact solvability

ÖZET

KISMİ ÇÖZÜLEBİLEN MATRİX MODELLERİNİN JAHN TELLER SİSTEMLER İÇİN ARAŞTIRILMASI

ÖZKEKLİKÇİ (KÖRCÜK), Eser
Doktora Tezi, Fizik Mühendisliği Bölümü
Tez Yöneticisi: Doç.Dr. Ramazan KOÇ
Tez Yöneticisi Yardımcısı: Doç.Dr. Hayriye TÜTÜNCÜLER
Ocak 2007, 82 sayfa

Lie cebiri, kuantum mekaniksel problemlerin çözümünde önemli role oynar. Tam ve kısmi çözülebilir sistemler cebirsel yaklaşım kullanarak Hamilton işlemcisini Lie cebirinin jeneratörleri türünden ifade ederek sınıflandırılabilir. Bu tezde bazı Jahn Teller (JT) sistemlerin ve kuantum mekaniksel potansiyellerin kısmi çözülebilirliği Lie (super) cebiri çerçevesinde tartışılmıştır.

Bu çalışma iki ana bölümü içermektedir. Birinci bölümde, kısmi çözülebilen kuantum mekaniksel potansiyellerin özdeğer ve özfonksiyonları dik polinomlar türünden bulunmuştur ve bu potansiyeller uygun dönüşüm ile birbirlerinden elde edilmiştir.

İkinci bölüm $E \otimes \epsilon$ and $T \otimes t$ JT Hamilton işlemcilerinin çözümlerini kapsamaktadır. JT etkisi (elektron-vibron çiftlenimi) yüksek simetrili sistemlerde moleküllerin ve katıların yapı ve dinamiğini anlamada önemli bir kavram olduğu iyi bilinmektedir. $E \otimes \epsilon$ JT Hamilton işlemcisi osp(2,2) Lie süpercebiri bağlamında kısmi bulunmuştur. Hamilton işlemcisi benzerlik dönüşüm tekniği tanımlanarak bir değişkenli diferansiyel denklem formuna indirgenmiştir. $T \otimes t$ JT Hamilton işlemcisi, Lie tipi dönüşümü temel alan ve JT problemlerinin matematiksel karmaşıklığını basitleştiren dönen dalga yaklaşım metodu kullanılarak çözülmüştür. Özdeğerler ve ilgili özfonksiyonları doğal titreşim frekansları çiftlenim sabitinden küçük olduğunda kapalı formda elde edilmiştir.Bu metodun uygulanabilirliği ilk önce literatürde Jaynes Cumming (JC) Hamilton işlemcisi olarak bilinen basit sistem için gösterilmiştir.

Bu metodlar çoklu bozon yada çoklu fermiyon-bozon sistemlerini içeren diğer JT Hamilton işlemcilerinin çözümü için genişletilebilir.

Anahtar kelimeler: Jahn Teller etkisi, Lie (süper)cebiri, Kısmi çözülebilirlik

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LIST OF SYMBOLS

$[.,.]$ Commutator

$\{.,.\}$ Anticommutator

a_i Annihilation operator of the field

$a_i^\dagger$ Creation operator of the field

$f, f^\dagger$ Fermions

σ_x, σ_y Pauli matrices

$\sigma_{\pm,0}$ Standart Pauli matrices

μ Level seperation

κ Jahn Teller coupling constant

ω Frequency of oscillator

N Number Operator

Γ Reducible representation

Γ_α Irreducible representation

$[\Gamma \otimes \Gamma]$ Symmetric direct product representation

$\{\Gamma \otimes \Gamma\}$ Antisymmetric direct product representation

$\hbar$ Planck costant

ΔE Energy difference between two states

E_{JT} Jahn Teller energy

$\chi_i(G)$ Charecter of representation

g_0 Order of the group

CHAPTER 1

INTRODUCTION

There exist a small number of exactly solvable Hamiltonians whose spectra and corresponding eigenfunctions can be computed in a purely algebraic way [1-7]. However, the choice of such Hamiltonians is too restricted to meet numerous requirements coming from different fields of the modern quantum physics. Over the past decade, a great deal of effort has been directed towards the construction of physically significant quantum mechanical system for which part of the spectrum can be computed exactly by algebraic methods. For this new class of spectral problems are called quasi-exactly solvable (QES). This class is characterized by the property that the Schrödinger operator is Lie algebraic i.e. expressible as a bilinear combinations of first order differential operators.

QES models have an amazingly wide range of applications in different fields of theoretical physics, including molecular physics, nuclear physics and conformable quantum field theories. There are appeared different approaches to constructing QES models, including the one based on their symmetries. The number of solutions can be related to the dimension of the irreducible representations of a Lie algebra.

Lie algebraic and Lie group theoretical methods have played a significant role in the development of quantum mechanics since its inception. In the classical applications, the Lie groups appears as a symmetry group of the Hamiltonian, and the associated representations theory provides an algebraic means for computing the spectrum. The basic problem of determining which potentials are QES, then, is to classify the Schrödinger operators which admit such a finite dimensional invariant subspace. Then this problem reduced by considering the Schrödinger operators that are expressed differential operators of the Lie algebra. In that case, Hamiltonian can be written as bilinear combinations of the group generators, these preserving the finite dimensional space of the solutions. Due to the preservation of this space, the associated Hamiltonian actually reduces to an algebraic equation.

The concept of a spectrum generating algebra appears to date back to a 1959 paper of Goshen and Lipkin[8]. Spectrum generating algebras were independently rediscovered in 1965 by two groups of theoretical physicist [9]. A survey of the history and contributions appears in the review paper of Bohm and Ne'eman[10]. The fundamental concept of a spectrum generating algebra was introduced by Arima and Iachello [11, 12]. Applications of spectrum generating algebras to molecular spectroscopy began in early 1980's with the work of Iachello, Levine, Alhassid, Gürsey and collaborates[13, 14] and to scattering theory [15, 16].

The first explicit examples of QES problems were found by Razavy [17] and by Singh-Rampal-Biswas-Datta [18]. In an explicit form a general idea of quasi -exactly solvability had been formulated at the first time in Turbiner [19, 20] and Turbiner shown that one dimensional QES Schrödinger operators related to space of polynomials [21].

In the late 1980's Shifman, Turbiner, Usheveridze, and their collaborators suggested the analysis of a significant new class of Schrödinger operators which they called "quasi-exactly-solvability" [22]. A connection of quasi-exactly-solvability and finite dimensional representations of sl_2 was mentioned at the first time by Zaslavskii-Ulyanov [23]. Usheveridze later proposed a different procedure [24] for generating QES systems. This method involves starting with a set of analytical functions that depend on some numerical parameters that are fitted to make the functions compatible with the Schrödinger equation being considered. From these functions one can obtain the QES Schrödinger operator and associated eigenfunctions simultaneously. The QES Hamiltonians were generalized multidimensional differential operators. Shifman shown that the Hamiltonian can be expressed matrix differential operators [25], Ogievetsky it can be expressed finite difference operators [26], and recently, to mixed operators containing differential operators by Turbiner [27].

In Morozov et all [28] it was described a connection of quasi-exactly - solvability with conformal quantum field theories, and in a brief review done by Shifman [29]. A general survey of a phenomenon of the quasi-exactly-solvability was done in Turbiner [30]. The QES problems attract much attention at the present time [31, 32, 33, 34]. Debergh and co-worker were shown that a general approach of QES Schrödinger equation [35]. They constructed a general algorithm generating the analytic eigenfuctions as well as eigenvalues of one dimensional stationary Schrödinger Hamiltonians. A new family of quasi solvable quantum many body system was obtained by using the Lie algebraic structure of $sl(M+1)$ [36]. F. Chafan and collaborates were develop new method which three body potential transformed into QES ones [37]. The solvability of the Dirac equation with a Lorenz scalar potential was examined relating to the $sl(2)$ Lie algebra Turbiner's classification [38].

The Jahn-Teller matrix Hamiltonians can be solved quasi-exactly by using matrix Lie algebras. Therefore it is necessary to develop a more general theory of quasi-exact solvability for Jahn-Teller systems.

The Jahn-Teller effect is concerned with one aspect of the fundamental problem of how to describe quantum systems in which electronic and nuclear degrees of freedom are coupled. It is an example of electron-phonon coupling that is very simple to understand in its primitive form and yet produces a rich variety of phenomena to study. The use of the term electron-phonon coupling implies that there are both heavy and light particles to be considered, with the heavy particles being discussed in terms of normal coordinates or phonons. The peculiarity of the Jahn-Teller interaction is that there must be a multiplicity of electronic states interacting with one or more normal modes of vibration. The Jahn -Teller theorem says that for almost any set of degenerate electronic states associated with a molecular configuration, there will exist a symmetry breaking interaction in which molecular distortion is associated with the removal of the electronic degeneracy.

The simplest proof of the Jahn-Teller theorem rests on group theory: One list all the possible point symmetry groups under which a system such as a molecule may be invariant, and one also lists all the normal modes of each system, classified by their symmetry. The energy must therefore be a minimum against small displacements of atoms from their equilibrium positions, otherwise the molecule would be unstable and would break up under the slightest external influence or by its thermal agitation's. In particular, since any general vibration of the molecule can be expressed as a sum of contributions from each of the normal modes, energy of the molecule must be a minimum with regard to displacements corresponding to any one of its normal modes. Suppose that there exist some electron state belonging to one of the degenerate representations of the point group of the molecule and that the atoms in the molecule are in their equilibrium positions. Then in any normal mode of vibration except the totally symmetrical mode the symmetry of the molecule is reduced when the atoms are in their displaced positions, and in general any electron energy level which was degenerate will have its degeneracy removed by this vibration. It can be shown that this splitting cannot occur if the molecule is to be stable for these displacements and, by studying the matrix elements which must vanish if the splitting is not to occur.

New interest in the Jahn Teller effect has followed on several recent discoveries in physics and chemistry:high temperature super conductivity , buckminsterfullerene (C_{60}), and the Bery phase all provide examples of vibronic Jahn Teller active system. Jahn Teller system has been studied by many authors.

In 1934 Landau, in a discussion with Teller [39], pointed out that if the electronic state of a certain symmetric nuclear configuration is degenerate, then this configuration is unstable with respect to nuclear displacements which remove the degeneracy. The Landau statement was afterwards verified by E. Teller and H. Jahn and more rigorously formulated as what is known as the Jahn Teller theorem [40]. Actually, not only degenerate but also relatively close in energy (quasi degenerate or pseudodegenerate) electronic terms can not be treated by the adiabatic approximation.

In 1950's development of the ESR technique made possible observations of fine structure effects in polyatomic systems. Even the first experiments on the ESR spectra of bivalent copper compounds in two-fold degenerate electronic states revealed an unusual fine and hyperfine structure of the spectrum and their rather complicated temperature dependence. These results could be explained only by taking account of the nuclear dynamics due to the Jahn Teller effect.

In the late 1950's and early 1960's the investigation of electronic and vibrational spectra taking account of vibronic coupling began. In particular, the expected fine structure of electronic transition bands was calculated, and the tunneling of the energy levels in Jahn Teller system with strong coupling was predicted. Meanwhile, it was shown that besides the proper Jahn Teller effect in systems with electronic degeneracy, similar effects are expected in the case of mixing of close in energy electronic states, which together with the Renner effect form the so called vibronic effects.

In the early 1960's it becomes clear that the interaction of dynamically unstable Jahn Teller centers in crystals at a certain temperature may result in an ordering of the local distortion manifested as a phase transition. Simultaneously it was shown that in the case of dipolar unstable centers in crystals such an ordering may lead to the spontaneous polarization of the crystal and ferro electric phase transition.

The $E \otimes \beta$ system, an electronic doublet coupled to a single mode of vibration, is introduced as an elementary example and is used to illustrate features characteristic of JT system. All such interactions can be reduced to same form of Hamiltonian, and so this system occurs widely. The type of Jahn Teller interaction depends on the symmetry of the complex in which it takes place, and this degree of simplicity will be expected if there is a relatively low symmetry to start with Bersuker [41]. The quasi exact solution of the $E \otimes \beta$ JT Hamiltonian have been obtained by Koç et all [42]. The analytical expressions were found for eigenstates and eigenvalues in terms of orthogonal polynomials. These solutions have a direct practical importance for checking the precision of analytical and numerical approximations.

The $E \otimes \epsilon$ JT Hamiltonian describes the vibronic coupling between a two fold degenerate electronic level and a pair of degenerate vibrational modes. In simple JT systems the energy eigenvalues depend on system parameters in a complicated way, and therefore they can be determined only numerically. In 1958 Longuet-Higgins [43] carried out the first diagonalization of this Hamiltonian within the adiabatic approximation. A more precise calculation was performed for $\Gamma_8 \otimes \tau_2$ by Thorson and Moffit (1968) [44], who noted several remarkable features in the energy level patterns. This phenomena was studied by Judd [45], who solved the Longuet Higgins recurrence relations for the $E \otimes \varepsilon$ and $\Gamma_8 \otimes \tau_2$ JT systems in closed rational form for isolated values of the interaction constant. The most complete and simple description of these solutions, also for the optical applications has been given by Reik [46, 47]. They observed that the isolated solutions can easily be obtained by using the Neumann series expansion for the eigenvectors in the Bargmann representation for the boson operators. Their results have been generalized for a wider class of JT systems by Loorits [48]. The exact isolated solutions for the class of quantum optical system, two or multi level interacting with the single radiation mode, have been obtained by Kus and Lewenstein without the use of a rotating wave approximation [49]. The same problem has been treated by Klenner in polar coordinates [50]. The canonical form of the $E \otimes \epsilon$ JT Hamiltonian has been found by Szopa and Ceulemans [51]. They shown that there exist a matrix transformation that maps the JT Hamiltonian into an exactly solvable Kummer problem and isolated solutions of the Hamiltonian correspond to special quantization of the canonical form. By using the operator methods, linear and quadratic coupling matrix element of the Hamiltonian have been evaluated by Bosnick [52]. In the weak coupling limit, the method leads to an analytical expression for the energy levels with the same spacing and degeneracy as the traditional expression for this limit. Numerically diagonalizing the complete linear and quadratic JT models generates eigenvalue spectra identical with his results.

The $T \otimes t$ JT Hamiltonian in which an electronic tripled is coupled to tripled vibrational modes. This interaction to be found in tetrahedral, octahedral and icosahedral symmetry. In standard analytical models for orbital triplet JT systems, a Hamiltonian is written down to describe the vibrational and interaction energies of the JT centre, which is a function of phonon coordinates and momenta. The Hamiltonian is then diagonalized in the adiabatic limit to produce eigenstates of energy.

The $T \otimes t$ Jahn Teller system has been studied previously by many authors.

Various methods have been developed to obtain its approximate solution. The most used methods are energy minimization procedure and unitary transformation method [54, 55, 56, 57, 58]. The method involved locating potential energy wells and obtain vibronic states localized in them in terms of phonon operators, rather than the more conventional electronic operators. The wells found were at positions corresponding to tetragonal, trigonal and orthorhombic symmetries. The main advantage of this method is the form of the states obtained readily allows overlaps and matrix elements between states in two wells of any symmetry to be evaluated. A unitary transformation U, which is a function of free parameters α_i, is applied to the Hamiltonian, and the transformed Hamiltonian divided into two parts. One parts is independent of the phonon operators, so is a good Hamiltonian for determining the ground states of the system. However, this method does not take into account the shape of the potential energy surface around the minima. If the full Hamiltonian is included, the degeneracy of the vibrational frequency of the phonons modes Hamiltonian is included, the degeneracy of the vibrational frequency of the phonon modes will be lifted and so anisotropy introduced into the system. This anisotropy alters the vibrational frequencies and hence the positions of the energy levels, and can be particularly significant when the barriers between wells are shallow. The anisotropy is important as Jahn Teller systems must be described by vibronic states containing both electronic and vibrational coordinates. The changes in frequency of the local modes will alter the vibrational contributions to the vibronic states, which in turn will affect other important properties of the system.

The frequencies of the local modes in the strong coupling limit can be determined using the method of ”Opik and Pryce [59]. States can then be written down to incorporate the effects of anisotropy by multiplying the states at the minima by harmonic oscillator functions reflecting the strong coupling frequencies. However, the results are only valid at strong coupling, and the advantages of the transformation approach are lost. YM Liu and co-worker [60] have shown that how the unitary transformation method can be modified to include anisotropy for all moderate to strong JT couplings by the addition of a new scale transformation.

The standard definition of a $T \otimes t$ Jahn Teller effect is one in which only the coupling to t_2 type phonon vibrations need to be considered. The e- type vibrations are assumed to be completely quenched by JT reduction factors. However, Bersuker and Polinger [61] showed that if the coupling to e-modes is only slightly weaker than that to the t_2 modes, the effect of the e-type coupling may not be negligible in determining Jahn Teller reduction factors. The idea of the Jahn Teller reduction factors was first develop by Ham [62] and O’Brein [63].

Since then, many papers have been published describing both calculations and measurement of reduction factors [64, 65, 66, 67, 68]. Although reduction factors for $T \otimes e$ Jahn Teller systems can be calculated analytically by Ham, reduction factors for $T \otimes t$, $T \otimes (e + t_2)$ and $E \otimes e$ Jahn Teller system can only be obtained using approximate method. Second order reduction factors for spin orbit coupling in the strongly coupled $T_1 \otimes t_2$ JT system have been calculated using the symmetry adapted excited states by Dunn and co-workers. The only other published calculation of second order Jahn Teller reduction factors for the $T \otimes t_2$ system appears to be numerical work of O'Brien [69].

The triplet electronic states interact with doubly degenerate e-type vibrations and three-fold degenerate t-type vibrations is known as the $T \otimes (e + t_2)$ problem. The adiabatic potentials of all the cubic systems in the subspace of $(e + t_2)$ vibrations possess the same symmetry , octahedral or tetrahedral. The simplest cubic molecule, the full vibrational representation of which contains only one e and one t irreducible representation, is the octahedral molecule of type ML_6. This problem was given earlier by Bates [70] based on the detailed theoretical calculations. Ham reduction factors and the quantum mechanically energy levels were found by using a cluster model [71]. The two phonon modes were taken to have equal coupling strengths and frequencies and four different quadratic couplings were included in the analysis, one by one. An approximate analytical treatment was given by Chancey and Judd [72] using the same assumption. A different approach was used by Lister and O'Brien [73] based on earlier work of O'Brien for strong coupling regime. By introducing an effective adiabatic potential surface they deduced specific properties of the system by studying its shape.

In quantum optics the simplest model which describes a two-level atom interacting with a single mode cavity field is the Jaynes-Cummings (JC) model [75]. It is quite natural generalization step to investigate the interaction of quantum fields with a groups of atoms. A considerable attention has been devoted to the interaction of a radiation field with atoms, since the paper of Dicke [76]. Such system is commonly termed as the Dicke model. In spite of its simplicity, the whole spectrum of the Dicke Hamiltonian can not be obtained exactly and usually it has been treated in the framework of RWA. Besides its solution with RWA, in some papers, an attempt is made to go beyond the RWA [77]. The continual integration methods are based on variational principles. The perturbative approach [78, 79] leads to more complicated mathematical treatments and the theory converges only for a certain relationship between parameters of the Hamiltonian. In a more recent study, Klimov and his co-workers[80] have developed a general perturbative approach to quantum optical models beyond the RWA, based on the Lie-type transformation.

Our thesis is based on quasi exact and approximate solution of the JT Hamiltonians and quantum mechanical potentials in the framework of the Lie algebra. The Lie algebra can be expressed differential equations for each systems. To do this Lie algebra is realized boson and fermion operators and the Hamiltonian can be written as combinations of generators of relevant symmetry group. Then the spectrum of the Hamiltonian can be found by using the suitable transformations. The structure of the thesis is organized as follows.

In the second chapter we deal with the Group Theory, Lie Algebra and Jahn Teller Effect and we have indicated that relationship between them. The application of group theory to the problems in physics can be classified in two categories. The first category is based on the symmetry of a crystal and the second category is based on eigenvalue problems where the differential equation are such of geometric nature that certain rotations or translations leave the problem unchanged. In this case it may happen that the eigenvalue connected with the solution of the problem is degenerate; that is more than one eigenfunction belongs to the same eigenvalue. Under this aspects we have devoted to the abstract group theory. We have explained the lie algebra which consists of the linear combinations of the differential operators; commutators are imposed on these linear combinations in the obvious way and then obey all the usual abstract properties of commutator brackets. Also we have discussed Jahn Teller effect which have proofed under the group theoretical approach. Construction of the JT Hamiltonian and generation matrix is introduced in this chapter.

In the third chapter, we give a set of the QES quantum mechanical potentials associated with the Pöschl-Teller and Eckart potential. These potentials can be solved by using the Lie algebraic technique. We show that QES Pöschl -Teller potential can be transformed into the generalized QES Pöschl-Teller, QES PT-Symmetric Scarf, Sextic Oscillator and, PT Symmetric Anharmonic Oscillator potential and Eckart Potential can be converted to the Hultén, Rosen Morse, Coulomb and, QES Harmonic Oscillator potentials. Their eigenfunctions and eigenvalues will be obtain in terms of the orthogonal polynomials for each potentials.

The fourth chapter of the thesis includes the solvability of the $E \otimes \epsilon$ JT Hamiltonian. We have shown that the $E \otimes \epsilon$ JT Hamiltonian becomes quasi exactly solvable with an underlying $osp(2,2)$ symmetry [53]. The construction of the boson fermion representations of $osp(2,2)$ superalgebra is presented. The Hamiltonian has two different realization under two similarity transformations then two recurrence relations can be obtained and its roots gives us the spectrum of the Hamiltonian.

In the fifth chapter, we have found the solution of the $T \otimes t$ JT Hamiltonian in the framework of the rotating wave approximating (RWA) method [74]. This is a useful method in determination of the eigenvalues and associated eigenfunctions of the various quantum optical Hamiltonians whose frequency associated with the free evaluation of the system is essentially bigger than the transmission frequencies induced by the interaction between subsystem or external source. Thus, the RWA method has been widely used when a quantum oscillator and multilevel atoms are excited by an external force and/or interact with the subsystem. Firstly this method is applied simplest JC model then applying same procedure into $T \otimes t$ JT Hamiltonian. An interesting and somewhat simpler form of the Hamiltonian is constructed by introducing a Lie-type similarity transformation and then we discuss the symmetry properties of the resultant Hamiltonian. We solve the Hamiltonian and give explicit expressions for its eigenvalues and eigenstates. The eigenvalues are displayed on a graph as a function of coupling constant.

