EXACT SUPERSYMMETRIC SOLUTION OF SCHRÖDINGER EQUATION FOR SOME POTENTIALS

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ABSTRACT

EXACT SUPERSYMMETRIC SOLUTION OF SCHRÖDINGER EQUATION FOR SOME POTENTIALS

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Exact solution of the Schrödinger equation with some potentials is obtained. The normal and supersymmetric cases are considered. Deformed ring-shaped potential is solved in the parabolic and spherical coordinates. By taking appropriate values for the parameter q, similar results are obtained for Hulthén and exponential type screened potentials. Similarly, Morse, Pöschl-Teller and Hulthén potentials are solved for the supersymmetric case. Supersymmetric solution of PT-/non-PT-symmetric and non-Hermitian Morse potential is also studied. The Nikiforov-Uvarov and Hamiltonian Hierarchy methods are used in the calculations. Eigenfunctions and corresponding energy eigenvalues are calculated analytically. Results are in good agreement with the ones obtained before.

Keywords: Supersymmetric Quantum Mechanics, Exactly Solvable Potentials, PT-Symmetric Quantum Mechanics, Hierarchy of Hamiltonian, Nikiforov-Uvarov Method.

ÖZ

BAZI POTANSİYELLERLE SCHRÖDİNGER DENKLEMİNİN SÜPERSİMETRİK TAM ÇÖZÜMLERİ

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Bazı potansiyellerle Schrödinger denkleminin tam çözümleri elde edildi. Normal ve süpersimetrik durumlar dikkate alındı. Parabolik ve küresel koordinatlarda deforme olmuş halka şekilli potansiyel çözüldü. q parametresi için uygun değerler alınarak, benzer sonuçlar Hulthén ve eksponansiyel tipteki perdelenmiş potansiyeller için elde edildi. Benzer şekilde süpersimetrik durum için Morse, Pöschl-Teller ve Hulthén potansiyelleri çözüldü. Ayrıca parite-zaman geri dönüşümlü, simetrik veya simetrik olmayan ve hermityen olmayan Morse potansiyelinin süpersimetrik çözümleri elde edildi. Bu hesaplamalarda Nikiforov-Uvarov ve Hamiltonyen hiyerarşi metodları kullanıldı. Özfonksiyonlar ve bunlara karşılık gelen enerji özdeğerleri analitik olarak hesaplandı. Sonuçlar, daha önceden elde edilenlerle iyi bir uyum içindedir.

Anahtar Kelimeler: Süpersimetrik Kuantum Mekaniği, Tam Çözülebilir Potansiyeller, Parite-Zaman Simetrik Kuantum Mekaniği, Hamiltonyen Hiyerarşi, Nikiforov-Uvarov Yöntemi.

...MY WIFE

and

MY SONS...