CHAPTER 2

GROUP THEORY AND JAHN TELLER EFFECT

In general group theory solves the problems in quantum mechanics where its degeneracy occurs. Because usually the degeneracy appears Schrödinger equation allows certain groups, i.e. the Schrödinger equation remains invariant if the system under consideration undergoes a set of tansformations on the variables that enter into the wave function and this set of transformations forms a group. We known that JT effect describes the interaction of degenerate electronic states with the vibrational modes of representation and this theorem implies that any molecule, except linear ones, having a degenerate ground level will lower its symmetry by lifting the degeneracy. JT interaction matrices can be found under the group invariance then the sepectrum of the Hamiltonians can be obtained by using the Lie algebra.

In this chapter, we will give general information about group theory and JT effect and their concepts. In order to, understand group phenomena it is necessary to describe the symmetry operations mechanics. One of the remarkable aspect of the this subject, is that define the properties of the reducible and irreducible representations and explain the character tables. We mentioned about the coupling of states and direct product of representation. And also we give basic properties of the Lie algebras and corresponding Lie groups. We have known that, one interesting and very useful application of group theory is JT effect. We will show that JT Hamiltonian of a molecule must be invariant under the symmetry operations of the molecule and construct the $T \otimes T, \quad E \otimes e, \ and \ E \otimes \beta$ JT Hamiltonian.

2.1 Definition of a Group

A group is defined as a set, or collection, of elements which a multiplication rule is somehow defined so that the following conditions are satisfied

1. Closure: The product of any two members of the group is itself a member of the group.

2. Associative: The multiplication must be associative, i.e.

$$(PQ)R = P(QR),$$

where $P,\ Q,\ and\ \ R$ are members of the group, and the products can therefore be written just as PQR are unique.

3. Identity: One of the operations of the group must be identity operation, called E, so that

$$ER = RE = R$$

for all operations, R, of the group.

4. Inverses:If R is a member of the group then there must be some element of the group which we can call the inverse of R namely R^{-1} where

$$R^{-1}R = E = R^{-1}R$$

The number of elements in a group is called its order. A group containing a finite number of element is called a finite group; a group containing an infinite number of element is called an infinite group. An infinite group may further be either discrete or continues.

2.2 Symmetry Operation

Symmetry operation is important for the application of group theory. If we start with the study of the symmetry of crystals there is only a finite number of different types symmetry operation which can occur, and when selections of them are combined together it is only possible to form a finite number of different groups.

Symmetry is possessed by atoms, molecules and infinite crystals. That is, we can operate on them with a symmetry operation which interchange the position of various atoms but results in the molecule or crystal looking exactly the same as before the symmetry operation. Another way an object is said to be symmetric, or to have a symmetry, if there is a transformation, rotation or reflection, whereby the object looks the same after the transformation. The symmetry operations are defined in Table 2.1. We can summarize them briefly in

E	Identity
i	Inversion
C_n	Rotation by $2\pi/n$ (proper rotation)
σ	Reflection
σ_n	Reflection in a horizontal plane
σ_v	Reflection in a vertical plane
σ_d	Reflection in a diagonal plane
S_n	Improper rotation ($S_n = \sigma_n C_n$

Table 2.1: Symmetry operations in Schoenflies notation

Schoenflies notation. Note that all the symmetry operations involve movement of the body. A symmetry element is a geometric entitle such as a center of inversion, an axis of rotation, or a plane. Symmetry operations can be carried out with respect to these symmetry elements or combinations of them.

2.3 Representations of Group

The group elements corresponding to symmetry operation which are carried out a spatial coordinates. The resulting matrix can be found at the end of this operation. These matrices form what is called a representation of the symmetry group with each element corresponding to a particular matrix.

A representation of dimension n of an group G is a homomorphism or isomorphism between the element of G and the group of non-singular matrices. (If the order of the two groups is the some. This mapping is said to be an isomorphism and the two groups are isomorphic to one another. If the order of the two groups is not the same, then the mapping is a homomorphism and the two groups are said to be homomorphic. An isomorphic representation is called a faithful representation and a homomorphic representation is called a unfaithful representation.

Representations of groups are important in quantum mechanics for several reasons. First, the eigenfunctions of a Hamiltonian will transform under the symmetry operations of that Hamiltonian according to a particular representation of that group. Second, quantum mechanical operators are often written in terms of their matrix elements. So it is convenient to write symmetry operations in the same kind of matrix representation.

Character tables include the reducible representation which have different dimension. A and B representation have one dimensional and correspond to ground state. Two dimensional representation is denoted by E. Three, four and five dimensional representation are denoted by T, G and H respectively. They are of less general occurrence, and since their subscription is less direct than that for lower dimensional representation. G and H representations occur only in icosahedral groups as do also T representations. The other T representations occur in the cubic group of tetrahedral and octahedral groups.

2.4 Character Tables

Essentially all the information we need in analyzing a physical system in terms of its symmetry properties is contained in the group character table. Knowledge of the properties of the character of representation will allow us to quickly determine reducibility or irreducibility, to analyse a general representation in terms of the irreducible representation it contains.

Character table gives us the special properties and information about the group. The compilation of character tables requires two types of input; the order of the group and the number of classes it contains. These quantities provide stringent restrictions on the number of irreducible representations and their dimensionless.

Generally the class labels label the columns of the table while the symbol indicating the appropriate irreducible representation label the rows. Since the number of classes equals the number of irreducible representations the table is square.

2.5 The Decomposition of Reducible Representations

One of the main uses of characters is in the decomposition of a given reducible representation $[\Gamma]$ into its constituent irreducible representations $[\Gamma_\alpha]$. Suppose the given a representation Γ is reducible. If it is, then by a suitable transformation it can be reduced to the point where it can be written as a sum of irreducible representations of the group in question

$$\Gamma = \Gamma_1 \oplus \Gamma_2 \oplus ... = \sum_\alpha c_\alpha \Gamma_\alpha \tag{2.1}$$

where c_α tell us how many times Γ_α occurs in Γ. Now although the above equation is a symbolic sum an equation for the character of a particular element can be written as

$$\chi(s) = \sum_\alpha c_\alpha \chi^{(\alpha)}(s) \tag{2.2}$$

Now, the characters of the various irreducible representations of G, we can determine c_β by multiplying $\chi(s)$ by $\chi^{(\beta)}(s)$ and summing over the group element s. The character orthogonality relation

$$\begin{aligned}\sum \chi^{(\beta)}(s)\chi(s) &= \sum c_\alpha \chi^{(\beta)}(s)\chi^{(\alpha)}(s) = c_\beta G \qquad (2.3)\\ c_\beta &= \frac{1}{G}\sum \chi^{(\beta)}(s)^*\chi(s) = \frac{1}{G}\sum \lambda_i \chi_i^{(\beta)}\chi_i\end{aligned}$$

the last two equations simply being the sum over elements or the weighted sum over classes. By a very simple process, then we can deduce the composition of any representation of group in terms of irreducible representations.

2.6 Direct Product

The direct product provides a way of enlarging the number of elements in a group while retaining the group properties. Direct product occur in several contexts. For example, if a Hamiltonian or Lagrangian contains different types of coordinates, such as spatial coordinates for contains different particles, or spatial and spin coordinates, then the symmetry operations on the different coordinates commute with each other. If there is a coupling between such degrees of freedom, such as particle interaction or a spin-orbit interaction, then the direct product is required to determine the appropriate irreducible representations of the resulting eigenstates.

Now, we define what is the meant by the direct product of two irreducible representations. This is a concept that is used often since it is related to products of wave functions. One is often concerned with the products of basis functions that transform as different or the same irreducible representations. Consider a set of basis functions $A_1,\ A_2, ..., Ap$ that transform as a $p-$dimensional irreducible representation and another set of basis functions $B_1, B_2, ...Bq$ for a $q-$dimensional irreducible representation of a group of order h. A symmetry operation R operating on any function, will yield a linear combination of is partners in the usual way

$$\begin{aligned}RA_j &= \sum_{j=1}^{p} A_j a_{ji} \qquad (2.4)\\ RB_m &= \sum_{n=1}^{q} B_n ab_{nm}\end{aligned}$$

where a_{ji} and b_{nm} are appropriate irreducible representations of the group. The complete set of all possible products of functions A_iB_m contains pq functions and forms a basis of a representation of the group. This representation called the direct product of the representation is of dimension pq.

2.7 Symmetric and Antisymmetric Direct Product

When both sets of functions transform as the same irreducible representation, $a_{ij} = b_{ij}$ and pq. For this case we show that there are symmetrized and antisymmetric products with respect to the interchange of the two sets of functions.

In general, the direct product of representation $\Gamma_n(R)$ with itself, can always be written in terms of a symmetric and antisymmetric part.

$$\Gamma_n(R) \otimes \Gamma_n(R) = [\Gamma_n(R) \otimes \Gamma_n(R)]_S + \{\Gamma_n(R) \otimes \Gamma_n(R)\}_{AS} \tag{2.5}$$

The character of the symmetric and antisymmetric part of the direct product representation can be written as

$$\begin{aligned} [\Gamma_n(R) \otimes \Gamma_n(R)]_S &= \frac{1}{2}\left[[\Gamma(R)]^2 + \Gamma(R^2)\right] \\ \{\Gamma_n(R) \otimes \Gamma_n(R)\}_{AS} &= \frac{1}{2}\left\{[\Gamma(R)]^2 - \Gamma(R^2)\right\} \end{aligned} \tag{2.6}$$

The first term indicates that character squared of the representation and the second term gives us the trace of the matrix squared of the representation. The result that the direct product of an irreducible representation with itself can be expressed as a symmetric and antisymmetric part as in Eq.(2.6) is a general case.

2.8 Lie Algebra

Consider an n parameter Lie group with the n generators $I_1, I_2, ..., I_n$ and the n parameter c_i. We have seen that any element of the Lie group can be expressed in the form

$$\exp\left(i \sum_{k=1}^{n} c_k I_k\right) \tag{2.7}$$

In the case of a finite group, we have seen that all the properties of the group can be obtained from the structure of its multiplication table. For a Lie group, the commutators of its generators determine the structure of the group. Thus, consider two particular elements of the lie group of the form

$$\begin{aligned} A &= \exp(ic_k I_k) \\ B &= \exp(ic_\ell I_\ell) \end{aligned} \tag{2.8}$$

The product of these two element must be belong to the group and hence must be expressible in the form of Eq. (2.7) with some values of the parameters

c_i. In general the generators of a Lie group do not, 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 which involves the commutator of I_k and I_ℓ. For the product $\exp(ic_k J_k)\exp(ic_\ell J_\ell)$ to belong to the group, it therefore follows that the commutator $[I_k, I_\ell]$ must be a linear combination of the generators, i.e.,

$$[I_k, I_\ell] = \sum_{j=1}^{n} a^j_{k\ell} I_j, \qquad 1 \leq k,\ \ell \leq n \tag{2.9}$$

where $a^j_{k\ell}$ are real coefficients. The commutators of pairs of generators of a Lie group determine the structure of the Lie group. The coefficients $a^j_{k\ell}$ are known as the structure constants of a Lie group. They are characteristic property of the Lie group and do not depend on any particular representation of the generators. However, they are not unique, since the generators of a Lie group are themselves not unique.

Any linear combination of the generators with real coefficients can also be used as a generator of the group. It is clear that the n generators of a Lie group are the bases for an n dimensional real linear vector space.

The equation (2.9) 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. The set of all real linear combinations of the generators of a Lie group is, in fact, a Lie algebra.

A Lie algebra L, is a vector space g over some field F together with a bilinear multiplication $L \times L \to L$ called the Lie bracket, which satisfies the following properties,

· $[x, y] = -[y, x]$ (Anticommutativity for all x, y in g)

· $[x[y, z]] = [[x, y], z] + [x, [y, z]]$ (Jacobi identity for all x, y, z in g)

· $[ax + by, z] = a[x, z] + b[y, z]$, $[z, ax + by] = a[z, x] + b[z, y]$ (Bilinearity for $a, b \in F$ and all $x, y, z \in g$)

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. Thus, if we are able to find a set of n square matrices all of order p, say, such that they satisfy the commutation relations Eq. (2.9) with the given structure constants. Using these for the I_k's in Eq. (2.7) we would generate a p dimensional representation of the Lie group. We can therefore 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.

Lie algebra is an incredibly exciting and interesting place to be. There are large numbers of important unsolved questions, there is a rich theory in place, and there are hordes of application. The some basic examples of Lie algebra is given by,

1. Every vector space becomes an abelian Lie algebra trivially if we define the Lie bracket to be identically zero.

2. Euclidean space R^3 becomes a Lie algebra with the Lie bracket given by the cross product of vectors.

3. If an associative algebra A with multiplication * is given, it can be turned into a Lie algebra by defining $[x, y] = x * y - y * x$. This expression is called the commutator of x and y.

4. Another important example of a Lie algebra comes from differential topology: the smooth vector field on a differentiable manifold form an infinite dimensional Lie algebra when equipped with the lie derivative as the Lie bracket. The Lie derivative identifies a vector field X with a partial differential operator acting on a smooth scalar field f by letting $X(f)$ be the directional derivative of f in the direction of X. Then in the expression $(YX)(f)$, the juxtaposition YX represents composition of partial differential operators. Then the Lie bracket $[X, Y]$ is defined by

$$[X, Y]f = (XY - YX)f \tag{2.10}$$

for every smooth function f on the manifold.

5. The vector space of left invariant vector fields on a Lie group is closed under this operation and is therefore a finite dimensional Lie algebra. The underlying vector space of the Lie algebra belonging to a Lie group as the tangent space at the groups identity element.

6. Consider the Lie group $sl(n, R)$ of all $n \times n$ matrices with real entries and determinant 1. The tangent space at the identity matrix may be identified with the space of all real $n \times n$ matrix with trace 0, and the Lie algebra structure coming from the Lie group coincides with the one arising from commutators of matrix multiplication

7. In quantum mechanic, the commutator relations between the x, y and z component of the angular momentum form the Lie algebra for the three dimensional rotation group, which is $Su(2)$ and $SO(3)$,

$$[J_1, J_2] = i\hbar J_3, \quad [J_2, J_3] = i\hbar J_1 \quad [J_3, J_1] = i\hbar J_2 \tag{2.11}$$

The list of the some Lie groups and their lie algebras are given by Table 2.2.

2.8.1 Orthogonal Groups

Many transformations in physical applications are required to preserve length in appropriate space. If that space is ordinary Euclidean $n-$dimensional

Lie group	Description	Lie algebra	Description	dim/R
GL(n,R)	General linear group:invertible nxn real matrices	M(n,R)	nxn matrices, with Lie bracket the commutator	n^2
SL(n,R)	Special linear group real matrices with determinant 1	sl(n,R)	Square matrices with trace 0, with Lie bracket the commutator	$n^2 - 1$
O(n,R)	orthogonal group: real orthogonal matrices	so(n,R)	skew symmetric square real matrices, with Lie bracket the commutator; so(3,R) ii isomorphic to Su(2)	$n(n-1)/2$
SO(n,R)	special orthogonal group: real orthogonal matrices with determinant 1	so(n,R)	skew symmetric square real matrices, with Lie bracket the commutator	$n(n-1)/2$
U(n)	Unitary group:complex unitary nxn matrices	u(n)	square complex matrices A satisfying $A = -A^*$,with Lie bracket the commutator	n^2
SU(n)	Special unitary group:complex unitary nxn matrices with determinant 1	su(n)	square complex matrices A with trace 0 satisfying $A = -A^*$,with Lie bracket the commutator	$n^2 - 1$

Table 2.2: List of real Lie groups and their Lie algebra

space. The restriction that lengths be preserved means that,

$$X_1'^2 + X_2'^2 + ... + X_n'^2 = X_1^2 + X_2^2 + ... + X_n^2 \tag{2.12}$$

The corresponding groups are called orthogonal and are denoted by $O(n)$. Consider the orthogonal group in two dimensions, i.e. $O(2)$ where the coordinates are x and y. The most general linear two dimensional transformations is $X' = AX$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{2.13}$$

By substituting Eq. (2.12) into Eq. (2.13) then we get,

$$\begin{aligned} x'^2 + y'^2 &= (a_{11}x + a_{12}y)^2 + (a_{21}x + a_{22}y)^2 \qquad (2.14) \\ &= \left(a_{11}^2 + a_{21}^2\right) x^2 + 2\left(a_{11}a_{12} + a_{21}a_{22}\right) xy + \left(a_{12}^2 + a_{22}^2\right) y^2 \end{aligned}$$

for the right hand side of this equation to be equal to $x^2 + y^2$ for all x and y, we must set

$$a_{11}^2 + a_{21}^2 = 1; \qquad a_{11}a_{12} + a_{21}a_{22} = 0; \qquad a_{12}^2 + a_{22}^2 = 1 \tag{2.15}$$

Thus we have three conditions imposed on four parameters, leaving one free parameter. These condition can be used to establish the following relation;

$$a_{11}a_{22} - a_{12}a_{21} = 1 \tag{2.16}$$

Recognizing the quantity in parentheses as the determinant of the transformation, this condition implies that $\det(A) = \pm 1$

If $\det(A) = 1$ then the parity of the coordinate system is not changed by the transformation; this correspond to an proper rotation. If $\det(A) = -1$, then the parity of the coordinate system is changed by the transformation; thus correspond to improper rotation. Both types of transformations are important in physical applications. If the proper rotations in two dimensions then this group is called special orthogonal group in two dimensions and is denoted by $SO(2)$, where "special" signifies the restrictions to proper rotations. The parameterisation of this group that we will use is

$$R(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \tag{2.17}$$

If the proper rotations in three dimensions then this group is called special orthogonal group in three dimensions and is denoted by $SO(3)$. There are three common ways to parameterise these rotations:

1) Successive rotations about three mutually orthogonal fixed axis.

2) Successive rotations about $z-$axis, about the new $y-$axis, and then about the new $z-$axis. These are called Euler angles.

3) The axis-angle representation, defined in terms of an axis whose direction is specified by a unit vector (two parameters) and a rotation about that axis (one parameter)

Consider the first rotations about the $x-$axis by an angle ϕ_1, the rotation matrix is

$$R_1(\phi_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi_1 & -\sin\phi_1 \\ 0 & \sin\phi_1 & \cos\phi_1 \end{pmatrix} \tag{2.18}$$

for rotations about $y-$axis by an angle ϕ_2,

$$R_2(\phi_2) = \begin{pmatrix} \cos\phi_2 & 0 & \sin\phi_2 \\ 0 & 1 & 0 \\ -\sin\phi_2 & 0 & \cos\phi_2 \end{pmatrix} \tag{2.19}$$

finally rotations about the $z-$axis by an angle ϕ_3, we have

$$R_3(\phi_3) = \begin{pmatrix} \cos\phi_3 & -\sin\phi_3 & 0 \\ \sin\phi_3 & \cos\phi_3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.20}$$

So we can find generators using the three matrices with the different angles for the $SO(3)$ group. Let A and B denote such generators. The generation relations of the finite subgroup of $SO(3)$ is given by,

$$A^p = B^q = C^r = Z \tag{2.21}$$

where $C = AB,\ Z^2 = 1$, (pqr) takes the values $(nn1)$ for the cyclic groups, $(n22)$ for the dihedral groups, for the tetrahedral,octahedral and icosahedral groups (332), (432), and (532) respectively. The normal operators of $SO(3)$ associated with the quantum theory of angular momentum, and corresponding commutation relation becomes

$$[J_1, J_2] = iJ_3; \quad [J_2, J_3] = iJ_1; \quad [J_3, J_1] = iJ_2 \tag{2.22}$$

The operators of $J_\pm$ can be expressed in terms of the J_1, J_2 and J_3;

$$J_\pm = \frac{1}{\sqrt{2}}(J_1 + iJ_2) \tag{2.23}$$

with the relation

$$[J_3, J_3] = 0; \quad [J_3, J_\pm] = \pm J_\pm; \quad [J_3, J_-] = J_3 \tag{2.24}$$

Finite subgroups of $SO(3)$	Generators	Generation relations
Cyclic (C_n)	$A = \exp i\frac{2\pi}{n} J_3$	$A^n = 1$
Dihedral (D_n)	$A = \exp i\frac{2\pi}{n} J_3,$ $B = \exp i\pi J_1$	$A^n = B^2 = C^2 = 1$
Tetrahedral (T)	$A = \exp i\frac{2\pi}{3\sqrt{3}}(J_1 + J_2 + J_3),$ $C = \exp i\pi J_1$	$A^3 = B^3 = C^2 = 1,$ $B = A^2C$
Octahedral (O)	$A = \exp i\frac{2\pi}{4} J_3,$ $B = \exp i\frac{2\pi}{3\sqrt{3}}(J_1 + J_2 + J_3)$	$A^4 = B^3 = C^2 = 1$
Icosahedral (I)	$A = \exp i\frac{2\pi}{5}\frac{\sigma J_1 + J_3}{\sqrt{2+\sigma}},$ $B = \exp i\frac{2\pi}{3\sqrt{3}}(-\sigma J_1 + \tau J_3)$	$A^5 = B^3 = C^2 = 1$

Table 2.3: The generators and generation relation of the polyhedral subgroup of SO(3)

The irreducible representations of $SO(3)$ are all real; up to an equivalence, there is only one such representation for each odd dimension $2j + 1$, where j is the angular momentum. An arbitrary group element of $SO(3)$ can be written as e^{iwJ} where J are the usual $(2j+1)(2j+1)$matrix representation. The matrix element of J are calculated from the relations

$$\begin{aligned} J_3 \left|jm\right\rangle &= m \left|jm\right\rangle \\ J_\pm \left|jm\right\rangle &= \sqrt{(j \mp m)(j \pm m + 1)} \left|j, m \pm 1\right\rangle \end{aligned} \tag{2.25}$$

where $|jm\rangle$ is the basis vectors of the $(2j + 1)$ dimensional irreducible representation of $SO(3)$, when j takes the values $0, 1/2, 1, 3/2...$ The generators and generator relation are summarized in the Table 2.3. Where $C = AB$, $Z = 1$, $\tau = \frac{1}{2}(1 + \sqrt{5})$, $\sigma = \frac{1}{2}(1 - \sqrt{5})$. Generation matrix of the each groups can be computed easily by the mathematica program which is given in the Appendix A.

2.8.2 Unitary Group

The irreducible representations of SO(3) are appropriate for describing the degeneracies of states of quantum mechanical systems which have rotational symmetry in three dimensions. But there are many systems must be supplemented by operations on internal degrees of freedom which have no classical analogue. For example, the Stern- Gerlach experiment showed that electrons are endowed with an internal degree of freedom called spin which has the properties of an angular momentum. The two spin states are therefore inconsistent with the dimensionless of the irreducible representations of SO(3), so another group SU(2) must be used to describe these states.

Consider a general complex transformation in two dimensions a $SU(2)$ group

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{2.26}$$

where $a,\ b,\ c,\ and\ d$ are complex numbers and hence transformation matrix involves eight parameters. Suppose we require the quantity $|x|\ ^2 + |y|^2$ to be invariant of such a transformation. Then,

$$|x|^2 + |y|^2 = |ax + by|^2 + |cx + dy|^2 \tag{2.27}$$

Since x and y are independent variables, this invariance necessitates setting the following conditions on the matrix elements

$$|a|^2 + |c|^2 = 1,\ |b|^2 + |d|^2 = 1,\quad ab^* + cd^* = 0 \tag{2.28}$$

These four conditions means that the original eight free parameters are reduced to four. By using Eq. (2.28), it can be deduced that the most general unitary matrix of order two involving four real parameters can be expressed in the form

$$\begin{pmatrix} \cos\theta e^{i\alpha} & \sin\theta e^{i\gamma} \\ -\sin\theta e^{i(\beta-\gamma)} & \cos\theta e^{i(\beta-\alpha)} \end{pmatrix} \tag{2.29}$$

whose determinant $\exp(i\beta)$. Here $\alpha,\ \beta, \gamma\ and\ \theta$ are the four real parameters. These transformations are analogous to orthogonal transformations of real coordinates and orthogonal transformation are also unitary. The group comprised of unitary matrices is denoted by U(2) and by U(N) for the N dimensional case.

In additions to the conditions, we require that the determinant of the transformation is unity, the transformation matrix must have the form

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix},\quad |a|^2 + |b|^2 = 1 \tag{2.30}$$

There are now three free parameters and the group of these matrices is denoted by special unitary group SU(2).

2.9 Jahn Teller Effect

Vibronic interactions effects constitute a new field of investigation in the physics and chemistry of molecules and crystals that combines all the phenomena and laws originating from the mixing of different electronic states by nuclear displacements. This field is based on a new concept which goes beyond the separate descriptions of electronic and nuclear motions. Publications on this topic appear under the title of the JT effect. The JT effect is over a sixty years old, and numerous different approaches have been taken in the analysis of the vibronic structure of the JT active molecules and providing a general approach to understanding the properties of molecules and crystals and their origins.

As it is well known, the fundamental laws of electronic and nuclear motions determining the structure and properties of molecules and crystals were revealed after the discovery of quantum mechanics. Because of mathematical difficulties encountered in the quantum mechanical description of polyatomic system, several essential approximation are usually employed in the solution of the appropriate Schrödinger equation, and among them the adiabatic or Born-Oppenheimer approximation is the most important. This approximation is based on difference in the masses of electrons and nuclei; due to this difference, for every position of the nuclei at any instant a stationary distribution of the electrons is attained. Without the adiabatic approximation the notation of the spatial structure becomes uncertain.

There are a number of physical phenomena which depend for their existence on the interplay between the two types of motion, the ionic electronic. Examples of these are the relaxation of electronic spins in a lattice, the high temperature electrical resistance of metals, superconductivity, ultrasonic attenuation, etc., in extended systems and some less spectacular but nevertheless important phenomena in localized systems. By localized systems we mean entities composed of an atom and a few of its close neighbors in a solid, such that some physical event is confined to these entities. Small or medium sized molecules are of course also localized systems. Then we know that phenomena like ligands field transitions in paramagnetic complexes or singlet absorptions in some hydrocarbons very frequently take place thanks to the coupling in localized systems the vibrations of the ions and the trajectory of the electrons. This coupling and the effects following from it are often called vibronic. This term is more commonly used for localized systems than in the solid state proper, where although the vibronic coupling is vital for existence of the phenomenon, there are a number of other effects which steal the limelight from the vibronic coupling. Another term which is frequently used for vibronic coupling is the breakdown of the Born-Oppenheimer approximation. This owes its origin to the circumstance that there are terms in the Hamiltonian H of the system which are neglected in that approximation but which re enter in vibronic effects. Frequently it is possible to explain the experimental data by regarding the vibronic coupling as small. One includes then the lowest order correction to the Born-Oppenheimer treatment, namely the term this term perturbationaly. In second order perturbation theory we should except an energy lowering of the order of $\kappa^2/\Delta E$, where ΔE is a characteristic energy difference between two states which are admixed by the linear term. As regards κ, this is simply meant to be a measure of the strength of the linear coupling, having dimensions of energy. In words, κ is the reduced matrix element of the linear coupling term, in which the vibrational coordinates have the amplitude of the zero point motion. To obtain a pure number which is a representative of the magnitude of the vibronic coupling we may divide $\kappa^2/\Delta E$ by an energy associated with the motion of either the heavy particles, the ions, or the light particles, the electrons. Since, however, our object is to find out when the perturbation approach breaks down, it is more pertinent to divide by the smaller of these quantities, by $\hbar\omega$ say, which is the energy quantum of a vibration involved in the coupling.

$$S^{'} = \frac{\kappa^2}{\hbar\omega\Delta E} \tag{2.31}$$

Characteristically, the magnitudes of κ and $\hbar\omega$ are similar, but there may be in exceptional cases fluctuations by a few orders of magnitude either way. As regards ΔE three cases arise,

1. When ΔE is an energy difference between electronic states, and this is large compared to either κ or $\hbar\omega$. Then the perturbational approach is justified, since even the lowest, second order perturbation alters the energy by only a small fraction of the whole.

2. When ΔE is an electronic energy difference which is however, in a rather uncharacteristic way, of the order of or smaller than κ. Then the ratio in equation Eq. (2.31) is of the order of unity or larger. It is an elementary to conclude that perturbation theory has to be abandoned and an exact solution of at least part of the vibronic problem is necessary.

3.When κ denotes the matrix elements between degenerate electronic states then the electronic part in ΔE is zero, by definition. Nevertheless, ΔE does not vanish but is one vibrational quantum since κ arises from a term in the Hamiltonian which is linear in a vibrational coordinate. The ratio $S^{'}$ in equation Eq. (2.31) will now be made precise by specifying the vibrational quantum $\hbar\omega$ and also by appending a number ν^{-1}which varies from each interaction i.e.,.$\nu = 4$ for $E \otimes \beta$, $\nu = 8$ for $E \otimes \epsilon$. The instead of equation Eq. (2.31)

$$\frac{1}{\nu}\frac{\kappa^2}{(\hbar\omega)^2} \equiv \frac{E_{JT}}{\hbar\omega} \equiv S \tag{2.32}$$

Here E_{JT} is the JT stabilization energy that for any molecular system whose electronic state is degenerate there is at least one linear term in the Hamiltonian such that κ is nonzero and consequently $E_{JT} \neq 0$.

From our earlier estimates of the relative magnitudes of κ and $\hbar\omega$ we now see that $E_{JT}/\hbar\omega$ can be small, of order of unity or large. There are two cases, which are the regimes for the operation of the JT effect. The case when $E_{JT}/\hbar\omega \gg 1$ is often called the strong coupling limit. In this case, frequently referred to as the static JT effect. This case, JT distortion is large it will result in a wavefunction localized around the minimum of the resulting potential energy surface, which occurs at the other then the symmetrical nuclear configuration. The vibronic and spin vibronic eigenvalues and eigenfunctions can be calculated much as for any other asymmetric molecule. Static effects can be seen in crystal structure, in spin resonance, in nuclear magnetic resonance, or in the Mössbauer effect. Such distortion also may be stabilized by effects such as strains in a crystals. A rather more interesting case is the weak coupling case $E_{JT}/\hbar\omega \ll 1$ and what is called dynamic JT effect. The result of the weak coupling case can always be obtained perturbationally, so that this case does not belong to the real of the JT effect which is essentially a non perturbational phenomenon.

The characteristic effect of vibronic coupling on electrically degenerate states by the following:

1.The electronic degeneracy is replaced by a vibronic degeneracy of the same type which possesses qualitatively (i.e. symmetry-wise) similar and quantitatively different electronic and vibrational properties from those of the vibronically uncoupled system.

2. Vibronically strongly coupled systems possess an extraordinarily great tendency to undergo distortion when stressed in some favorable direction. The stress may be applied externally or may be due to some internal irregularity in the lattice.

3. In the limit of strong coupling, the distorted state, which comes about owing to the stress, displays a considerable stability with respect to transitions between equivalent distorted configurations. The transitions may be of two kinds: real transitions (reorientations) caused by time dependent forces or strains, and virtual transitions (a term proper to quantum mechanics) which means the admixture into the state localized in one distorted configuration state localized in a second configuration. The rates of both transitions are reduced by the JT effect, as a result of which the distortion becomes more or less static.

The adjective static has been given in the past to the strong JT effect. We understand now that a static situation may come about by the characteristic (2) and (3). However, as a consequence of the terminology the strong JT effect has been regarded as equivalent to or even synonymous with a distorted configuration. However, a distorted situations amounts to a reduction of the symmetry of the systems and this can not occur as a result of internal interaction but only presence of a low symmetry external field.

2.10 Group Theoretical Approach to the Jahn Teller Systems

Let us formulate the JT theorem as follows. For all possible molecules, except linear ones, and for all degenerate terms $\overline{\Gamma}$, except the two fold Kramers degeneracy, there are nuclear displacement q_Γ for which the matrix elements $\left\langle \Psi_{\overline{\Gamma}}(r) \left| V_\Gamma(r) \right| \Psi_{\overline{\Gamma}_2}(r) \right\rangle$ are non zero. Here, $V_\Gamma(r)$ is the operator of the linear vibronic coupling to q_Γ and the $\Psi_{\overline{\Gamma}}(r)$ are electronic wave functions of the degenerate electronic term $\overline{\Gamma}$. Kramers degeneracy is determined by the symmetry with respect to the time reversal. This symmetry cannot be destroyed by any type of nuclear configuration distortion. Kramers degeneracy cannot be removed by nuclear displacements; it remains over the whole range of q_Γ values. For the matrix elements $\left\langle \Psi_{\overline{\Gamma}}(r) \left| V_\Gamma(r) \right| \Psi_{\overline{\Gamma}_2}(r) \right\rangle$ to be nonzero it is necessary that the expansion

$$\left[\overline{\Gamma}^2\right] = \sum_{i=1}^{k} n_i \Gamma_i \tag{2.33}$$

contains one of the low symmetry representation Γ of the full vibrational representation. In Eq. (2.33) all the irreducible representations of the group G_0 are labelled by i, Γ_1 is the totally symmetric representation, k is the number of different irreducible representations of the group G_0, equal to number of classes, and n_i is the coefficient of Γ_i in $\left[\overline{\Gamma}^2\right]$:

$$n_i = \frac{1}{g_0} \sum_{G_0} \left[\chi^2(G)\right] \chi_i(G) \tag{2.34}$$

Here g_0 is the order of the group G_0, $[\chi^2(G)]$ is the character of the symmetrized (or anti symmetrized , for double group representation) square of the representation $\overline{\Gamma}$, and $\chi_i(G)$ is the character of representation Γ_i. All the characters are real due to the fact that the representations of the group G_0 are real or can be made real.

For polyatamic systems possessing orbital degeneracy the reference symmetry group G_0 has at least one $n-fold$ rotational axis C_n or one axis of rotation reflection S_n with $n \geq 3$. This means that among the transitive set of atoms of the molecule under consideration there is at least one which contains s atoms that do not lie on the symmetry axis C_n or S_n and $s \geq 3$.Let us assume that G_0 is a point group, and consider the displacement of one of the atoms of this transitive set along its position vector with respect to the center of the system. Under the symmetry operations of the group G_0 this displacement transforms into other equivalent displacements generating the basis of some, in general, reducible representation Γ_D. Since any operation G_0 which changes the position of the given nucleus transforms its displacements of another equivalent nucleus (from the remaining $s-1$ ones), and displacements of the different nuclei are linearly independent, the dimension of the representation Γ_D is s.In the case of the three and more equivalent atoms the radial displacements $u_1, u_2, ...$forming the basis of Γ_D cannot produce rotations of the system as a whole, but these displacements contain, in most cases, degrees of freedom which remove the degeneracy. Although the representation Γ_D contains also translational degrees of freedom (in addition to vibrational ones) these, as shown below. The expansion for Γ_D is

$$\Gamma_D = \sum_{i=1}^{k} m_i \Gamma_i \tag{2.35}$$

It follows from Eq. (2.35) that for any element G from G_0

$$\chi_D(G) = \sum_{i=1}^{k} m_i \chi_i(G) \tag{2.36}$$

Multiplying Eq. (2.34) by m_i,summing over i, and using Eq. (2.36) we have

$$\sum_{i=1}^{k} n_i m_i = \frac{1}{g_0} \sum_{G_0} \left[\chi^2(G)\right] \chi_D(G) \tag{2.37}$$

or, separating the term $n_1 m_1$, we obtain

$$\sum_{i=2}^{k} n_i m_i = \frac{1}{g_0} \sum_{G_0} \left[\chi^2(G)\right] \chi_D(G) - n_1 m_1 \tag{2.38}$$

The numbers n_i and m_i, being coefficients of Γ_i from G_0 in the reducible representations $\left[\overline{\Gamma}^2\right]$ and Γ_D,respectively, are either positive integers or zero, and therefore the sum on the left-hand side of Eq. (2.38) is also either positive or zero. The latter case is possible if the low symmetric representations of the expansion Eq. (2.33) are not present in the expansion Eq. (2.35).

The fact that this sum is positive means that there are radial displacements which remove the degeneracy in first-order perturbation theory. Since $\Gamma_D$belongs to the full vibrational representation, the JT theorem will be proved if one proves the inequality

$$\frac{1}{g_0} \sum_{G_0} \left[\chi^2(G)\right] \chi_D(G) > n_1 m_1 \tag{2.39}$$

For all the point groups the symmetrized square of the irreducible representation $\left[\overline{\Gamma}^2\right]$ contains the totally symmetric representation Γ_1 only once. This means that $n_1 = 1$. Therefore,

$$\frac{1}{g_0} \sum_{G_0} \left[\chi^2(G)\right] \chi_D(G) > m_1 \tag{2.40}$$

It follows from Eq. (2.35) and from the fact that the Γ_i are real that

$$m_1 = \frac{1}{g_0} \sum_{G_0} \chi_D(G)\chi_1(G) \tag{2.41}$$

and, since $\chi_1(G) = 1$ for all the elements G of the group $G_{0,}$

$$m_1 = \frac{1}{g_0} \sum_{G_0} \chi_D(G) \tag{2.42}$$

Consider the representation Γ_D, in general , operation G from G_0 transforms each of the s displacements u_i into a linear combination as follows:

$$Gu_i = \sum_{J=1}^{s} G_{ji}u_i$$

The set of coefficients G_{ji} forms the matrix of the representation Γ_D. On the other hand, the symmetry operation over the radial displacements just interchanges their positions, and hence $G_{ji} = \delta(u_j, Gu_i)$, where $\delta(x, y)$ is the Kronecker symbol $[\delta(x, y) = 0 \ for \ x \neq y, \ and \ \delta(x, y) = 1 \ for \ x = y]$. Therefore

$$\chi_D(G) = \sum_{i=1}^{s} G_{ii} = \sum_{i=1}^{s} \delta(u_i, Gu_i) \tag{2.43}$$

Consider now the right-hand side of Eq. (2.42) . Using Eq. (2.43), it can be rewritten

$$m_1 = \frac{1}{g_0} \sum_{i=1}^{s} \sum_{G_0} \delta(u_i, Gu_i) \tag{2.44}$$

Among the elements of the group G_0 there are operations which leave the $i$the atom unmoved. The set of these operations H_i is a subgroup of the group G_0, while all the s sets of H_i with different i values form s classes:H_1, $H_2 = G_2H_1$, $H_3 = G_3H_1, ...$, where $G_2, G_3, ..$, are the elements of the group which transform the position of atom 1 to that of $2, 3, ..., s$, respectively. The order h of each of the isomorphous subgroups H_i is g_0/s since s is the index of the subgroup H_i in the group G_0.Taking into account the isomorphism of the subgroups H_i one can rewrite Eq. (2.44) as

$$m_1 = \frac{s}{g_0} \sum_{H_a} \delta(u_a, Gu_a) = \frac{s}{g_0} h = 1 \tag{2.45}$$

Here the index a correspond to any of the equivalent atoms of the transitive set under consideration.

Insert Eq. (2.43) into the left hand side of Eq. (2.42). Using an argument similar to that employed above we have

$$\frac{s}{g_0} \sum_{G_0} \left[\chi^2(G)\right] = \frac{1}{h} \sum_{H_a} \left[\chi^2(G)\right] \chi_1^{(a)}(G) \tag{2.46}$$

Here the notation $\chi_1^{(a)}(G)$ has been introduced for the characters of the irreducible representations $\Gamma_i^{(a)}$of the group $H_a, \Gamma_1^{(a)}$ being the totally symmetric representation. Taking account of Eq. (2.45) and Eq. (2.46), the inequality Eq. (2.42) can be rewritten

$$\frac{1}{h}\sum_{H_a}\left[\chi^2(G)\right]\chi_1^{(a)}(G) > 1 \tag{2.47}$$

Thus, if the symmetrized square $\left[\overline{\Gamma}^2\right]$ contains more than one totally symmetric representation $\Gamma_1^{(a)}$of the group H_a,then the left hand side of Eq. (2.38) is positive and the JT theorem is proved. There are two possible cases:

A)The representation $\overline{\Gamma}$ of the group G_0 is reducible in the subgroup H_a. In this case the expansion

$$\overline{\Gamma} = \sum_{j=1}^{k_a} \ell_j \Gamma_j^{(a)} \tag{2.48}$$

where k_a is the number of different irreducible representations of H_a, contains more than one term. It follows from the expansion Eq. (2.48) that

$$\overline{\Gamma} \otimes \overline{\Gamma} = \sum_{i=1}^{k_a}\sum_{j=1}^{k_a} \ell_i \ell_j \Gamma_i^{(a)} \otimes \Gamma_j^{(a)} \tag{2.49}$$

Hence in $\left[\overline{\Gamma}^2\right]$there are terms of the type

$$\sum_{i=1}^{k_a} \ell_i^2 [\Gamma_i^{(a)2}] \tag{2.50}$$

Each symmetrized square $[\Gamma_i^{(a)2}]$ contains one totally symmetric representation $\Gamma_1^{(a)}$, and taking into account that in Eq. (2.48) there is more than one term, we come to conclusion that the symmetrized square $\left[\overline{\Gamma}^2\right]$ contains more than one totally symmetric representation. Thus the inequality Eq. (2.47) and the JT theorem are proved for this case.

B) The representation $\overline{\Gamma}$ of the group G_0 is irreducible in the subgroup H_a. In this case the expansion Eq. (2.48) contains only one term, i.e., $\overline{\Gamma} = \Gamma_i^{(a)}$ and $\left[\overline{\Gamma}^2\right] = [\Gamma_i^{(a)2}]$ contains only one totally symmetric representation $\Gamma_1^{(a)}$.Consequently,

$$\frac{1}{h}\sum_{H_a}\left[\chi^2(G)\right]\chi_1^{(a)}(G) = 1 \tag{2.51}$$

and Eq. (2.47) is invalid. This means that within the space of the radial displacements there are no totally symmetric ones which remove the degeneracy of $\overline{\Gamma}$ in first order perturbation theory. In this case the remaining vibrational degrees of freedom have to be tried to see whether they contain displacements which remove the degeneracy in the first order. So far no general procedure for the solution of this problem has been worked out but, as shown below, there are only three cases belonging to the case B, and the problem for these cases can be solved by direct verification, as has been done by Jahn and Teller.

For situations belonging to case B, the subgroup H_a is either an axial group (for linear molecules) or its subgroups C_n or C_{nv}, $n \geq 3$. All these groups possess no irreducible representations of more than two dimensions, and hence the case B contains more than doubly degenerate terms. Several cases are possible here.

a) $\overline{\Gamma}$ is one of the two valued representations of a double group. The case of a two-dimensional representation corresponds to the Kramers degeneracy that cannot be removed by nuclear displacements. It is one of the exception to the JT theorem mentioned above. The double valued representations of higher dimensionality are not irreducible in the subgroup H_a, and therefore they belong to the case A considered above.

b) The molecule is linear. The representations E of the axial group are characterized by the quantum number L of the momentum describing the rotations around the axis of the molecule, and $L \geq 1$. In this case $[E_L^2] = A_1 + E_{2L}$, whereas all the nontotally symmetric nuclear displacement transform as E_L with $L = 1$. Thus, linear molecules are the second exception to the JT theorem.

c) The subgroup H_a coincides with C_n and C_{nv}. Here, in addition to the limitation $n \geq 3$ mentioned above, there is another one: $n \leq 5$. This is due to the fact that there are no regular polyhedra with equivalent apexes with one lying on the axis of symmetry C_n for $n > 5$. Hence there are three possible cases : $n = 3, 4, 5$. The fifth order axis is possible only for icosahedral groups I and I_h that have no other two-dimensional representations than Kramers double-valued ones.

The cases $n = 3, 4$ are present only for cubic groups $T, T_d, T_h O, O_h$. In all these groups the cases $n = 4$ belong to the case A, since their E representations are not irreducible, they decompose into two one dimensional representations. Thus, only the cases $n = 3$ remain, i.e.,the cases of an E term in a cubic molecule in which the equivalent atoms lie on the threefold axis of symmetry. This case is possible when four atoms of the transitive set occupy the apexes of a regular cube so as to form a regular tetrahedron. The direct verification of these two cases by means of the method of Jahn and Teller proves that there exist non totally symmetric vibrational degrees of freedom which remove the electronic degeneracy of the E term in first-order perturbation theory.

To prove the theorem as a whole, it remains to show that the inequality Eq.(2.42) is full filled due to the contribution of vibrational degrees of freedom to the representation Γ_D. The rotational degrees of freedom, as mentioned above, are excluded. To exclude translational degrees of freedom one can use symmetry considerations as follows. Since all the positions of a polyatomic systems in space are equivalent, we can state that its Hamiltonian is invariant with respect to translational, rotation or inversion of the space. This means that the fully symmetry group G_0 of the system contains the subgroup of continues three-dimensional orthogonal transformations including inversion. This statement becomes convincing when one passes to the center of mass coordinate system. If the additional operation of space inversion is taken into account, all the irreducible representations are also characterized by parity.

The translational displacement of the system is defined by a vector, i.e., all the translational degrees of freedom change sign on inversion of the space, and hence they belong to odd representations. The representation $\left[\overline{\Gamma}^2\right]$ is defined in the basis of products $\Psi^*_{\overline{\Gamma}_1}(r)\Psi_{\overline{\Gamma}_2}(r)$ which do not change sign on inversion, i.e., the expansion Eq. (2.33) contains only even representations. Thus the odd representations in the expansion Eq. (2.35) are not present in the left hand side of Eq. (2.37) and hence the translational degrees of freedom do not contribute to the inequality Eq. (2.42). The JT theorem is proved.

Now, we can obtain the $T \otimes T, \;\; E \otimes e, \; and \; E \otimes \beta$ JT Hamiltonian. First of all, we start with the $T \otimes t$ JT Hamiltonian. So we have concentrate of the character table of octahedral groups which is given by Table 2.4. For using the character table have been found symmetric and antisymmetric part of the three dimensional direct product for octahedral group. The matrix generator of the octahedral group is given by [82].

$$\begin{aligned} C_3 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad & C_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad (2.52) \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad & R = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \end{aligned}$$

The character of the symmetric and antisymmetric part of the direct product representation is

$$\begin{aligned} (T_1 \otimes T_1)_S &= A_1 + T_2 + E \qquad (2.53) \\ (T_1 \otimes T_1)_{AS} &= T_1 \end{aligned}$$

We concentrate only symmetric part of the three dimensional direct product of equation Eq. (2.53). The totally symmetric part of direct product of an irreducible representation of a finite group, which describes the properties of JT

O	E	$8C_3$	$6C_2'$	$6C_4$	$3C_2$
A_1	1	1	1	1	1
A_2	1	1	-1	-1	1
E	2	-1	0	0	2
T_1	3	0	-1	1	-1
T_2	3	0	1	-1	-1

Table 2.4: Character tables of octahedral group

surfaces,is written in the form of

$$[\Gamma^{\ell} \otimes \Gamma^{\ell}] = \Gamma^{\ell 1} \oplus \Gamma^{\ell 2} \oplus .... \oplus .\Gamma^{\ell n} \tag{2.54}$$

where ℓ is the angular momentum quantum number. Decomposition of $[\Gamma^{\ell} \otimes \Gamma^{\ell}]$ implies that the JT Hamiltonian can be written in the following way

$$H_{JT} = H^{\ell 1} + H^{\ell 2} + ... + H^{\ell n} \tag{2.55}$$

where H^{ℓ} is the JT Hamiltonian and it is invariant under the symmetry operations of corresponding finite group, for the $2\ell + 1$ dimensional representation. The decomposition of representation are in the Table 2.5 for different ℓ values.

So the JT Hamiltonian we consider has the following structure,

$$H_{JT} = H^0 + H^2 \tag{2.56}$$

This problem can be investigated by two parts. The first part is H^0 which vibration shift energies but it does not cause splitting and it can be solved exactly. Remaining vibrations substend the configuration space, which contains all distorted configuration, may be reached by JT active coordinates. As seen from Table 2.5, the second part of the Hamiltonian H^2 corresponds to the direct sum of $E \oplus T_2$ vibrational levels. The two parts of the Hamiltonian must be separately $T \otimes t$ and $T \otimes e$ couplings which are invariant under octahedral symmetry.

Now, we want to construct a polynomial function in electronic and nuclear configuration space, to examine symmetry properties of potential energy surface.

ℓ	Octahedral(O)
0	A_1
1	T_1
2	$E + T_2$
3	$E + T_1 + T_2$

Table 2.5: The representation of O with $\ell < 4$ are splitted by the octahedral point group

A polynomial function, which has been produced for this purpose, is in the form

$$P_{\ell m}(x,q)=\sum_{i,j=1}^{2\ell+1}\sum_{k=1}^{2m+1}F_{ijk}x_ix_jq_k \tag{2.57}$$

In this expression x_i and x_j correspond to electronic coordinates and q_k correspond to nuclear coordinates. F_{ijk} is force elements or coupling coefficients should be chosen appropriately for each coupling. For $T\otimes t$ coupling ℓ and m take value 1, for $T\otimes e$ case ℓ and m take value 1 and 1/2. The polynomial function can be obtained by using octahedral generator matrix. The double differential of $P_{11}(x,Q)$ with respect to electronic coordinates x_i and x_j produce linear JT interaction matrix. In general we can write

$$(B_m)_{ij}=\frac{\partial^2 P_{2m}}{\partial x_i \partial x_j} \tag{2.58}$$

The equation Eq. (2.57) is solved for F_{ijk}. The double differentiation of $P_{\ell m}(x,q)$ with respect to electronic coordinates gives JT interaction matrix for $T\otimes t$ coupling as in the form

$$JT_1=\begin{pmatrix} 0 & q_3 & q_2 \\ q_3 & 0 & q_1 \\ q_2 & q_1 & 0 \end{pmatrix} \tag{2.59}$$

For $T\otimes e$, JT interaction matrix is

$$JT_2=\frac{1}{2}\begin{pmatrix} -q_2 & 0 & 0 \\ 0 & -\sqrt{3}q_1+q_2 & 0 \\ 0 & 0 & \sqrt{3}q_1+q_2 \end{pmatrix} \tag{2.60}$$

and $T\otimes T$ JT Hamiltonian

$$H=H_0I-\frac{V_E}{2}JT_2-\frac{\sqrt{3}V_T}{2}JT_2 \tag{2.61}$$

$$H_0=-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}+\frac{\partial^2}{\partial q_3^2}+\frac{\partial^2}{\partial \varepsilon^2}+\frac{\partial^2}{\partial \xi^2}\right)+\frac{1}{2}\mu\omega_E^2\left(\varepsilon^2+\xi^2\right)+\frac{1}{2}\mu\omega_T^2\left(q_1^2+q_2^2+q_3^2\right) \tag{2.62}$$

The JT interaction matrices for two fold $E\otimes E$ coupling system requires the inclusion in the theory of spin-orbit interaction between states. The symmetric part of the direct product of two fold degenerate states is in the form

$$[E\otimes E]=A_1+E \tag{2.63}$$

In here, also the first part of the direct product representation does not cause splitting just shift the energies. Then Hamiltonian reduced $E\otimes\epsilon$ form which is

D_4	E	$2C_4$	C_2	$2C_2^{'}$	$2C_2^{''}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Table 2.6: Character table of D_4 group

invariant under the octahedral symmetry. The matrix generators of its Hamiltonian is

$$C_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad C_3 = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix} \tag{2.64}$$

JT interaction matrix can be obtained by applying the same procedure and it is given by

$$JT_3 = \begin{pmatrix} -q_1 & q_2 \\ q_2 & q_1 \end{pmatrix} \tag{2.65}$$

and $E \otimes \epsilon$ JT Hamiltonian is

$$H = H_0^{'} I - \frac{1}{2}\kappa JT_3 \tag{2.66}$$

$$H_0^{'} = \frac{1}{2}\hbar\omega\left(\frac{d^2}{dq_1^2} + \frac{d^2}{dq_2^2} + q_1^2 + q_2^2\right) \tag{2.67}$$

The $E \otimes \beta$ Hamiltonian is invariant under the D_4 group. Dihedral group includes one and two dimensional representation and its character table is given by Table 2.6.

The symmetric part of the direct product of $E \otimes E$ coupling is

$$[E \otimes E] = A_1 + B_1 + B_2 \tag{2.68}$$

This interaction can be examined three parts which are $E \otimes a$, $E \otimes b_1$ and $E \otimes b_2$. Consider $E \otimes \beta$ ($E \otimes b_1$) coupling and its generators are given by

$$C_4 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad C_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}; \; C_4 = -1; \; C_2^{'} = 1 \tag{2.69}$$

Two dimensional matrix generators interact with the $E-$state, one dimensional matrix generators interact with B_1 states. After the all statements do it and we get $E \otimes \beta$ JT interaction matrix

$$JT_4 = \begin{pmatrix} -q & 0 \\ 0 & q \end{pmatrix} \tag{2.70}$$

and the $E \otimes \beta$ JT Hamiltonian

$$H = H_0^{''} I - \frac{1}{\sqrt{2}} \kappa q J T_4 \tag{2.71}$$

$$H_0^{''} = -\frac{1}{2} \hbar\omega \left(\frac{d^2}{dq^2} - q^2 \right) \tag{2.72}$$

The mathematica program given by Appendix B. JT interaction matrices can be computed by using this program.

CHAPTER 3

QUASI EXACTLY SOLVABLE PHYSICAL POTENTIALS

Quantum mechanical potentials are said to be QES if a finite part of the energy spectrum and associated eigenfunctions can be found exactly and closed form. QES systems can be classified using an algebraic approach in which the Hamiltonian is expressed in terms of the generators of a Lie algebra.

In this chapter, we have discussed quasi exact solvability and related to the Lie algebra. A set of the QES quantum mechanical potentials have been studied. Solutions of the Schrödinger equation for each potential have been determined and the eigenstates are expressed in terms of the orthogonal polynomials. We have obtained the generation and solution of the QES Pöschl-Teller like potential. Then the QES generalized Pöschl-Teller potential and QES PT symmetric Scarf-like potentials are obtained from the QES Pöschl-Teller like potential by replacing coordinate $x \rightarrow x/2$, and $x \rightarrow x/2 + i\pi/4$ respectively. Transformations of QES Pöschl-Teller like potential to the sextic oscillator potential and to the QES PT symmetric anharmonic oscillator potential are discussed. Secondly, the QES Eckart like potential is constructed by using the $s\ell(2, R)$ algebra and then we transform it to the QES Hultén like and the QES Rosen-Morse like potentials by a linear transformation on the coordinate. The relation between the QES Eckart like potential and the QES Coulomb like potential is discussed. We also show that a specific form of the QES Coulomb like potential corresponds to the Coulomb correlation problem for a system of two electrons in an external oscillator potential.

3.1 Quasi Exact Solvability

In the quantum mechanics, the state of a system is characterized by a wavefunction ψ which is the solution of the second order linear partial differential

Schrödinger equation

$$H\psi = E\psi \tag{3.1}$$

where H is a second order linear differential operator, known as Schrödinger operator and E is the eigenvalue of the equation. The operator H may correspond to any physical observable such as position, momentum, angular momentum, and so on. The wave function ψ can be interpreted as the probability amplitude of the particle's position. For a system consisting of only one particle in three dimensions interacting with a potential $V(x, y, z)$ the form of H is,

$$H = -\nabla^2 + V(x, y, z) = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z) \tag{3.2}$$

where $\hbar^2/2m = 1$. In general the Schrödinger equation cannot be solved exactly to obtain the whole spectrum of eigenvalues except for a small number of potentials, i.e., the harmonic oscillator and the hydrogen atom potentials. For most potentials, the equation must be solved numerically to obtain the spectrum. However recent research has discovered an intermediate class of potentials, in which it is possible to obtain a finite part of the eigenvalue spectrum algebraically. For this reason they are named to QES potentials. These potentials are characterized by the fact that for them, the operator H can be expressed a second or higher degree polynomial in the generators of a finite dimensional Lie algebra that possesses a finite dimensional representation space.

In order to describe the general form of a QES problem, we begin with a finite dimensional Lie algebra g spanned by r linearly independent first order differential operators

$$T_a = \sum_{i=1}^{n} \xi_{ai}(x)\frac{\partial}{\partial x_i} + \eta_a(x), \quad a = 1, \ldots, r \tag{3.3}$$

whose coefficients ξ_{ai}, η_a are smooth functions of x. The Lie algebra assumption requires that the commutator between two such operators can be written as a linear combination of the operators

$$[T_a, T_b] = T_aT_b - T_bT_a = \sum_c C_{ab}T_c \tag{3.4}$$

where C_{ab} are the structure constants of the Lie algebra.

A differential operator is said to be Lie algebraic means that, it can be expressed as a polynomial in the operators T_a. In particular, a second order differential operator is Lie algebraic then, it can be written as a quadratic combination

$$H = \sum_{a,b} c_{ab}T_aT_b + \sum_a c_aT_a + c_0 \tag{3.5}$$

for certain constants $c_{ab},\ c_a,\ c_0$.

There are additional constraint on the Lie algebra for condition of QES. A Lie algebra of first order differential operators g will be called QES if it possesses a finite dimensional representation space (or module) $N \subset C^{\infty}$ consisting of smooth functions; this means that if $\psi \in N$ and $T_a \in g$,then $T_a(\psi) \in N$. A differential operator H is called QES if it lies in the universal enveloping algebra of a QES Lie algebra of differential operators. Clearly, the space N is an invariant space for the Hamiltonian H, *i.e.*, $H(N) \subset N$, and hence H restricts to a linear matrix operator on N. We will call the eigenvalues and corresponding eigenfunctions for the restriction $H \mid N$ algebraic since they can be computed by algebraic methods for matrix eigenvalue problems.

It is of great interest to know when a given differential operator is in Lie algebraic or QES form. There is a direct test on the operator in question. Consequently, the best approach to this problem is to effect a complete classification of such operators under an appropriate notion of equivalence. So as to classify Lie algebras of differential operators, and hence Lie algebraic and QES Schrödinger operators, we need to precisely specify the allowable changes of variables.

Two differential operators are equivalent if they can be mapped into each other by a combination of change of independent variable,

$$x' = \varphi(x) \tag{3.6}$$

and similarity transformation

$$H' = e^{\sigma(x)} H e^{-\sigma(x)} \tag{3.7}$$

This transformations have two key properties. First, they respect the commutator between differential operators, and therefore preserve their Lie algebra structure. Second, they preserve the spectral problem associated with the differential operator H, so that if $\psi(x)$ is an eigenfunction of H with eigenvalue E, then the transformed function

$$\psi'(x') = e^{\sigma(x)} \psi(x) \tag{3.8}$$

is the corresponding eigenfunction of H' having the same eigenvalue. Therefore this notion of equivalence is completely adapted to the problem of classifying QES Schrödinger operators.

3.2 QES Pöschl-Teller Like Potential

The QES Pöschl Teller like potential can be generated by several methods [83, 84, 85]. One method is to use the Lie algebraic technique. The linear and bilinear combinations of the operators of the $sl(2,R)$ Lie algebra with the standart realization [83, 34, 85], leads to the following differential equation,

$$z(1-z)\frac{d^2\Re_j(z)}{dz^2}+(L+\frac{3}{2}+z\left(B+4j-qA^2z\right))\frac{d\Re_j(z)}{dz}-\left(\lambda-2jqA^2z\right)\Re_j(z)=0 \tag{3.9}$$

where L, q, A and λ are constants and $j=0,1/2,1,....$ The differential equation Eq. (3.9) becomes QES, provided B is taken as:

$$B=-\frac{1}{2}\left(2L+8j+5-\sqrt{1+4A(A+1+(2L+8j+5)qA}\right) \tag{3.10}$$

Moreover, it becomes exactly solvable with the condition $q=0$. The function $\Re_j(z)$ is a polynomial of degree $2j$. In order to obtain the QES quantum mechanical potentials we can transform Eq. (3.9) in the form of Schrödinger equation by introducing the variable

$$z=-\sinh^2\alpha x \tag{3.11}$$

Now we define the wave function as follows:

$$\psi(x)=(\cosh\alpha x)^{qA^2-B-L-4j-2}(\sinh\alpha x)^{1+L}e^{-\frac{1}{4}qA^2\cosh 2\alpha x}\Re_j(-\sinh^2\alpha x) \tag{3.12}$$

Substituting Eq. (3.11) and Eq. (3.12) in Eq. (3.9) we obtain the Schrödinger equation with ($\hbar=2m=1$):

$$-\frac{d^2\psi(x)}{dx^2}+(V(x)-E)\psi(x)=0 \tag{3.13}$$

where the potential $V(x)$ is given by

$$\begin{aligned} V(x) &= L(L+1)\alpha^2\csc h^2\alpha x-A(A+1)\alpha^2\sec h^2\alpha x+ \\ &\quad q(2BA^2\sin h^2\alpha x+qA^4\sin h^4\alpha x)\alpha^2\tan h^2\alpha x \end{aligned} \tag{3.14}$$

The eigenvalues of energy are given by the expression

$$E=\left[-(L-A+2m+1)^2+(L-A+B+4j+2)(2L+4m+3)+4\lambda\right]\alpha^2 \tag{3.15}$$

One can check that for $q=0$ the potential given in Eq. (3.14) is exactly solvable Pöschl -Teller potential and the eigenstates of the Schrödinger equation can be expressed in terms of the Jacobi polynomials. It is easy to see that the equalities $B=A-L-4j-2$ and $\lambda=4m(L-M+m+1)$ hold when $q=0$. Then the eigenvalues of the Schrödinger equation take the form

$$E=-\alpha^2\left[(L-A+2m+1)^2+4m(L-M+m+1)\right] \tag{3.16}$$

Next task is now to determine the eigenfunctions of the QES Schrödinger equation Eq. (3.13). Therefore, we search for a solution of Eq. (3.9) by substituting the polynomial

$$\Re_j(z=\sum_{m=0}^{2j}a_m z^m \tag{3.17}$$

which leads to an expression for the coefficients a_m

$$a_m = \frac{(4qA^2)^m (2j)!(2L+1)!(L+m)!}{2m!(2j-m)!(2L+2m+1)!} P_m(\lambda). \tag{3.18}$$

The polynomial $P_m(\lambda)$ satisfies the following three term recurrence relation

$$\begin{aligned} 2(2j-m)qA^2 P_{m+1}(\lambda) + m(2L+2m+1)P_{m-1}(\lambda) \quad & - \\ 2(\lambda + m(B+4j-m+1))P_m(\lambda) = 0 & \end{aligned} \tag{3.19}$$

with initial condition $P_0(\lambda) = 1$. The polynomial $P_m(\lambda)$ vanishes for $m \geq 2j+1$ and the roots of $P_{2j+1}(\lambda) = 0$ corresponds to the λ eigenvalues of the Schrödinger equation Eq. (3.13). The first three of these polynomials are given by

$$\begin{aligned} P_1 &= \lambda \\ P_2 &= \lambda^2 - (B-4j)\lambda - j(2L+3)qA^2 \qquad (3.20) \\ P_3 &= \lambda^3 - 4(9Bj-1)\lambda^2 + [2B(B-2) + 16j(B+2j-1) + (2L - j(6L+13)+5)qA^2]\lambda \\ &\quad +2j(2L+3)(B+4j-2)qA^2 \end{aligned}$$

The recurrence relation Eq. (3.19) can also be put into matrix form. The diagonal matrix characterizes the system,

$$\begin{pmatrix} \beta_0 - 4\lambda & \mu_{2j} & & & \\ \gamma_1 & \beta_1 - 4\lambda & \mu_{2j-1} & & \\ & .. & .. & .. & \\ & & \gamma_{2j-1} & \beta_{2j-1} - 4\lambda & \mu_1 \\ & & & \gamma_{2j} & \beta_{2j} - 4\lambda \end{pmatrix} \begin{pmatrix} P_0 \\ P_1 \\ . \\ P_{2j-1} \\ P_{2j} \end{pmatrix} = 0 \tag{3.21}$$

where the parameters in matrix element are given by

$$\gamma_m = 2m(2L+2m+1), \quad \mu_m = 4mqA^2, \; \textit{and} \; \; \beta_m = 4m(B+4j-m+1) \tag{3.22}$$

Analytical solutions of the recurrence relation Eq. (3.19) and the determinant of Eq. (3.21) for λ are available only for the first few values of $j \leq 2$. For $j > 2$ the solutions become numerical, and the numerical errors grow rapidly. The solutions take simpler forms and the precision becomes better for $A >> q$, in which case B takes the value

$$B \approx 2(\lambda + m(L - A + m + 1)) - m(2L + 8j + 5)qA \tag{3.23}$$

In this approximation the QES Pöschl-Teller like potential in Eq. (3.15) becomes comparable with the perturbed Pöschl-Teller potential, a specific form of which has been studied in [86].

3.3 Generalized QES Pöschl-Teller Potential

In this section we present a procedure that relates the QES Pöschl-Teller like potential to the generalized QES Pöschl-Teller potential. It is amusing to observe that when the coordinate x of the Pöschl-Teller like potential is replaced by $x \to x/2$, the QES Pöschl-Teller like potential transforms to the generalized QES Pöschl-Teller potential

$$\begin{aligned} V(x) &= \frac{\alpha^2}{2}\left[(L(L+1)+A(A+1)\csc h^2\alpha x+(L-A)(L+A+1)\coth\alpha x\csc h\alpha x\right] \\ &\quad +q(2BA^2\sinh^2\frac{\alpha x}{2}+qA^4\sinh^4\frac{\alpha x}{2})\alpha^2\tanh^2\frac{\alpha x}{2} \end{aligned} \tag{3.24}$$

Obviously when $q=0$ this potential reduces to the exactly solvable generalized Pöschl-Teller potential. The wave function corresponding to the solution of Eq. (3.13) with the potential of Eq. (3.24) now takes the form

$$\begin{aligned} \psi(x) &= \left(\cosh\frac{\alpha x}{2}\right)^{qA^2-B-L-4j-2}\left(\sinh\frac{\alpha x}{2}\right)^{1+L} \\ &\quad e^{-\frac{1}{4}qA^2\cosh\alpha x}\Re_j\left(-\sinh^2\frac{\alpha x}{2}\right) \end{aligned} \tag{3.25}$$

The corresponding energies are determined as

$$E^{'}=\frac{E}{4}+m(B+4j-m+1)\alpha^2 \tag{3.26}$$

where E is the eigenvalue of the Schrödinger equation with the QES Pöschl-Teller like potential given by Eq. (3.15). It is clear that the same recurrence relation in Eq. (3.19) for the polynomial $P_m(\lambda)$ holds true.

3.4 QES PT Symmetric Scarf Like Potential

It is interesting to observe that one can transform the QES Pöschl-Teller like potential to the PT symmetric QES Scarf like potential by replacing x by the complex variable

$$x \to \frac{x}{2}+\frac{i\pi}{4\alpha} \tag{3.27}$$

Then one obtains the following potential

$$\begin{aligned} V(x) &= -\frac{\alpha^2}{2}[L(L+1)+A(A+1))\sec h^2\alpha x+ \\ &\quad i(L-A)(L+A+1)\tanh\alpha x\sec h\alpha x] \\ &\quad +\frac{\alpha^2}{4}(2qBA^2\sinh^2\left(\frac{\alpha x}{2}+\frac{i\pi}{4}\right)+ \\ &\quad q^2A^4\sinh^4\left(\frac{\alpha x}{2}+\frac{i\pi}{4}\right))\tanh^2\left(\frac{\alpha x}{2}+\frac{i\pi}{4}\right) \end{aligned} \tag{3.28}$$

This is the QES form of the PT symmetric Scarf like potential which has not been discussed in the literature. The exactly solvable part of the potential has been discussed recently by Bagchi[87]. The energy eigenvalues are the same as in Eq. (3.26) obtained for the generalized QES Pöschl-Teller like potential. But the wave function now reads

$$\begin{aligned}\psi(x) &= \left(\frac{i+\tanh\alpha x}{i-\tanh\alpha x}\right)^{\frac{1}{2}\left(B+2L-qA^2+4j+3\right)}(\cosh\alpha x)^{\frac{1}{2}\left(qA^2-4j-B-1\right)}\times \\ &\quad e^{-\frac{i}{4}qA^2\sinh\alpha x}\Re_j\left(-\sinh\left(\frac{\alpha x}{2}+\frac{i\pi}{4}\right)\right)\end{aligned} \tag{3.29}$$

Here again the polynomial $P_m(\lambda)$ satisfies the same recurrence relation defined in Eq. (3.19).

The method described in this section in order to transform one type of potential to another type may be further generalized. The transformation $x \rightarrow ax+ib$,where a and b, are arbitrary real parameters, preserves the PT symmetry. The energy eigenvalues of the new potential involves further terms in addition to the scaled energy eigenvalues of the QES Pöschl-Teller like potential. The corresponding wave function is obtained from the former wave function of the Pöschl-Teller potential by replacing $x \rightarrow ax+ib$, and the polynomial $P_m(\lambda)$ obeys the same recurrence relation of Eq. (3.19). This transformation has been discussed in the literature [86] for the exactly solvable potentials.

3.5 The Sextic Oscıllator

In this section we discuss a method about the transformation of the QES Pöschle-Teller like potential to the sextic oscillator potential. The QES Pöschl-Teller like potential can be converted to the radial sextic oscillator potential by redefining the parameters and taking suitable limits while keeping the variable x intact. If we redefine the parameters in Eq. (3.14) and Eq. (3.15) by introducing

$$B=\frac{b}{\alpha^2},\quad A=\frac{a}{\alpha^2},\quad \lambda=\frac{\varepsilon-mb}{\alpha^2} \tag{3.30}$$

and taking the limit of the $(V(x)-E)$ term in the Schrödinger equation for $\alpha \rightarrow 0$ the Pöschl-Teller like potential transforms to the radial sextic harmonic oscillator potential,

$$V=\frac{L(L+1)}{x^2}+(b^2-(2L+8j+5)qa^2)x^2+2bqa^2x^4+q^2\alpha^4x^6 \tag{3.31}$$

The ground state wavefunction Eq. (3.12) takes the form

$$\psi(x)=x^{1+L}e^{-\frac{b}{2}x^2-\frac{q}{4}x^4} \tag{3.32}$$

and the energy eigenvalue is given by

$$E = 4\varepsilon + (2L+3)b \tag{3.33}$$

The general solutions of the Schrödinger equation with the sextic oscillator potential can be obtained by substituting into the Schrödinger equation Eq. (3.13)

$$\psi(x) = x^{1+L} e^{-\frac{b}{2}x^2 - \frac{q}{4}x^4} \Re_j(x^2) \tag{3.34}$$

By rearranging the terms one can obtain,

$$\Re_j(x^2) = \sum_{m=0}^{2j} \frac{(2j)!(2L+1)!(L+m)!}{2m!(2j-m)!(2L+1+2m)!} P_m(\varepsilon)(4qa^2x^2)^m \tag{3.35}$$

along with the recurrence relation satisfied by $P_m(\varepsilon)$

$$2(2j-m)qa^2 P_{m+1}(\varepsilon) + 2(\varepsilon - bm)P_m(\varepsilon) - m(2L+2m+1)P_{m-1}(\varepsilon) = 0 \tag{3.36}$$

The first four polynomials are given by

$$\begin{aligned}
P_1(\varepsilon) &= \varepsilon \\
P_2(\varepsilon) &= \varepsilon^2 - b\varepsilon - \frac{1}{2}\left(3+2L\right)qa^2 \\
P_3(\varepsilon) &= \varepsilon^3 - 3b\varepsilon^2 - 2(b^2 - 2(L+2))\varepsilon + 2b(3+2L)qa^2 \\
P_4(\varepsilon) &= \varepsilon^4 - 6b\varepsilon^3 + (11b^2 - 5(2L+5)qa^2\varepsilon^2 + 3b(-2b^2 + (10L+21)qa^2\varepsilon + \\
&\quad 9\left[-b^2(2L+3) + \frac{1}{4}\left(4L(5L+1)+21\right)q^2a^4\right]
\end{aligned} \tag{3.37}$$

They agree with the polynomials given in reference [88] and [89]. We have also compared our results with the numerical solutions obtained in the reference [90], for the potentials,

$$\begin{aligned}
V_1(x) &= x^2 + \frac{x^4}{2(7.625)^{3/2}} + \frac{x^6}{7442} \\
V_2(x) &= x^2 + \frac{x^4}{2(7.375)^{3/2}} + \frac{x^6}{6962} \\
V_3(x) &= x^2 + \frac{x^4}{2(7.125)^{3/2}} + \frac{x^6}{6498}
\end{aligned} \tag{3.38}$$

where we have obtained exactly the same results of [90], for the energy eigenvalues

$$E_1 = 2.897143, \quad E_2 = 5.891677, \quad \textit{and } E_3 = 8.991223 \tag{3.39}$$

corresponding to the potentials $V_1(x),\ V_2(x),\ \textit{and}\ \ V_3(x)$ respectively.

3.6 PT Symmetric Anharmonic Oscillator Potential

In order to transform the potential given in Eq. (3.28) to the PT symmetric anharmonic oscillator potential we substitute in the parameters in Eq. (3.26) and Eq. (3.28)

$$\begin{aligned} A &= \sqrt{17}\frac{qa^2}{\alpha^3} + \frac{7}{\sqrt{17}}\frac{b}{\alpha^2}, \quad L = \frac{1}{2}\left(3 - \sqrt{17} + \left(1 - \frac{7}{\sqrt{17}}\right)\frac{\alpha b}{qa^2}\right) \\ \lambda &= \frac{\varepsilon + 2jb}{\alpha^2} + \frac{4jq\alpha^2}{\alpha^3}, \ q \to \frac{4qa^2}{\alpha^3} - \frac{1}{17}\left(1 + \frac{7}{\sqrt{17}}\right)\frac{2b^2 + 17\ell qa^2}{qa^2\alpha} \end{aligned} \tag{3.40}$$

and taking the limit of the $(V(x) - E)$ given in Eq. (3.26) and Eq. (3.28) when $\alpha \to 0$, we obtain the PT symmetric anharmonic oscillator potential,

$$V = 2i(b\ell - (1+2j)qa^2)x + (b^2 - 2\ell qa^2)x^2 + 2iqba^2x^3 - q^2a^4x^4 \tag{3.41}$$

This leads to the energy eigenvalues,

$$E = \varepsilon + b(1+2j) + \ell^2 \tag{3.42}$$

The ground state wave function of the potential can be obtained from Eq. (3.29) by using the same limiting procedure as introduced in Eq. (3.40),

$$\psi(x) = e^{\left(-ix - \frac{1}{2}bx^2 - \frac{2i}{3}qA^2x^3\right)} \tag{3.43}$$

The wave function for any j can be obtained by letting

$$\psi(x) = e^{\left(-ix - \frac{1}{2}bx^2 - \frac{2i}{3}qA^2x^3\right)} \sum_{m=0}^{2j} a_m x^{2m} \tag{3.44}$$

Here we obtain a four term recurrence relation for the energy,

$$\begin{aligned} 2i(2j - m)qa^2 P_{m+1}(\varepsilon) + (\varepsilon - 2b(m-j))^2 P_m(\varepsilon) - \\ 2im\ell P_{m-1} + m(m-1)P_{m-2}(\varepsilon) = 0 \end{aligned} \tag{3.45}$$

The first four P_m is given by

$$\begin{aligned} P_1(\varepsilon) &= \varepsilon \\ P_2(\varepsilon) &= \varepsilon^2 - b^2 - 4qa^2\ell \\ P_3(\varepsilon) &= \varepsilon^3 - 4(b^2 - 4qa^2\ell)\varepsilon - 16q^2a^4 \\ P_4(\varepsilon) &= \varepsilon^4 - 10(b^2 - 4qa^2\ell)\varepsilon^2 - 96q^2a^4\varepsilon + 9(b^4 + 8qb^2a^2\ell + 16q^2a^4\ell^2) \end{aligned} \tag{3.46}$$

The result are in agreement with those given in [91].

3.7 QES Eckart Like Potential

The QES potentials have been constructed by employing a variety of approaches [21, 83, 85]. In this section we obtain the QES Eckart like potential, which can be generated by using the Lie algebraic method, widely used in the literature. Let us consider the second order differential equation which can be obtained by using linear and bilinear combinations of the operators of the $s\ell(2,R)$. The QES Eckart like potential given in this study can be obtained by transforming the following linear and bilinear combination of the operators of the $s\ell(2,R)$ Lie algebra,

$$\begin{aligned}&2J_-J_+ + 2J_-J_3 - (\lambda + 2(2L + j + 3))J_- + \lambda J_3 - qJ_+ + \\ &(\lambda(L + j + 1) + (2(L(L + 3) + 2j(L + 1 - A)\end{aligned} \tag{3.47}$$

in the form of Schrödinger equation. The generators of the Lie algebra satisfy the standard differential realization of the $s\ell(2,R)$[21, 83, 85], with standard realization,

$$\begin{aligned}&2z(1-z)\frac{d^2\Re_j(z)}{dz^2} + (4(jz - L - j - 1) + \lambda(z-1) + 2qz^2)\frac{d\Re_j(z)}{dz} + \\ &(\lambda(L+1) + 2L(L+3) - A + 4j(L - qz + 1) + 4)\Re_j(z)\end{aligned} \tag{3.48}$$

which possesses the polynomial solution. Here L, q, A *and* λ are constant, and $j = 0, 1/2, 1\ldots.$ The function $\Re_j(z)$ forms a basis function for the $s\ell(2,R)$ algebra and preserve the space of polynomials of order $2j$. The differential equation Eq. (3.48) is exactly solvable under the condition $q = 0$. In order to generate the QES quantum mechanical potentials, two step procedure can be employed to transform Eq.(3.48) into the Schrödinger equation. We introduce a new variable,

$$z = e^{-2\alpha x} \tag{3.49}$$

as well as define a new function,

$$\psi(x) = (e^{-2\alpha x} - 1)^{L-\frac{q}{2}}(1 - e^{2\alpha x})\times\exp\left(\frac{1}{2}\alpha x(4L + 4j + 2 + \lambda) - \frac{1}{2}qe^{-2\alpha x}\right)\Re_j(e^{-2\alpha x}) \tag{3.50}$$

to eliminate the first order differential term in Eq. (3.48). The equation is converted to the Schödinger equation

$$\frac{d^2\psi(x)}{dx^2} + (V(x) - E)\psi(x) = 0 \tag{3.51}$$

Here the potential $V(x)$ is in the form

$$\begin{aligned}V(x) &= [L(L+1)\alpha^2 \csc h^2\alpha x + A\alpha^2 \coth \alpha x + \\ &\quad \frac{q\alpha^2}{(e^{2\alpha x} - 1)^2}\left(qe^{-4\alpha x} + (\lambda - 4j)\,e^{-2\alpha x} - (4L - 4j + \lambda + 2)\right)\end{aligned} \tag{3.52}$$

The energy eigenvalues for this potential can be determined as

$$E = (A - (2L + \lambda/2 + 4j + 3)^2)\alpha^2 \tag{3.53}$$

If we choose $q = 0$ in Eq. (3.52), the remaining term is Eckart potential.

$$\lambda = \frac{A}{L + m + 1} - 2(L + 2j - m + 2) \tag{3.54}$$

then we obtain the exact solution of the Schrödinger equation where the eigenvalue Eq. (3.53) of the Schrödinger equation can be expressed in the closed form

$$E_e = \frac{\alpha^2}{4}\left(\left(\frac{A}{L + m + 1}\right)^2 + 4(L + m + 1)^2\right) \tag{3.55}$$

and the eigenfunctions can be expressed in terms of the Jacobi polynomials. As it was stated before, for the differential equation Eq. (3.48) to possess polynomial solutions for non negative integer and half integer values of j, $\Re_j(z)$ can be written as a polynomial of degree $2j$

$$\Re_j(z) = \sum_{m=0}^{2j} a_m z^m \tag{3.56}$$

The coefficient a_m is related to the parameters of the potential. Let us redefine the coefficient a_m such that the parameter λ factors out from the other parameters

$$a_m = f_m(L, A, q) P_m(\lambda) \tag{3.57}$$

The coefficient, $f_m(L, A, q)$ is independent of λ and plays the role of the normalization constant. After a straight forward calculation one can obtain a three-term recurrence relation for the polynomial $P_m(\lambda)$

$$\begin{aligned} &2q(2j - m)P_{m+1}(\lambda) - ((\lambda + 2(L + 2j - m + 2)) \\ &(L + m + 1) - A)P_m(\lambda) + m/4L + 4j - 2m + 6 + \lambda)P_{m-1}(\lambda) \end{aligned} \tag{3.58}$$

with the initial condition $P_0(\lambda) = 1$.The polynomial P_{2j+1} vanishes and the roots λ belong to the eigenvalues of the Schrödinger equation. Analytical solution of the recurrence relation Eq. (3.58), for λ, depends on the values of the parameters $A, L,$ *and* q. In general, for $j \geq 2$ the values of λ can be determined numerically.

3.8 QES Hultén Like Potential

In this section we discuss the transformation of QES Eckart like potential to the QES Hultén like potential, the exactly solvable form of which has been widely discussed in the literature [92, 93]. The QES Eckart like potential can be converted to the QES Hultén like potential by replacing $x \to x/2$. Under these conditions, we obtain QES Hultén like potential,

$$\begin{aligned} V(x) &= \frac{\alpha^2}{2}\left(2L(L+1)+A\right)\frac{e^{-\alpha x}}{1-e^{-\alpha x}} + L(L+1)A\left(\frac{\alpha e^{-\alpha x}}{1-e^{-\alpha x}}\right)^2 \\ &\quad + \frac{q\alpha^2}{4(e^{2\alpha x}-1)^2}\left(qe^{-2\alpha x} + (\lambda-4j)e^{-\alpha x} - (4L-4j+\lambda+2)\right) \end{aligned} \tag{3.59}$$

The energy values of the Schrödinger equation with QES Hultén like potential Eq. (3.59) is given by

$$E' = \frac{1}{4}\left(E_e + A\alpha^2\right) \tag{3.60}$$

where E is the energy eigenvalues of the Schrödinger equation with QES Eckart like potential. It is obvious that the corresponding eigenfunction is then given by

$$\psi_{HL}(x) = \psi(x/2) \tag{3.61}$$

where $\psi(x)$ is the wave function of the Schrödinger equation with the QES Eckart like potential. It obvious that the corresponding polynomial $P_m(\lambda)$ satisfies the same recurrence relation of Eq. (3.58). Under the conditions that $q = 0$ and λ takes the value of Eq. (3.54), the Hultén like potential is exactly solvable and eigenvalues of the Schrödinger equation read

$$E'_e = \frac{1}{4}\left(E_e + A\alpha^2\right) \tag{3.62}$$

where E_e given in Eq. (3.55).

3.9 QES Rosen-Morse Like Potential

The QES Eckart like potential can be transformed to the Rosen-Morse like potential by shifting the coordinate $x \to x + i\pi/4\alpha$. Then the corresponding potential is given by

$$\begin{aligned} V(x) &= \left[-L(L+1)\alpha^2 \sec h^2 \alpha x + A\alpha^2 \tan \alpha x\right] \\ &\quad + \frac{q\alpha^2}{(e^{2\alpha x}-1)^2}\left(qe^{-4\alpha x} + (\lambda-4j)e^{-2\alpha x} - (4L-4j+\lambda+2)\right) \end{aligned} \tag{3.63}$$

The energy eigenvalues are the same as in the QES Eckart like potential. The corresponding wave function is $\psi_{RM}(x) = \psi(-x)$. The polynomials in the coefficient of the eigenfunction of the QES Rosen-Morse like potential obey the same recurrence relation given in Eq. (3.58).

3.10 QES Coulomb Like Potential

The QES Eckart like potential Eq. (3.52) can be transformed to the QES Coulomb like potential by a suitable change of parameters. Let us redefine the parameters by

$$q \to \frac{q}{2\alpha^2}, \quad L \to \ell + \frac{q}{4\alpha^2}, \quad \lambda \to 2 + 4j + \frac{a+\varepsilon}{\alpha} - \frac{2q}{\alpha^2}, \quad A = \frac{a}{\alpha} - \frac{q\ell}{\alpha^2} + \frac{4aq}{\alpha^3} - \frac{3q^2}{8\alpha^4} \tag{3.64}$$

and substitute them in Eq. (3.52) and Eq. (3.53); when we take the limit of the $(V(x) - E)$, as $\alpha \to 0$, the potential is transformed to the perturbed Coulomb like potential,

$$V(x) = \frac{\ell(\ell+1)}{x^2} + \frac{a}{x} - q(\varepsilon + a)x + q^2x^2 \tag{3.65}$$

This relation indicates that the QES Eckart like potential and QES Coulomb like potential possesses similar behavior in a certain range of variable x. The ground state wave function of the perturbed Coulomb like potential is given by

$$\psi(x) = x^{\ell+1} \exp\left(\frac{1}{2}x(\varepsilon + a - qx)\right) \tag{3.66}$$

and the energy eigenvalue reads as

$$E = -\frac{(\varepsilon + a)^2}{4} + 2q\left(\ell + 2j + \frac{3}{2}\right) \tag{3.67}$$

The parameter ε is obtained from the recurrence relation

$$2q(2j-m)P_{m+1}(\varepsilon) + ((\varepsilon + a)(\ell + m + 1) + a)P_m(\varepsilon) + m(2\ell + m + 1)P_{m-1}(\varepsilon) = 0 \tag{3.68}$$

When $q = 0$, the potential is exactly solvable and from Eq. (3.68) we obtain

$$\varepsilon = -a\left(1 + \frac{1}{\ell + m + 1}\right) \tag{3.69}$$

Then energy eigenvalue Eq. (3.67) takes the form

$$E = \left(\frac{a/2}{\ell + m + 1}\right)^2 \tag{3.70}$$

With the substitution Eq. (3.65) and $\alpha \to 0$ one can transform the QES Hultèn like potential into the perturbed Coulomb potential. We note that, with a special choice of $\varepsilon = -a$ the QES Coulomb like potential corresponds to the potential describing a two electron system in an external oscillator potential [22, 94] where the eigenvalue of the Schrödinger equation reads

$$E = 2q\left(\ell + 2j + \frac{3}{2}\right) \tag{3.71}$$

If we substitute the $\varepsilon = -a$ in Eq. (3.68), then the recurrence relation simplifies to

$$2q(2j - m)P_{m+1}(\varepsilon) - \varepsilon P_m(\varepsilon) + m(2\ell + m + 1)P_{m-1}(\varepsilon) = 0 \qquad (3.72)$$

The parameter a ($\varepsilon = -a$) is the effective charge of the inter electronic interaction and it can be changed by the atomic number Z. The effective charge can be obtained by solving the recurrence relation. The first four of this relation is given by

$$\begin{aligned} P_1(\varepsilon) &= \varepsilon \\ P_2(\varepsilon) &= \varepsilon^2 - 8qj(\ell + 1) \\ P_3(\varepsilon) &= \varepsilon[\varepsilon^2 + 4q(2\ell + 3 - 2j(3\ell + 4))] \\ P_4(\varepsilon) &= \varepsilon^4 + 4q(8\ell + 15 - 4j(4\ell + 5))\varepsilon^2 + 192j8j - 1)(\ell^2 + 3\ell + 2)q^2 \end{aligned} \qquad (3.73)$$

The roots of the polynomial $P_{2j+1}(\varepsilon) = 0$ can be written for a few values of j

$$\begin{aligned} j &= 0, \quad \varepsilon = 0 \\ j &= \frac{1}{2}, \quad \varepsilon = \pm 2\sqrt{q(\ell + 1)} \\ j &= 1, \quad \varepsilon = \left\{ \pm 2\sqrt{q(4\ell + 5)}, \;\; 0 \right\} \\ j &= \frac{3}{2}, \quad \varepsilon = \left\{ \pm\sqrt{2q\left(5(2\ell + 3) \pm \sqrt{153 + 64\ell(\ell + 3)}\right)} \right\} \end{aligned} \qquad (3.74)$$

As noted in the paper [95], there exists equal number of positive and negative eigenvalues. This implies that electron-electron correlation energy is related with the electron-positron correlation energy.

3.11 QES Anharmonic Oscillator Potential

In order to obtain the anharmonic oscillator potential from the Rosen-Morse like potential we redefine the parameters

$$\begin{aligned} q &\to \frac{q}{2\alpha^3}, \quad L \to -\frac{\ell}{4\alpha} + \frac{a}{2\alpha^2} - \frac{3q}{2\alpha^3} \\ \lambda &\to \varepsilon + \frac{3\ell}{2\alpha} - \frac{a}{\alpha^2} + \frac{2q}{\alpha^3} \\ A &\to \frac{2a\alpha - q(3\varepsilon + 4j + 10)}{4\alpha^3} - \frac{7q\ell}{8\alpha^4} + \frac{qa}{4\alpha^5} - \frac{3q^2}{8\alpha^6} \end{aligned} \qquad (3.75)$$

Substituting Eq. (3.75) into Eq. (3.63), taking the limit of $(V(x) - E)$ when $\alpha \to 0$, we obtain the potential,

$$V(x) = \left(\frac{a\ell}{2} - 2q(1 + 2j)\right)x + \left(\frac{a^2}{4} - q\ell\right)x^2 - qax^3 + q^2x^4 \qquad (3.76)$$

The ground state wave function is given by

$$\psi(x) = \exp\left(\frac{\ell}{2}x + \frac{a}{4}x^2 - \frac{q}{3}x^3\right) \tag{3.77}$$

and the energy is obtained as

$$E = \frac{1}{2}(\varepsilon + 4j + 5)a \tag{3.78}$$

As noted before ε is determined from the recurrence relation

$$2q(m-2j)P_{m+1}(\varepsilon)+\frac{1}{4}(2a(\varepsilon+4j-2m+4)-\ell^2)P_m(\varepsilon)-m\ell P_{m-1}(\varepsilon)-m(m-1)P_{m-2}(\varepsilon) = 0 \tag{3.79}$$

This transformation shows that the QES Rosen-Morse like and the anharmonic oscillator potentials have similar behavior in a certain range of variable x.

3.12 Result and Discussion

We have developed a general procedure to obtain the eigenstates of some QES potentials in terms of the orthogonal polynomials as well as the eigenvalues. These potentials can be expressed operators of the $sl(2,R)$ Lie algebra. We have shown that QES Pöschl -Teller like potential can be transformed into QES PT symmetric Scarf like potential, QES Sextic Oscillator, and QES Eckart like potential can be transformed into QES Hultén like, QES Rosen-Morse like, QES Coulomb like potentials by redefining parameters, changing the coordinates and applying an appropriate limiting procedure.

CHAPTER 4

QUASI EXACT SOLUTION OF THE $E \otimes \epsilon$ JAHN TELLER HAMILTONIAN

In this chapter, we deal with solution of the generalized $E \otimes \varepsilon$ JT Hamiltonian in the context of QES spectral problems. The Hamiltonian has been solved in the Bargmann-Fock space by obtaining an expressions as linear and bilinear combinations of the generators of the $osp(2,2)$ Lie algebra.

4.1 The $E \otimes \epsilon$ Jahn Teller Hamiltonian

The $E \otimes \varepsilon$ JT Hamiltonian describing a two level fermionic subsystem coupled to two boson modes which are obtained by [46]. The well known form of the Hamiltonian is given by

$$H = a_1^\dagger a_1 + a_2^\dagger a_2 + 1 + \left(\frac{1}{2} + 2\mu\right)\sigma_0 + 2\kappa\left[\left(a_1 + a_2^\dagger\right)\sigma_+ + \left(a_1^\dagger + a_2\right)\sigma_-\right] \quad (4.1)$$

where $\frac{1}{2} + 2\mu$ is the level separation, and κ is the coupling strength. The Pauli matrices $\sigma_{\mp,0}$ are given by

$$\sigma_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \sigma_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (4.2)$$

and they satisfy the commutation relations

$$[\sigma_+, \sigma_-] = \sigma_0, \qquad [\sigma_0, \sigma_\mp] = \mp 2\sigma_\mp \quad (4.3)$$

The annihilation and creation operators, a_i and $a_i^\dagger$ satisfy the usual commutation relations

$$\left[a_i^\dagger, a_j^\dagger\right] = [a_i, a_j] = 0, \quad \left[a_i, a_j^\dagger\right] = \delta_{ij}. \quad (4.4)$$

The Hamiltonian can be written as this form by Reik [46],

$$\frac{1}{2}H = \frac{1}{2}J + \frac{1}{2} + h \quad (4.5)$$

where J represents the angular momentum of the system and is given by

$$J = a_1^\dagger a_1 - a_2^\dagger a_2 + \frac{1}{2}\sigma_0 \tag{4.6}$$

and h,

$$h = a_2^\dagger a_2 + \mu\sigma_0 + \kappa[(a_1 + a_2^\dagger)\sigma_+ + (a_2 + a_1^\dagger)\sigma_-] \tag{4.7}$$

Clearly the Hamiltonian conserves the number of particles in the system, they have same eigenfunction when J commutes with h, then the eigenvalue problem of the angular momentum part can be easily solved. It reads

$$J\left|\psi\right\rangle_{j+\frac{1}{2}} = \left(j + \frac{1}{2}\right)\left|\psi\right\rangle_{j+\frac{1}{2}}, \qquad (j = 0, 1, 2.....) \tag{4.8}$$

with the eigenfunctions

$$\left|\psi\right\rangle_{j+\frac{1}{2}} = (a_1^\dagger)^j \phi_1(a_1^\dagger a_2^\dagger)\left|0\right\rangle\left|\uparrow\right\rangle + (a_1^\dagger)^{j+1}\phi_2(a_1^\dagger a_2^\dagger)\left|0\right\rangle\left|\downarrow\right\rangle \tag{4.9}$$

where $\left|0\right\rangle$ is the vacuum state for both bosons. Here $\left|\uparrow\right\rangle$ and $\left|\downarrow\right\rangle$ are the eigenstates of the operators σ_0, and ϕ_1 and ϕ_2 are arbitrary functions of $a_1^\dagger a_2^\dagger$. The eigenfunctions Eq. (4.8) are also the eigenfunctions of the Hamiltonian Eq. (4.1)because of the properties of the commutation relations. Therefore, we can write the eigenvalue equation

$$H\left|\psi\right\rangle_{j+\frac{1}{2}} = E\left|\psi\right\rangle_{j+\frac{1}{2}} \tag{4.10}$$

and the equivalent Schrödinger equation

$$h\left|\psi\right\rangle_{j+\frac{1}{2}} = \epsilon\left|\psi\right\rangle_{j+\frac{1}{2}} \tag{4.11}$$

where the eigenvalue ϵ is related to E by Eq. (4.7)

$$E = 2\epsilon + j + \frac{3}{2} \tag{4.12}$$

It is found that the solution of the Schrödinger equation Eq. (4.1) can be reduced to the solution of Eq. (4.11) under this consideration. Now, we use Bargmann's method (Bargmann 1961, Schweber 1967, Perelomov 1986 and Skagerstam 1985) for the solution of the eigenvalue problem Eq. (4.10). Then the Hamiltonian h and the eigenfunctions ψ can be expressed in the Bargman-Fock space by using the realizations of the bosonic operators

$$a_i^\dagger = z_i, \quad a_i = \frac{d}{dz_i}, \quad i = 1, 2. \tag{4.13}$$

$$\begin{aligned} h &= \begin{bmatrix} z_2\frac{d}{dz_2} + \mu & \kappa\left[\frac{d}{dz_1} + z_2\right] \\ \kappa\left[\frac{d}{dz_2} + z_1\right] & z_2\frac{d}{dz_2} - \mu \end{bmatrix} \qquad (4.14) \\ \left|\psi\right\rangle_{j+\frac{1}{2}} &= z_1^j\phi_1(\xi)\left|0\right\rangle\left|\uparrow\right\rangle + z_1^{j+1}\phi_2(\xi)\left|0\right\rangle\left|\downarrow\right\rangle \end{aligned}$$

In this formulation, the Hamiltonian h consists of two independent sets of first-order linear differential equation. Substituting Eq. (4.9) and Eq. (4.13) into Eq. (4.11) and defining $\xi = z_1.z_2$, after some algebraic manipulations we can obtain the following two linear differential equations satisfy by the functions $\phi_1$and ϕ_2 :

$$\begin{aligned} \left[\xi\frac{d}{d\xi} - (\epsilon - \mu)\right]\phi_1 + \kappa\left[\xi\frac{d}{d\xi} + (\xi + j + 1)\right]\phi_2 &= 0 \qquad (4.15)\\ \kappa\left[\frac{d}{d\xi} + 1\right]\phi_1 + \left[\xi\frac{d}{d\xi} - (\epsilon + \mu)\right]\phi_2 &= 0 \qquad (4.16) \end{aligned}$$

These coupled differential equations represent the Schrödinger equation of the $E \otimes \epsilon$ system in Bargmann's Hilbert space.

4.2 Construction of the boson fermion representations of the osp(2,2) superalgebra

Lie superalgebras have attracted considerable interest from both mathematical and physical point of view. Their representations and realizations play a key role to study physical models. Two level models play an important role in the research of the interaction of photon or phonon with condensed matter. The natural step to relate the physical systems and Lie superalgebras is to express the generators of the Lie superalgebra interms of bosons and/or fermions. The Hamiltonians can be written as combinations of the generators of a relevant symmetry group. Hence one can able to compute a part of spectrum by performing a suitable transformation of the generators. The key to the QES of the physical Hamiltonians lie in the studying finite dimensional inhomogeneous differential realizations of the Lie superalgebras.

Now, we derive inhomogeneous, one variable differential realizations of the osp(2,2) superalgebra whose representations consists of two bosons and one fermion. The supergroup $osp(2,2)$ is one of the major symmetry group candidates for spin one-half particles which has four even and four odd generators. Its even generators can be represented by bosons while odd generators are represented by combinations of the fermions and bosons. In order to construct $osp(2,2)$ superalgebra let us start by introducing three generators of the $su(1,1)$ algebra,

$$\begin{aligned} J_+ &= a_1^\dagger a_2^\dagger, \quad J_- = a_2 a_1 \qquad (4.17)\\ J_0 &= \frac{1}{2}\left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right) \end{aligned}$$

and its number operator is given by,

$$N = a_1^\dagger a_1 - a_2^\dagger a_2 \qquad (4.18)$$

which commutes with the $su(1,1)$ generators. The superalgebra $osp(2,2)$ might be constructed by extending $su(1,1)$ algebra with the fermionic generators. Its possible to express to set of fermionic generators to extend the $su(1,1)$ algebra to the $osp(2,2)$ algebra. These are given by

$$V_+ = f^\dagger a_2^\dagger, \quad V_- = f^\dagger a_1, \quad W_+ = f a_1^\dagger, \quad W_- = f a_2 \tag{4.19}$$

where $f^\dagger$ and f are fermions and in order to relate the $osp(2,2)$ algebraic structure with the two dimensional 2×2 matrix Hamiltonians one can use standard matrix representations of the fermions are given by,

$$\left\{f, f^\dagger\right\} = 1, \quad f = \sigma_-, \quad f^\dagger = \sigma_+, \quad ff^\dagger - f^\dagger f = \sigma_0 \tag{4.20}$$

The superalgebra $osp(2,2)$ can be constructed with the boson and fermion generators. The total number operator J of the system and it is given by

$$J = \frac{1}{2}N + \frac{1}{2}\left(f^\dagger f - ff^\dagger\right) \tag{4.21}$$

The generators of the $osp(2,2)$ superalgebra satisfy the following commutation and and anticommutation relations.

$$\begin{array}{rcllll}
[J_+, J_-] &=& -2J_0, & [J_0, J_\pm] = \pm J_\pm, & [J, J_\pm] = 0, \\
[J, J_0] &=& 0, & [J_0, V_\pm] = \pm\frac{1}{2}V_\pm, & [J_0, W_\pm] = \pm\frac{1}{2}W_\pm, \\
[J_\pm, V_\mp] &=& V_\pm, & [J_\pm, W_\mp] = W_\mp, & [J, W_\pm] = -\frac{1}{2}W_\pm, \\
[J, V_\pm] &=& \frac{1}{2}V_\pm, & [J_\pm, V_\pm] = 0, & [J_\pm, W_\pm] = 0, \\
\{V_\pm, W_\pm\} &=& J_\pm, & \{V_\pm, W_\mp\} = \pm J_0 - J, & \{V_\pm, V_\pm\} = \{V_\pm, V_\mp\} = 0, \\
\{W_\pm, W_\pm\} &=& \{W_\pm, W_\mp\} = 0 & &
\end{array} \tag{4.22}$$

The Hamiltonian of a physical system, with an underlying $osp(2,2)$ symmetry, has been expressed in terms of the operators of the corresponding algebra. In general, the Hamiltonian is exactly solved and the spectrum of the physical system can be calculated in a closed form when the Hamiltonian of the system can be written in terms of number operator and diagonal operator J_0, it can be diagonalized within the representation N. The abstract boson and /or fermion algebra can be associated with the exactly solvable Schrödinger equations by using the differential operator realizations of boson operators. Thus the combinations of operators Eq. (4.22) have direct physical meaning, being related to the quantum spin systems. In general, the solution of the such Hamiltonians can be obtained approximately or by means of numerical methods. However, if the Hamiltonian is transformed in a proper way, in some cases a finite dimensional closed subspace can be found and part of its spectrum can be obtained. In order to obtain a quasi exactly solvable Hamiltonian, in the next section, we prepare a suitable transformations procedure.

4.3 Transformation of the Operators

In this section we discuss transformation of the fermion boson representations of the $osp(2,2)$ algebra and its connection with the QES systems. This can be done by introducing the following similarity transformation induced by the metric

$$S = (a_2^\dagger)^{-a_1^\dagger a_1 + \alpha\sigma_+\sigma_-} \tag{4.23}$$

where α is a constant. Since a_1 and a_2 commute and $\sigma_{\pm,0}$ also commute with the bosonic operators, the transformation of a_1 and $a_1^\dagger$ under S can be obtained by writing $a_2^\dagger = e^b$, with $[a_1, b] = \left[a_1^\dagger, b\right] = 0$,

$$\begin{aligned} Sa_1S^{-1} &= a_1a_2^\dagger \\ Sa_1^\dagger S^{-1} &= a_1^\dagger(a_2^\dagger)^{-1} \end{aligned} \tag{4.24}$$

the transformation of a_2 and $a_2^\dagger$ is as follows

$$\begin{aligned} Sa_2S^{-1} &= a_2 - n(a_2^\dagger)^{-1} \\ Sa_2^\dagger S^{-1} &= a_2^\dagger \end{aligned} \tag{4.25}$$

and the transformations of the $\sigma_\pm$ are given by

$$S\sigma_\pm S^{-1} = \sigma_\pm(a_2^\dagger)^{\pm\alpha} \tag{4.26}$$

where n is given by

$$n = -a_1^\dagger a_1 + \alpha\sigma_\pm \tag{4.27}$$

The transformation of the bosons and fermions Eq. (4.24) through Eq. (4.27) plays a key role to construct QES one variable 2 × 2 matrix Hamiltonians. For two different values of the $\alpha = \pm 1$ the two component polynomial spinors form a basis function for the generators of the $osp(2,2)$ algebra. Consequently, we obtain two class of Hamiltonians which can be solved quasi exactly under some certain conditions.

Before constructing differential realizations of the $osp(2,2)$ superalgebra, let us consider the other transformation operators

$$T = (a_2)^{a_1^\dagger a_1 + \eta\sigma_+\sigma_-} \tag{4.28}$$

where η is a constant. By using the similar treatments given in the previous transformation operations one can easily obtain the following transformations.

$$\begin{aligned} Ta_1T^{-1} &= a_1(a_2^\dagger)^{-1} \\ Ta_1^\dagger T^{-1} &= a_1^\dagger a_2 \\ Ta_2T^{-1} &= a_2 \\ Ta_2^\dagger T^{-1} &= a_2^\dagger + n(a_2)^{-1} \\ T\sigma_\pm T^{-1} &= \sigma_\pm(a_2^\dagger)^{\pm\eta} \end{aligned} \tag{4.29}$$

These transformations leads to the various differential realizations of the $osp(2,2)$ superalgebra, depending on the choice of α and η. Now, we obtained the one variable differential realizations of the $osp(2,2)$ algebra for the choice of $\alpha = -1$,

$$\begin{aligned}
J_+^{'} &= SJ_+S^{-1} = a_1^\dagger \\
J_-^{'} &= SJ_-S^{-1} = a_1(a_1^\dagger a_1 + a_2^\dagger a_2 + \sigma_+\sigma_-) \\
J_0^{'} &= SJ_0S^{-1} = \frac{1}{2}(2a_1^\dagger a_1 + a_2^\dagger a_2 + 1 + \sigma_+\sigma_-) \\
J^{'} &= SJS^{-1} = \frac{1}{2}(-a_2^\dagger a_2 - \sigma_-\sigma_+) \\
V_+^{'} &= SV_+S^{-1} = \sigma_+ \\
V_-^{'} &= SV_-S^{-1} = \sigma_+a_1 \\
W_+^{'} &= SW_+S^{-1} = \sigma_-a_1^\dagger \\
W_-^{'} &= SW_-S^{-1} = \sigma_-(a_1^\dagger a_1 + a_2^\dagger a_2 + \sigma_+\sigma_-)
\end{aligned} \tag{4.30}$$

The representations Eq. (4.30) of $osp(2,2)$ can be characterized by a fixed number $a_2^\dagger a_2 = -j - 1$. Here j takes integer or half integer values. Therefore the realization Eq. (4.30) of the $osp(2,2)$ include one boson operator and generators can be expressed in terms of one boson operator a_1, and yield the following realization,

$$\begin{aligned}
J_+^{'} &= SJ_+S^{-1} = a_1^\dagger \\
J_-^{'} &= SJ_-S^{-1} = a_1(a_1^\dagger a_1 - j - 1 + \sigma_+\sigma_-) \\
J_0^{'} &= SJ_0S^{-1} = \frac{1}{2}(2a_1^\dagger a_1 - j + \sigma_+\sigma_-) \\
J^{'} &= SJS^{-1} = \frac{1}{2}(j + 1 - \sigma_-\sigma_+) \\
V_+^{'} &= SV_+S^{-1} = \sigma_+ \\
V_-^{'} &= SV_-S^{-1} = \sigma_+a_1 \\
W_+^{'} &= SW_+S^{-1} = \sigma_-a_1^\dagger \\
W_-^{'} &= SW_-S^{-1} = \sigma_-(a_1^\dagger a_1 - j - 1 + \sigma_+\sigma_-)
\end{aligned} \tag{4.31}$$

These generators play an important role in the quasi exact solution of the matrix Schrödinger equation. The generators of the $osp(2,2)$ algebra can be expressed as differential equation in the Bargmann Fock space by defining the bosonic operators,

$$a_1 = \frac{d}{dx}, \quad a_1^\dagger = x \tag{4.32}$$

The two component polynomials of degree j and $j+1$ form a basis function for the generators of the $osp(2,2)$ algebra in the Bargmann Fock space,

$$P_{n+1,n}(x) = \begin{pmatrix} x^0, x^1, \ldots .x^{n+1} \\ x^0, x^1, \ldots .x^n \end{pmatrix} \tag{4.33}$$

In the case of $\eta = 1$, under the transformation T, the generators of the $osp(2,2)$ algebra take the form,

$$\begin{aligned}
J_+^{'} &= TJ_-T^{-1} = a_1^\dagger(a_1a_1 + a_2^\dagger a_2 + 1 + \sigma_+\sigma_-) \\
J_-^{'} &= TJ_-T^{-1} = a_1 \\
J_0^{'} &= TJ_0T^{-1} = \frac{1}{2}(2a_1^\dagger a_1 + a_2^\dagger a_2 + 1 + \sigma_+\sigma_-) \\
J^{'} &= TJT^{-1} = \frac{1}{2}(-a_2^\dagger a_2 - \sigma_-\sigma_+) \\
V_+^{'} &= TV_+T^{-1} = \sigma_+(a_1^\dagger a_1 + a_2^\dagger a_2 + 1 + \sigma_+\sigma_-) \\
V_-^{'} &= TV_-T^{-1} = \sigma_+a_1 \\
W_+^{'} &= TW_+T^{-1} = \sigma_-a_1^\dagger \\
W_-^{'} &= TW_-T^{-1} = \sigma_-
\end{aligned} \tag{4.34}$$

This realization can also be characterized by $a_2^\dagger a_2 = -j - 1$.The basis function of this structure is same Eq. (4.33). The general QES operator can be obtained by linear and bilinear combinations of the generators of the $osp(2,2)$ superalgebra. Action of the QES operator on the basis function Eq. (4.33) gives us recurrence relation, therefore, the wavefunction is itself the generating function of the energy polynomials. The eigenvalues are then produced by the roots of such polynomials.

4.4 Solvability of the $E\otimes\epsilon$ Jahn Teller Hamiltonian

In this section we will demonstrate the Hamiltonian Eq. (4.1) posses $osp(2,2)$ symmetry and by the transformation procedure given in the previous section it can be solved in the framework of the QES. It will be shown that our approach relatively very simple when compared previous approaches. The Hamiltonian Eq. (4.1) can be expressed in terms of the generators of the $osp(2,2)$ algebra,

$$H = 2J_0 + \left(\frac{1}{2} + 2\mu\right)(2J - N) + 2\kappa\left[V_+ + V_- + W_+ + W_-\right] \tag{4.35}$$

The general procedure to solve a differential equation in terms of the generators of a given Lie algebra having a finite dimensional invariant subspace and use the algebraic operations. Under the transformation S and T , the Hamiltonian has two different realization in the Bargmann Fock space. The first transformation by S leads to the following one variable differential realization,

$$\begin{aligned} H_1 &= \left(2x\frac{d}{dx} - j + \sigma_+\sigma_-\right) - \left(\frac{1}{2} + 2\mu\right)\sigma_-\sigma_+ + \\ & 2\kappa\left[\sigma_+\left(1 + \frac{d}{dx}\right) + \sigma_-\left(x + x\frac{d}{dx} - j - 1 + \sigma_+\sigma_-\right)\right] \end{aligned} \tag{4.36}$$

and the second realization can be obtained by transforming the Hamiltonian by T,

$$\begin{aligned} H_2 &= \left(2x\frac{d}{dx} - j + \sigma_+\sigma_-\right) - \left(\frac{1}{2} + 2\mu\right)\sigma_-\sigma_+ + \\ & 2\kappa\left[\sigma_+\left(\frac{d}{dx} + x\frac{d}{dx} - j + \sigma_+\sigma_-\right) + \sigma_-(x+1)\right] \end{aligned} \tag{4.37}$$

The eigenvalue problem can be expressed as

$$H\varphi(x) = E\varphi(x), \qquad \varphi(x) = \begin{bmatrix} \nu_n(x) \\ \omega_m(x) \end{bmatrix} \tag{4.38}$$

where $\nu_n(x)$ and $\omega_m(x)$ are polynomials of degree n and m respectively. The action of the H_1 on the basis function $\varphi(x)$ gives the following recurrence relation,

$$\begin{aligned} (2n - j + 1 - E)\,\nu_n + 2\kappa\,(\omega_m + m\omega_{m-1}) &= 0 \\ \left(2m - j - \frac{1}{2} - 2\mu - E\right)\omega_m + 2\kappa\,(\nu_{n+1} + (n-j)\,\nu_n) &= 0 \end{aligned} \tag{4.39}$$

Similarly when the Hamiltonian H_2 acts on the basis function we obtain the recurrence relation ,

$$\begin{aligned} (2n - j + 1 - E)\,\nu_n + 2\kappa\,(m\omega_{m-1} + (m-j)\omega_m) &= 0 \\ \left(2m - j - \frac{1}{2} - 2\mu - E\right)\omega_m + 2\kappa\,(\nu_n + \nu_{n+1}) &= 0 \end{aligned} \tag{4.40}$$

It is requiring that the determinant of these sets are equal to zero giving the compatibility conditions which establish the QES systems. According to the Eq. (4.33) one can construct a QES system if $n = m + 1$. Restricted values of the m is given by

$$m = 0, \frac{1}{2}, 1, ..., j. \tag{4.41}$$

The recurrence relation implies that the wavefunction is itself the generating function of the energy polynomials. The eigenvalues are then produced just by the roots of such polynomials. If E is a root of the recurrence relation then the eigenfunction truncates for a certain values of j and E belong to the spectrum of the Hamiltonian. The initial conditions of the recurrence relation is given by

$$\nu_m = 0 \quad for \quad j < m < 1 \quad and \quad \omega_m = 0 \quad for \quad j < m < 0 \tag{4.42}$$

with these initial conditions solution of Eq. (4.39) gives us the following relation for the energy when $j = 0$,

$$E = \frac{1}{4}\left(5 - 4\mu \pm \sqrt{64\kappa^2 + (7 + 4\mu^2)}\right) \tag{4.43}$$

and for $j = 1/2$

$$E = \frac{1}{4}\left(3 - 4\mu \pm \sqrt{32\kappa^2 + (7 + 4\mu^2)}\right),\ E = \frac{1}{4}\left(7 - 4\mu \pm \sqrt{64\kappa^2 + (7 + 4\mu^2)}\right) \tag{4.44}$$

The same energy eigenvalues can be obtained by using the recurrence relation Eq. (4.40). In this case eigenvalues shifted $E \to E - 1$ and j takes negative integer and half integer values.

By using the different strategy we have obtained the solution of the differential equation Eq.(4.15,4.16) which have been expressed bosonic and fermionic generators then we have obtained the recurrence relations. To do this first of all we introduce a new variable,

$$\xi = \kappa^2(1 + x) \tag{4.45}$$

and redefine the functions

$$\phi_2(\xi) = -\frac{1}{\kappa}\varphi_2(x), \qquad \phi_1(\xi) = \varphi_1(x) + \varphi_2(x) \tag{4.46}$$

to obtain the following systems of differential equations:

$$\left[-x\frac{d}{dx} + \left(\epsilon + \kappa^2 - \mu\right)\right]\varphi_1(x) + \left[-x\frac{d}{dx} + 2\epsilon + 2\kappa^2 + 1 + j + \kappa^2 x\right]\varphi_2(x) = 0 \tag{4.47a}$$

$$\left[\frac{d}{dx} + \kappa^2\right]\varphi_1(x) + \left[-x\frac{d}{dx} + \left(\epsilon + \kappa^2 + \mu\right)\right]\varphi_2(x) = 0 \tag{4.47b}$$

The new bosonic and fermionic generators are defined by [3]

$$\begin{aligned}
J_- &= x\frac{d^2}{dx^2} - 2k\frac{d}{dx} + \sigma_-\sigma_+, \quad J_+ = x, \\
J_0 &= x\frac{d}{dx} - k + \frac{1}{2}\sigma_-\sigma_+, \qquad J = k + \frac{1}{2}\sigma_-\sigma_+ \\
f_1 &= \sigma_-, \qquad f_2 = \sigma_-\frac{d}{dx} \\
\overline{f}_1 &= -\sigma_+ x\frac{d}{dx} + 2k\sigma_+, \quad \overline{f}_2 = x\sigma_+
\end{aligned} \tag{4.48}$$

These generators form the $osp(2,2)$ algebra. The bosonic generators form $sl_2(R)$ algebra,

$$[J_+, J_-] = -2J_0 \qquad [J_0, J_\pm] = \pm\ J_\pm \tag{4.49}$$

and the fermionic generators satisfy the anticoagulation relations

$$\{f_i, f_j\} = \{\overline{f}_i, \overline{f}_j\} = 0, \quad i = 1, 2 \tag{4.50}$$

The number operators of the system are given by

$$N_1 = \{f_1, \overline{f}_1\} = 2k - x\frac{d}{dx}, \quad N_2 = \{f_2, \overline{f}_2\} = \sigma_-\sigma_+ + x\frac{d}{dx} \tag{4.51}$$

and the action of the number operators on the fermionic generators is defined as

$$\begin{aligned} [N_1, f_1] &= \left[N_1, \overline{f}_1\right] = 0, \quad [N_1, f_2] = f_2, \quad \left[N_1, \overline{f}_2\right] = -\overline{f}_2, \\ [N_2, f_2] &= \left[N_2, \overline{f}_2\right] = 0, \quad [N_2, f_1] = f_1, \quad \left[N_2, \overline{f}_1\right] = -\overline{f}_1. \end{aligned} \tag{4.52}$$

The linear and bilinear combinations of the operators given in Eq. (4.49) are QES, when the space is defined as $P_{n+1,n}$ [3]. Let us consider the following linear combinations of the fermionic generators:

$$L = 2\mu N_1 + (1 + 2\mu)N_2 + \kappa^2(f_1 + \overline{f}_2) + f_2 + \overline{f}_1 \tag{4.53}$$

Then the eigenvalue problem can be expressed as

$$L\varphi(x) = \lambda\varphi(x) \tag{4.54}$$

where

$$\varphi(x) = \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \end{bmatrix} \tag{4.55}$$

is a two component spinor.

The algebraic structure of $osp(2,2)$ has been studied previously [3, 19]. It is obvious that the fermionic generators of $osp(2,2)$ with number operators N_1 and N_2 form a subalgebra of $osp(2,2)$. Inserting the differential realization Eq. (4.49) into Eq. (4.54) and comparing the equations Eq. (4.54) with Eq. (4.15) and Eq. (4.16), we can show that the equations are identical when the following hold:

$$\begin{aligned} \lambda &= \frac{1}{2}\left(1 + j + 2\mu + 2k(1 + 4\mu)\right), \\ \epsilon &= k - \frac{j}{2} - \frac{1}{2} - \kappa^2. \end{aligned} \tag{4.56}$$

The restricted values of ϵ are the same as those of well known results [45]. When the generators acts on the space $P_{n+1,n}$, we can obtain the two recurrence relations

$$n\upsilon_n + \left(k - n + \mu - \frac{1}{2} - \frac{j}{2}\right)\omega_n + \kappa^2\upsilon_{n+1} = 0 \tag{4.57a}$$

$$(2k - n)\,\omega_n + \left(k - n + \mu - \frac{1}{2} - \frac{j}{2}\right)\upsilon_{n+1} + \kappa^2\omega_{n+1} = 0 \tag{4.57b}$$

The polynomials are related to the eigenfunction as

$$(P_{n+1}, P_n) = (\varphi_1, \varphi_2) = (\upsilon_{n+1}, \omega_n) \tag{4.58}$$

$\mu = 0$	$j = 0$	displaced harmonic oscillator
$\mu = 0$	j half integer	$E \otimes \epsilon$ JT system
$\mu = 0$	j integer	$\Gamma_8 \otimes \tau_2$ and $\Gamma_8 \otimes (\varepsilon + \tau_2)$ systems
$\mu \neq 0$	$j = 0$	dimer
$\mu \neq 0$	j half integer	$E \otimes \varepsilon$ JT system in an external field

Table 4.1: The physical systems described by recurrence relations

If κ_j is a root of the polynomial $(\upsilon_{n+1}, \omega_n)$, the wavefunction is truncated at $n = 2k$ and belongs to the spectrum of the Hamiltonian L.The recurrence relations in Eq. (4.58) and Eq. (4.59), depending on the choice of the parameters μ and j, describe a number of physical systems [48]. These recurrence relations can be given in the matrix form:

$$\begin{bmatrix} k+\mu-\frac{1+j}{2} & \kappa^2 & 0 & 0 & 0 & . \\ 2k & k-\mu-\frac{1+j}{2} & \kappa^2 & 0 & 0 & . \\ 0 & 1 & k+\mu-\frac{3+j}{2} & \kappa^2 & 0 & . \\ 0 & 0 & 2k-1 & k-\mu-\frac{3+j}{2} & \kappa^2 & . \\ 0 & 0 & 0 & 2 & . & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} \omega_0 \\ \upsilon_1 \\ \omega_1 \\ \upsilon_2 \\ \omega_2 \\ . \\ . \end{bmatrix} = 0 \tag{4.59}$$

4.5 Result and Discussion

We have shown that quasi-exact solutions of a class of JT problems can be obtained as the roots of the determinant of a matrix of order $2k$. The matrix Hamiltonian is identical with the results obtained by Looorits [48]. When we replace j by $-j-1$ and set $2\mu = G$. If $\mu = 0$ and j is replaced by $-j-1$,then our results are identical to Judd's result [45]. The physical system described by the recurrence relations in Eq. (4.58) and Eq. (4.59) after replacing j by $-j-1$,are summarized in Table 4.1. The first case correspond to displaced one-dimensional harmonic oscillator for which the energy equation (4.12) hold for all κ :

$$E = \left(2k + \frac{3}{2}\right) - \kappa^2 \tag{4.60}$$

In the second and third cases which correspond to three octahedral JT systems, have common features. The form of all the determinants is the same for all three systems, provided that in the $\Gamma_8 \otimes (\varepsilon + \tau_2)$ system, the two modes ε and τ_2 are equally coupled to the electronic state Γ_8. The case $j = 0$, as the limiting case in the $E \otimes \varepsilon$ JT system,indicates relationship between $E \otimes \varepsilon$ JT and the Rabi system. It is known that the Rabi system and the $E \otimes \beta$ JT system occur in the resonant excitation of double molecules and dimers. The $E \otimes \beta$ JT system possesses $sl_2(R)$ symmetries [42], which is a subgroup of $osp(2,2)$.

In the presence of an external field, the energies of the generalized $E \otimes \varepsilon$ JT system can be obtained by solving the recurrence relations Eq. (4.58) and Eq. (4.59), without any restriction. We have defined $j = -(\eta + \rho + 2)/2$ and $\mu = (\eta - \rho)/4$. And then the first few recurrence relations form polynomials in κ are given by

$$\begin{aligned} P_1(\kappa) &= \eta \\ P_2(\kappa) &= 8\eta\kappa^2 - (\rho+1)(\eta^2-1) \qquad (4.61) \\ P_3(\kappa) &= 128\eta\kappa^2 - 8(\eta(3\eta(\rho+1)-4) - 4(\rho+1))\kappa^2 + \eta\rho(\rho+2)(\eta^2-4) \end{aligned}$$

for the values $k = 0, 1/2$ and 1, respectively. The roots of these polynomials belong to the spectrum of the Hamiltonian Eq. (4.1).

CHAPTER 5

A SOLUTION OF THE $T \otimes T$ JAHN TELLER HAMILTONIAN WITH THE ROTATING WAVE APPROXIMATION

In this chapter, we develop a new approximation method known as rotating wave approximation (RWA) which is based on the Lie type similarity transformation. This method gives an accurate results when the frequency associated with the free evaluation of the system is essentially bigger than the transmission frequencies induced by the interaction between subsystem or external source. In this case the resultant Hamiltonian is associated with the Dicke Hamiltonian. The whole spectrum of the Dicke Hamiltonian can not be obtained exactly and usually it has been treated in the framework of the RWA. In a particular case it is demonstrated that Jaynes Cumming (JC) and $T \otimes t$ JT Hamiltonians can easily be solved within the framework of the suggested approximation.

5.1 The Jaynes-Cummings Hamiltonian

The Jaynes-Cumming (JC) model is one of the major paradigms describes the interaction between a two level atom and the quantized single mode electromagnetic field. It was introduced as a highly simplified model to explain qualitatively , the salient features of the interaction of matter with quantized radiation field in a cavity. Despite the fact that it considers matter in the highly simplified form of a two level atom and radiation in the form of a single mode field it demonstrates quite a few uniquely quantum mechanical features.

There are many approaches to solve JC model. Recently some algebraic techniques which improve both analytical and numerical solutions of the problems, have been suggested and developed for some quantum optical systems. It is well known that the Lie algebraic techniques are very powerful in describing many physical problems. In our study, we demonstrate our procedure on the JC model. The JC Hamiltonian can be written as

$$H = \omega a^\dagger a + \omega_0 \sigma_0 + \kappa(\sigma_+ + \sigma_-)(a^\dagger + a) \tag{5.1}$$

where $\sigma_0, \sigma_+$and $\sigma_-$are the usual Pauli matrices, $a^\dagger$and a are the boson creation and annihilation operators, respectively; κ is the interaction constant, ω is the frequency of the oscillator, the two atomic levels separated by an energy difference ω_0. The Hamiltonian Eq. (5.1) can be solved in the framework of quasi-exactly solvable problems or by using numerical diagonalization method. It is analytically solvable due to the neglect of the counter-rotating terms, so called RWA. In order to obtain rotating wave approximated form of the JC Hamiltonian, we use similarity transformation by introducing the operator

$$T = \frac{\kappa}{\omega + \omega_0} \left(\sigma_+ a^\dagger - \sigma_- a \right), \tag{5.2}$$

and imposing the condition $\omega + \omega_0 \gg \kappa$, which usually holds in quantum-optical interactions, transformation of the Hamiltonian (5.1), yields that

$$\begin{aligned} \widetilde{H} &= e^T H e^{-T} \approx \omega a^\dagger a + \omega_0 \sigma_0 + \kappa(\sigma_+ a + \sigma_- a^\dagger) + \\ &\frac{2\kappa^2}{\omega + \omega_0} \left[\left(a^\dagger a + a^{\dagger 2} + a^2 \right) \sigma_0 - \sigma_- \sigma_+ \right] + O\left(\frac{\kappa^3}{\omega^2 - \omega_0^2} \right), \end{aligned} \tag{5.3}$$

Since $\frac{\kappa^2}{\omega + \omega_0} \ll 1$ is a small parameter, neglected of the last term confirms the well known result;

$$\widetilde{H} \approx \omega a^\dagger a + \omega_0 \sigma_0 + \kappa(\sigma_+ a + \sigma_- a^\dagger) \tag{5.4}$$

The eigenvalue problem can be written as

$$\widetilde{H} \left| \psi \right\rangle = E \left| \psi \right\rangle \tag{5.5}$$

where $\left| \psi \right\rangle$ is the two component eigenstate

$$\left| \psi \right\rangle = \begin{pmatrix} c_1 \left| n \right\rangle \\ c_2 \left| n+1 \right\rangle \end{pmatrix}, \tag{5.6}$$

here $\left| n \right\rangle$ is the eigenstate and $c_1$and c_2 are normalization constant. Acting of $\widetilde{H}$ on ψ yields the following expressions

$$\begin{aligned} c_1 \left(\omega n + \frac{\omega_0}{2} \right) \left| n \right\rangle + c_2 \kappa \sqrt{n+1} \left| n \right\rangle &= c_1 E \left| n \right\rangle \qquad \text{(5.7a)} \\ c_2 \left(\omega(n+1) - \frac{\omega_0}{2} \right) \left| n+1 \right\rangle + c_1 \kappa \sqrt{n+1} \left| n+1 \right\rangle &= c_2 E \left| n+1 \right\rangle . \end{aligned}$$

Eliminating c_1 and c_2 between two equations and solving the resultant equation for E, we obtain

$$E = \left(n + \frac{1}{2}\right)\omega \pm \frac{1}{2}\sqrt{4\kappa^2(n+1) + (\omega_0 - \omega)^2}. \tag{5.8}$$

The eigenstates can be easily written by using boson operators, acting on a vacuum state$|0\rangle$;

$$|\psi\rangle = \left[c_1 a^{\dagger n}|0\rangle, c_2 a^{\dagger n+1}|0\rangle\right]^T. \tag{5.9}$$

In the following section we develop a similar procedure that leads to the analytical solution of the $T \otimes t$ JT Hamiltonian.

5.2 The $T \otimes t$ Jahn Teller Hamiltonian

The JT Hamiltonian for a T_1 ion in tetrahedral cluster interacting with e and t_2-types vibrational modes. In terms of the coordinates, ε and ξ belonging to the representation E and x, y, and z belonging to the representation T the Hamiltonian can be written as

$$H = H_0 I - \frac{V_E}{2}\begin{pmatrix} \sqrt{3}\xi - \varepsilon & 0 & 0 \\ 0 & \sqrt{3}\xi - \varepsilon & 0 \\ 0 & 0 & 2\varepsilon \end{pmatrix} - \frac{\sqrt{3}V_T}{2}\begin{pmatrix} 0 & x & z \\ x & 0 & y \\ z & y & 0 \end{pmatrix} \tag{5.10}$$

where V_E and V_T are JT coupling coefficients, I is the 3×3 unit matrix and the harmonic part of the Hamiltonian, H_0, is given by

$$H_0 = -\frac{\hbar^2}{2\mu}\left(\partial_x^2 + \partial_y^2 + \partial_z^2 + \partial_\varepsilon^2 + \partial_\xi^2\right) + \frac{1}{2}\mu\omega_E^2\left(\varepsilon^2 + \xi^2\right) + \frac{1}{2}\mu\omega_T^2\left(x^2 + y^2 + z^2\right). \tag{5.11}$$

The other terms describes the vibronic JT Hamiltonian which are rotationally invariant linear coupling between the electronic state and the vibrational mode.

In the standard JT theories [59, 61, 62], the Hamiltonian Eq. (5.10) can be diagonalized in the adiabatic limit to produce the eigenstates of energy. For systems with strong coupling between the electrons and associated vibrational modes, the system undergoes a static distortion to a new configuration of minimum energy. The vibronic JT states are constructed by multiplying the orbital states. Either these states or linear combinations of them are good eigenstates of the system. The energy is obtained in terms of the coordinates whose values are obtained by minimizing energy. Before going further let us discuss the solvability of the Hamiltonian Eq. (5.10).

In the particular cases when the vibronic interaction with one of the two types of vibrations E or T, is negligible,The Hamiltonian of the degrees of freedom involved in the vibronic interaction depends on a smaller number of variables and the corresponding adiabatic potentials are surfaces in the space of lower dimensionality. For instance, when the coupling of $E-$ mode alone exist in the system, the solution of the Hamiltonian H is diagonal and its eigenvalues may be represented by rotational paraboloid centered at the tetragonal extreme points. Then this system reduced to linear $T \otimes e$ JT Hamiltonian. The explicit form of the such Hamiltonian is,

$$\begin{aligned}
\left[-\frac{\hbar^2}{2\mu}\left(\partial_\varepsilon^2+\partial_\xi^2\right)+\frac{1}{2}\mu\omega_E^2\left(\varepsilon^2+\xi^2\right)+\frac{V_E}{2}\left(\varepsilon-\sqrt{3}\xi\right)-E\right]\psi_1\left(\varepsilon,\xi\right) &= 0\\
\left[-\frac{\hbar^2}{2\mu}\left(\partial_\varepsilon^2+\partial_\xi^2\right)+\frac{1}{2}\mu\omega_E^2\left(\varepsilon^2+\xi^2\right)+\frac{V_E}{2}\left(\varepsilon+\sqrt{3}\xi\right)-E\right]\psi_2\left(\varepsilon,\xi\right) &= 0\\
\left[-\frac{\hbar^2}{2\mu}\left(\partial_\varepsilon^2+\partial_\xi^2\right)+\frac{1}{2}\mu\omega_E^2\left(\varepsilon^2+\xi^2\right)+\frac{V_E}{2}\varepsilon-E\right]\psi_3\left(\varepsilon,\xi\right) &= 0
\end{aligned} \tag{5.12}$$

The wave function is

$$\Psi\left(\varepsilon,\xi\right)=\psi_1\left(\varepsilon,\xi\right)\psi_2\left(\varepsilon,\xi\right)\psi_3\left(\varepsilon,\xi\right) \tag{5.13}$$

In order to solve this type of the equations there are different types of the methods. In here we change the variables and the wave functions. $\varepsilon \to \sqrt{\frac{\hbar}{m\omega_E}}\varepsilon$, $\xi \to \sqrt{\frac{\hbar}{m\omega_E}}\xi$

$$\begin{aligned}
\psi_1(\varepsilon,\xi) &= e^{\frac{1}{2}(\frac{V_E}{2}+\varepsilon)^2}e^{\frac{1}{2}(\frac{\sqrt{3}V_E}{2}-\xi)^2}g_1(\xi)f_1(\varepsilon)\\
\psi_2(\varepsilon,\xi) &= e^{\frac{1}{2}(\frac{V_E}{2}+\varepsilon)^2}e^{\frac{1}{2}(\frac{\sqrt{3}V_E}{2}+\xi)^2}g_2(\xi)f_2(\varepsilon)\\
\psi_3(\varepsilon,\xi) &= e^{\frac{1}{2}(V_E-\varepsilon)^2}e^{\frac{1}{2}\xi^2}g_3(\xi)f_3(\varepsilon)
\end{aligned} \tag{5.14}$$

Insert these equations into the original Hamiltonian we get new equations

$$\begin{aligned}
\frac{f_1''(\varepsilon)-(V_E+2\varepsilon)f_1'(\varepsilon)}{f_1(\varepsilon)}+\frac{g_1''(\xi)+(\sqrt{3}V_E-2\xi)g_1'(\xi)}{g_1(y)}-2+\epsilon+V_E^2 &= 0\\
\frac{f_2''(\varepsilon)-(V_E+2\varepsilon)f_2'(\varepsilon)}{f_2(\varepsilon)}+\frac{g_2''(\xi)-(\sqrt{3}V_E+2\xi)g_2'(\xi)}{g_2(y)}-2+\epsilon+V_E^2 &= 0\\
\frac{f_3''(\varepsilon)+(V_E-\varepsilon)2f_3'(\varepsilon)}{f_3(\varepsilon)}+\frac{g_3''(y)-2\xi g_3'(\xi)}{g_3(\xi)}-2+\epsilon+V_E^2 &= 0
\end{aligned} \tag{5.15}$$

where $\epsilon = \frac{2}{\hbar\omega}E$. We seen that equation Eq. (5.15) can be solvable. Each of these equations are separated two parts. These are,

$$\begin{aligned}
f_1''(\varepsilon)-(V_E+2x)f_1^{'}(\varepsilon)+\alpha f_1(\varepsilon) &= 0\\
g_1''(\xi)+(\sqrt{3}V_E-2\xi)g_1^{'}(\xi)+\beta g_1(\xi) &= 0\\
\alpha+\beta-V_E^2+2 &= \varepsilon
\end{aligned} \tag{5.16}$$

and compared the equation Eq. (5.16) with the Hermite polynomial then we have obtained the wave function and energy of the system.

$$\begin{aligned}
f_1(\varepsilon) &= H_n\left(\frac{2\varepsilon+V_E}{2}\right);\ g_1(\xi)=H_n\left(\frac{2\xi-\sqrt{3}V_E}{2}\right);\\
f_2(\varepsilon) &= H_n\left(\frac{2\varepsilon+V_E}{2}\right);\ \ g_2(\xi)=H_n\left(\frac{2\xi+\sqrt{3}V_E}{2}\right);\\
f_3(\varepsilon) &= H_n\left(\frac{\varepsilon-V_E}{2}\right);\ \ \ g_3(\xi)=H_n\left(\xi\right)\\
E &= \hbar\omega_E(n_\varepsilon+n_\xi)-(V_E^2/2\mu\omega_E^2)
\end{aligned} \tag{5.17}$$

It seems that the solution of the $T\otimes e$ Hamiltonian H is very simple leading only shifted harmonic oscillator and all energy levels uniformly shifted.

On the other hand if only the coupling of the $T-$mode exist in the system, the Hamiltonian can not be solved exactly. In this case the Hamiltonian is not characterized by a vibronic angular momentum; the potential energy surfaces for nuclear motion have octahedral symmetry rather than spherical symmetry. An accidental spherical symmetry occurs only in the second order perturbation approximation. If the coupling is less strong, the zero-point vibrational energy is comparable with the JT energy. Thus no static distortion occurs, but the system exhibits a coupled motion of the electrons and vibrational modes. This situation is known as the dynamical JT effect.

Recently, Bates and Dunn have developed an alternative approach to solve the Hamiltonian H, including $T-$ modes couplings. In the theory of Bates' the coordinates x, y, z and momentums p_x, p_y, p_z are treated as quantum mechanical operators rather than dynamical constant. They applied a unitary transformation including a free parameter which minimize the energy of the transformed Hamiltonian. Here we develop a procedure that produces eigenvalues and eigenfunctions of the Hamiltonian Eq. (5.10) including only $T-$type interactions when the coupling is small.

Firstly we bosonise the Hamiltonian H by introducing appropriate differential realizations of the bosons. For our purpose, let us express the Hamiltonian Eq. (2.41) in a different basis by introducing the transformation matrix,

$$A=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1\\ 0 & \sqrt{2} & 0\\ -i & 0 & i \end{pmatrix}; \tag{5.18}$$

then $A^{-1}HA$ takes the form

$$\begin{aligned}
H &= \left[-\frac{\hbar^2}{2\mu}\left(\partial_x^2+\partial_y^2+\partial_z^2\right)+\frac{1}{2}\mu\omega_T^2\left(x^2+y^2+z^2\right)\right]I- \\
&\frac{\sqrt{3}V_T}{4}\left[S_+(x+iy)+S_-(x-iy)+(S_+^2-S_-^2)iz\right]
\end{aligned} \tag{5.19}$$

where S_+, S_- and S_0 are the 3×3 representations of the $SU(2)$ group and they are given by

$$S_+ = \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \; ; \; S_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \; ; \; S_- = S_+^T. \tag{5.20}$$

Our task is now to express the Hamiltonian Eq. (5.10) with the usual bosons. The relation can be obtained by realizing boson creation and annihilation operators as differential operators,

$$\begin{aligned}
a_1^\dagger &= \sqrt{\frac{\mu\omega}{4\hbar}}\,(x+iy) - \sqrt{\frac{\hbar}{4\mu\omega}}\,(\partial_x + i\partial_y), \\
a_1 &= \sqrt{\frac{\mu\omega}{4\hbar}}\,(x-iy) + \sqrt{\frac{\hbar}{4\mu\omega}}\,(\partial_x - i\partial_y), \\
a_2^\dagger &= \sqrt{\frac{\mu\omega}{4\hbar}}\,(x-iy) - \sqrt{\frac{\hbar}{4\mu\omega}}\,(\partial_x - i\partial_y), \\
a_2 &= \sqrt{\frac{\mu\omega}{4\hbar}}\,(x+iy) + \sqrt{\frac{\hbar}{4\mu\omega}}\,(\partial_x + i\partial_y), \\
a_3^\dagger &= \sqrt{\frac{\mu\omega}{2\hbar}}\,iz - \sqrt{\frac{\hbar}{2\mu\omega}}\,i\partial_z, \\
a_3 &= -\sqrt{\frac{m\omega}{2\hbar}}\,iz - \sqrt{\frac{\hbar}{2\mu\omega}}\,i\partial_z.
\end{aligned} \tag{5.21}$$

In terms of the bosons the JT Hamiltonian is given by

$$\begin{aligned}
H &= \hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3 + \frac{3}{2}\right) + \\
&\quad \frac{\sqrt{3}\hbar V_T}{4\sqrt{\mu\omega}}\left[S_+(a_1^\dagger + a_2) + S_-(a_1 + a_2^\dagger) + \frac{1}{\sqrt{2}}(S_+^2 - S_-^2)(a_3^\dagger - a_3)\right].
\end{aligned} \tag{5.22}$$

As we mentioned before, the Hamiltonian Eq. (5.22) is not spherically symmetric. When the term $(S_+^2 - S_-^2)(a_3^\dagger - a_3)$ is ignored the Hamiltonian H becomes spherically symmetric and its "isolated exact" or "quasi-exact" solutions can be obtained. In fact, the effect of the last term is small compared with the other terms.

Here we develop a different procedure to obtain approximate diagonal form of H by applying an appropriate Lie-type transformation. Consider the following transformation operator:

$$T = -\frac{\kappa}{\omega}\left[S_+(a_1^\dagger + a_1 + a_3) - S_-(a_1^\dagger + a_1 + a_3^\dagger) + \frac{1}{\sqrt{2}}(S_+^2 - S_-^2)(a_3^\dagger + a_3)\right] \tag{5.23}$$

The constant κ is defined by

$$\kappa = \frac{\sqrt{3}\hbar V_T}{4\sqrt{\mu\omega}}. \tag{5.24}$$

Under T, the Hamiltonian Eq. (5.22) transforms according to

$$\begin{aligned} \widetilde{H} &= e^T H e^{-T} \\ &\approx \omega \sum_{i=1}^{3} \left[\left(a_i^\dagger a_i + \frac{3}{2} \right) - \kappa \left(S_+ a_i + S_- a_i^\dagger \right) \right] + O\left(\frac{\kappa^2}{\omega^2} \right). \end{aligned} \tag{5.25}$$

The transformation of H is easily proven by using the identity

$$e^T H e^{-T} = H - [H, T] + \frac{1}{2!}[[H, T], T] - \cdots . \tag{5.26}$$

We assume that the coupling constant κ is smaller than ω, thus $\frac{\kappa^2}{\omega^2} \ll 1$, therefore we can neglect the higher order terms in Eq. (5.25). Amazingly interesting that the resultant Hamiltonian Eq. (5.25) is same as Dicke Hamiltonian with RWA and it can analytically be solved.

We conclude that t_2 type tetrahedral structure consists of three oscillator and they interact with T_1 ion. We have proven that when the interaction between T_1 ion and t_2-modes are weak then $T \otimes t$ JT Hamiltonian can be expressed as the sum of three Dicke Hamiltonian. Our formalism provides a solution of the problem which allows us to discuss the JT effects in the Dicke model.

5.3 Results and Discussion

In this section, we present a procedure to solve the Hamiltonian Eq. (5.25). There are several methods to obtain exact solution of $\widetilde{H}$. Constant of motion commutes with the Hamiltonian, $\widetilde{H}$, is given by

$$N = \sum_{i=1}^{3} a_i^\dagger a_i + S_0. \tag{5.27}$$

We note that $\widetilde{H}$ possesses $SU(2)$ symmetry. The total number operator N is a diagonal operator and its states can exactly be obtained. Since $\widetilde{H}$ and N commutes, they have the same eigenstates. It is obvious that the eigenstates of N can be obtained from the eigenvalue equation $N\psi = n\psi$, where n is the total quantum number. Let us consider the following form of the eigenstate:

$$|\psi\rangle = \left[c_1 |n_1, n_2, n_3\rangle, \quad c_2 |m_1, m_2, m_3\rangle, \quad c_3 |\ell_1, \ell_2, \ell_3\rangle\right]^T \tag{5.28}$$

where c_i are normalization constants and superscript T stands for transpose of the row vector. The expression Eq. (5.28) becomes the eigenstate of N, when the vibrational quantum numbers constrained to:

$$\sum_{i=1}^{3} n_i + 1 = \sum_{i=1}^{3} m_i = \sum_{i=1}^{3} \ell_i - 1 = n \tag{5.29}$$

In order to obtain a simplified results, the bosons are rotated by the operator

$$U = \exp\left(\beta(a_1^\dagger a_3 - a_3^\dagger a_1)\right) \exp\left(\alpha(a_1^\dagger a_2 - a_2^\dagger a_1)\right) \tag{5.30}$$

and provides the following expressions

$$\begin{aligned} U(a_1 + a_2 + a_3)U^{-1} &= \sqrt{3}a_1 \qquad (5.31\text{a}) \\ U(a_1^\dagger + a_2^\dagger + a_3^\dagger)U^{-1} &= \sqrt{3}a_1^\dagger \end{aligned}$$

when $\alpha = \pi/4$ and $\beta = \cos^{-1}\left(\sqrt{2/3}\right)$. The term $a_i^\dagger a_i$ is invariant under U, then the Hamiltonian takes the form

$$\widetilde{H} = \sum_{i=1}^{3} \omega \left(a_i^\dagger a_i + \frac{3}{2}\right) + \sqrt{3}\kappa \left(S_+ a_1 + S_- a_1^\dagger\right). \tag{5.32}$$

The solution of the Eq. (5.32) is straightforward. Since the Hamiltonian $\widetilde{H}$ is transformed to a different basis, the eigenstate (5.28) should be reexpressed for the Hamiltonian Eq. (5.32). For this purpose we introduce the following eigenstate

$$|\psi\rangle = \left[c_1 |n_1 - 1\rangle |n_2, n_3\rangle\,,\ c_2 |n_1\rangle |m_2, m_3\rangle\,,\ c_3 |n_1 + 1\rangle |\ell_2, \ell_3\rangle\right]^T \tag{5.33}$$

Action of the bosons on the state is given by

$$a_i |n_i\rangle = \sqrt{n_i}\, |n_i - 1\rangle\,; \quad a_i^\dagger |n_i\rangle = \sqrt{n_i + 1}\, |n_i + 1\rangle \tag{5.34}$$

then, the eigenvalue equation $\widetilde{H}\,|\psi\rangle = E\,|\psi\rangle$ leads to the following equations:

$$\begin{aligned} \left[c_1(\omega(n + \frac{1}{2}) - E)\, |n_2, n_3\rangle + c_2\sqrt{6}\kappa\sqrt{n_1}\, |m_2, m_3\rangle\right] &= 0 \\ \left[c_2(\omega(n + \frac{3}{2}) - E)\, |m_2, m_3\rangle + \sqrt{6}\kappa\left(c_1\sqrt{n_1}\, |n_2, n_3\rangle + c_3\sqrt{n_1 + 1}\, |\ell_2, \ell_3\rangle\right)\right] &= 0 \qquad (5.35) \\ \left[c_3(\omega(n + \frac{5}{2}) - E)\, |\ell_2, \ell_3\rangle + c_2\sqrt{6}\kappa\sqrt{n_1 + 1}\, |m_2, m_3\rangle\right] &= 0 \end{aligned}$$

Eliminating $c_1 |n_2, n_3\rangle\,,\ c_2 |m_2, m_3\rangle\,,\ c_3 |\ell_2, \ell_3\rangle$ between Eq. (5.35) and solving the set of equation for energy E, we obtain

$$E = \begin{cases} \left(n + \frac{3}{2}\right)\omega + (-1)^{1/3}\,\frac{P}{3^{2/3}} - \frac{(-1)^{2/3}Q}{3^{1/3}P} \\ \left(n + \frac{1}{2}\right)\omega - \frac{P}{3^{2/3}} - \frac{Q}{3^{1/3}P} \\ \left(n + \frac{5}{2}\right)\omega - (-1/3)^{2/3}\,P + \frac{(-1/3)^{1/3}Q}{P} \end{cases} \tag{5.36}$$

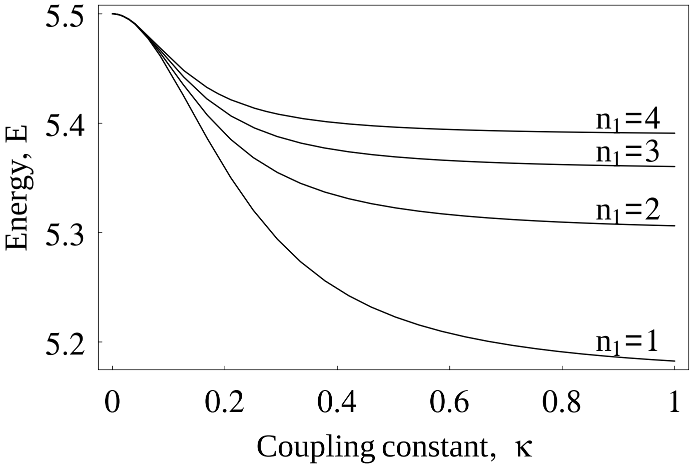

Figure 5.1: Plots of the energy E against the JT coupling strengt κ. Unit of the energy is $\hbar\omega$.Total vibrational quantum number $N = 4$.

where Q and P are given by

$$\begin{aligned} Q &= 6\kappa^2(2n_1+1)+\omega^2 \\ P &= \left[-27\omega\kappa^2+\sqrt{729\omega^2\kappa^4(2n_1+1)-3Q^3}\right]^{1/3}. \end{aligned} \tag{5.37}$$

When $\kappa = 0$, the eigenvalues reduces to the eigenvalues of the 3−level shifted harmonic oscillator with the eigenvalues

$$E = \begin{cases} \left(n+\frac{3}{2}\right)\omega \\ \left(n+\frac{1}{2}\right)\omega \\ \left(n+\frac{5}{2}\right)\omega \end{cases}. \tag{5.38}$$

Plots are made for the energy levels for which $n = 4$ and $n_1 = 1, 2, 3, 4$ in FIG 1.

The eigenstates $|\psi\rangle$ can easily be written using boson operators acting on the vacuum state $|0\rangle$:

$$|\psi\rangle = \left[c_1 a_1^{\dagger n_1-1} a_2^{\dagger n_2} a_3^{\dagger n_3}, c_2 a_1^{\dagger n_1} a_2^{\dagger n_2} a_3^{\dagger n_3}, c_3 a_1^{\dagger n_1+1} a_2^{\dagger n_2} a_3^{\dagger n_3}\right]^T |0,0,0\rangle \tag{5.39}$$

Approximate eigenstate of the original Hamiltonian Eq. (5.32) can be obtained from the relation

$$|n_1, n_2, n_3\rangle = Ue^{-T}|\psi\rangle \approx U(1-T)|\psi\rangle \tag{5.40}$$

The results of our study show that the eigenvalues and eigenstates of the $T \otimes t$ JT Hamiltonian can be approximately described when the frequency ω of the oscillation larger than the interaction constant.

CHAPTER 6

CONCLUSION

In this thesis, we have found the spectrum of the JT Hamiltonian and some quantum mechanical potentials by using the Lie algebraic technique. Generally,the physical systems can be expressed of generators of the Lie (super)algebra in terms of boson and fermions. The Hamiltonians of the various physical systems can be written as combinations of the generators of the symmetry group. We known that general formalism of the JT effect, a degenerate electronic state corresponding to a representation of Γ of symmetry group G of the molecule interact with the vibrational modes corresponding representations contained in the symmetric part of the direct product $\Gamma\otimes\Gamma$. In this aspect $T\otimes t,\ T\otimes e,\ \ E\otimes\epsilon\ and\ E\otimes\beta$ JT matrices and JT Hamiltonians have been obtained.

We have developed a general procedure to obtain the eigenstates and eigenvalues of the various potentials in terms of the orthogonal polynomials. The recurrence relations of the polynomials which represent the eigenstates of the corresponding potentials are obtained. We have proven that these potentials can be obtained from each other by suitable transformations. It is interesting to observe that the polynomial of energy occurring in the eigenfunctions of the QES Eckart, QES Hultén and the QES Rosen-Morse potentials satisfy the same recurrence relation. We have also proven that the QES Eckart and QES Rosen Morse potentials can be related to the QES Coulomb and anharmonic oscillator potentials.

We have presented a quasi exact solution of the $E\otimes\epsilon$ JT Hamiltonian which has invariant under the $osp(2,2)$ Lie superalgebra by using two different ways. The first way, JT Hamiltonian is reduced two independent sets of first order Schrödinger equation in the Bargmann's Hilbert space then the Hamiltonian is expressed combinations of the generators of $osp(2,2)$ algebra. In the second way instead of this tedious transformations, the fermion boson realization of the $osp(2,2)$ algebra have been constructed in the form of one variable two dimensional differential equation then the $E\otimes\epsilon$ JT Hamiltonian can be expressed in terms of the generators of the corresponding algebra. We have obtained the recurrence relation, eigenstates and eigenvalues of the Hamiltonian for each ways. These methods given in this thesis constitutes the most general Lie algebraic analysis of the JT interaction for $E \otimes \epsilon$ system. The success of our analysis leads us to connection between isolated exact and quasi exact solutions. We conclude that it is possible to study isolate, exactly solvable optical systems in the framework of quasi-exact solvability. In this way, isolated exact solutions of the JT Hamiltonians are put in the correspondence with the solutions of the QES Hamiltonians.

Also in this thesis $T \otimes t$ and JC Hamiltonians can be solved by developing a transformation procedure using the RWA. In quantum physics the application of the RWA usually leads to symmetry breaking: the representation space of the whole system is then divided into invariant subspaces, which strongly simplifies the mathematical complexity of the problem and usually provides the exact solution of the Hamiltonian. An approximate form of the Hamiltonians have been found in the framework of the RWA. The resultant Hamiltonians can be solved analytically and its eigenvalues can be obtained in closed form. We have shown that in the weak coupling limit the JT models may be recognized as the Dicke model. The method presented here is comparatively simple and can easily be used to obtain approximate solutions of the other JT systems.

In the future we hope that, all the suggested methods can be generalized in various directions. Invariant subspaces of the multi-boson and multi-fermion and other JT systems can be obtained by extending the method given in this study.

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APPENDIX A

MATHEMATICA PROGRAM TO OBTAIN MATRIX GENERATORS OF SO(3) GROUPS

This program computes the matrix generators of SO(3) group and its subgroup. JP and JM are ladder operators of J_+ and J_-. $J3$ is the z component of the angular momentum quantum operator and j is the angular momentum quantum number.

$$\begin{aligned}
j &= 1 \\
m &= 2j+1 \\
JP &= Table[0,\{i,1,m\},\{k,1,m\}]; \\
J3 &= JP; \\
Do[ii &= j-1;\ JP[[i,i+1]] = \sqrt{j(j+1)-ii(ii+1)},\{i,1,m-1\}; \\
Do[J3[[i,i]] &= j-i+1,\{i,1,m\}; \\
JM &= Transpose[JP]; \\
J1 &= \frac{1}{2}(JP+JM); \\
J2 &= \frac{1}{2I}(JP-JM); \\
A &= FullSimplify[MatrixExp[2IPi(J1+J2+J3)/3\sqrt{3}] \\
B &= FullSimplify[MatrixExp[2IPiJ3/4]
\end{aligned}$$

A and B corresponding to the octohedral matrix generators.

APPENDIX B

MATHEMATICA PROGRAM TO OBTAIN THE JAHN TELLER INTERACTION MATRICES

The coupling states of the Jahn Teller potential form is $V = \sum_{i=1}^{m}\sum_{j=1}^{m}\sum_{k=1}^{n} F_{i,j,k}x_i x_j q_k$. x_i and x_j refer to electronic coordinates and, q_k refer to nuclear coordinates. m and n corresponding dimension of couplings. For $E \otimes \beta$ the value of $m = 2$ and $n = 1$, for $E \otimes e$, the value of $m = 2$ and $n = 2$, for $T \otimes e$, the value of $m = 3$ and $n = 2$, for $T \otimes t$, the value of $m = 3$ and $n = 3$. $G_m[1]$ and $G_n[2]$ are the generators which have calculated by using the mathematica program which are given in appendix A. We have also given these generators in Chapter 3 for each couplings.

$$\begin{aligned}
m &= 3;\ n = 3;\\
V &= \sum_{i=1}^{m}\sum_{j=1}^{m}\sum_{k=1}^{n} F_{i,j,k} x_i x_j q_k;\\
T &= Flatten[Table[F_{i,j,k}, \{i,1,m\}, \{j,1,m\}, \{k,1,n\}]\\
S1 &= Simplify[Join[Table[x_i \to Sum[G_m[1][[i,j]]x_j, \{j,1,m\}, \{i,1,m\}],\\
Table[q_i &\to Sum[G_n[2][[i,j]]q_j, \{j,1,n\}, \{i,1,n\}]]]\\
S2 &= Simplify[Join[Table[x_i \to Sum[G_m[1][[i,j]]x_j, \{j,1,m\}, \{i,1,m\}],\\
Table[q_i &\to Sum[G_n[2][[i,j]]q_j, \{j,1,n\}, \{i,1,n\}]]]\\
VF &= Expand[V/.S1] - V;\\
SVF &= Table[D[VF, x_i, x_j, q_k] == 0, \{i,1,m\}, \{j,1,m\}, \{k,1,n\}]//Flatten;\\
L1 &= Flatten[Solve[SVF, T]];\\
L1 &= Expand[L1];\\
V &= V/.L1;\\
V &= Expand[V]\\
VF &= Expand[V/.S2] - V;\\
SVF &= Table[D[VF, x_i, x_j, q_k] == 0, \{i,1,m\}, \{j,1,m\}, \{k,1,n\}]//Flatten\\
L1 &= Flatten[Solve[SVF, T]];\\
L1 &= Expand[L1];\\
V &= V/.L1;\\
V &= Expand[V]\\
JTM &= Table[D[V, x_i, x_j], \{i,1,m\}, \{j,1,m\}];
\end{aligned}$$

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