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CHAPTER 1

INTRODUCTION

Supersymmetry is a new type of symmetry which expands our understanding of the symmetry of physical systems. Supersymmetry (SUSY) concept plays an important role for understanding the relationship between the fermions and bosons as well. Supersymmetric models provide unified description which means a Grand Unified Theory (GUT) for all basic interactions of nature such as strong, weak, electromagnetic and gravitational. This model is a necessary ingredient for any unifying approach. In SUSY, a graded Lie algebra exists. This kind of algebra satisfies certain commutation and anti-commutation relations. Supersymmetry was first discovered by Gelfand Likhtman as a work on the superalgebra in the space-time within the framework of the Poincaré algebra [1]. Later, it was reconsidered for a non-renormalizable form of supersymmetry in field theory by Volkov and Akulov [2]. Wess and Zumino introduced a model on renormalizable supersymmetric field theory [3]. SUSY is also responsible for unifying the space-time and internal symmetries of the S-matrix. The no-go theorem of Coleman and Mandula [4] which is based on the assumption of a Lie algebra is not allowed in the matrix. In addition, by incorporating SUSY to the theory of gravity, we realize the supergravity [5, 6]. Furthermore, the general theory of relativity discovered by Einstein is a necessary consequence of a local gauged SUSY. The local SUSY theories allow us to unify the gravity with the other fundamental interactions in nature. Although, no experimental evidence of SUSY has so far existed in nature, the ideas of SUSY have been applied as a new model to all branches of physics, such as atomic, molecular, nuclear, statistical, condensed matter physics and nonrelativistic quantum mechanical systems. In a supersymmetric system, supersymmetry might be broken (spontaneously broken) or unbroken. If the SUSY is unbroken, this leads to a degeneracy between the spectra of the fermions and bosons in a unified field theory. The breaking scale is of the order of the electroweak scale of 100 GeV. The conceptual problem of the symmetry breaking scale is the gravitational or Planck scale which is of the order of 10^{19} GeV. The simplest case of SUSY quantum mechanics has first been examined for a class of the dynamically broken supersymmetric quantum mechanical models by Witten [7] and Cooper and Freedman [8]. Various methods for estimating the ground state energy, including the instanton, have been applied by several workers [9, 10]. In the Witten model of SUSYQM, the Hamiltonian of a certain quantum mechanical system is denoted by a pair of $\hat{H}_{1,2}$, for which all energy levels except for the ground state energy are doubly degenerate for both $\hat{H}_{1,2}$. Various properties of the topological index (the Witten index) introduced by Witten were studied for the non-perturbative mechanism of SUSY breaking [11-23]. Using a general formalism for the nonlinear quantum mechanical σ model, a mechanism of spontaneous breaking of the supersymmetry at the quantum level related to the uncertainty of the operator has been obtained [24]. The mechanism of spontaneous breaking of the supersymmetry has also been investigated [25]. The ideas of SUSY have aroused new approaches in physics [9]. For a dynamical SUSY of even-even and even-odd nuclei, evidence has been found. A path integral formulation of SUSYQM was first given [9]. The path integrals and the Langevin equation was then used to prove algorithms about the stochastic quantization. Afterwards, the tunneling rate through double-well barriers could be determined [26-29]. The SUSYQM concepts extended to higher dimensional systems, and to systems for large number of particles are studied by several groups [30-38]. A simple realization of a SUSY algebra involving the fermionic and bosonic operators is considered in SUSYQM. The fermionic operators commute with the Hamiltonian which means that they are invariant. Thus, there is a relationship between the energy eigenvalues and the eigenfunctions of the S-matrices. It can here be noted that the degenerate Wess-Zumino field theory has not been interpreted in the context of SUSYQM. Furthermore, one has attempted for solving of some well-known potentials in SUSYQM. Recently, the exact multi-soliton solutions to certain Hamiltonians have been governed by higher order partial equations such as Korteweg de Vries and sine-Gordon equations. The solution of these equations is based on the inverse scattering methods whose potential is the solution itself. In fact, these solutions correspond to a new potential. They are related to potentials which are isospectral to the single soliton potential. The soliton solutions have been investigated for field equations defined in space-time. The kinks in field theory are an example of soliton in $1+1$ dimensions [39-43]. In SUSYQM formalism, the Dirac equation have been studied for several aspects [44-46]. This formalism has also been extended as a model for parasupersymmetric quantum mechanics [47-49] and orthosupersymmetric quantum mechanics [50]. The other notable aspect of SUSYQM is the Hamiltonian Hierarchy method also known as the factorization method introduced first by Schrödinger [51] to solve the hydrogen atom problem algebraically. This method was recognized as a rediscovery of a technique attributable to Darboux [52]. Later, Infeld and Hull [53] generalized the method to obtain a wide class of solvable potentials by considering six different forms. Gendenshtein [54] introduced the shape invariance concept. If a potential is shape invariant, then its SUSY partner potential has the same spatial dependence as the original potential with a translation parameter. The formulation of SUSYQM has also been developed by several groups [55, 56]. Using both the factorization method and the concept of shape invariance, the nonlinear first-order Riccati equation is reformulated for obtaining the exact eigenvalue spectra [57]. In this approach, the solution of the second order Schrödinger equation for a given potential reduces to the first-order Riccati equation involving the superpotential $W(x)$. The solutions of this equation are the result of the superpotential $W(x)$ of a given potential $V(x)$. Several methods have been developed in the framework of SUSYQM [58-62]. Because of the interesting properties of SUSYQM, it has also been applied to other branches of physics. As an example, the Jaynes-Cummings model for a two-level atom interacting with an electromagnetic field is analyzed in terms of SUSYQM [63]. Recently, PT-symmetric quantum systems have been studied within the context of SUSYQM [64, 65]. For scattering states, the SUSYQM formalism has been applied in nonrelativistic quantum mechanics [66, 67].

The thesis is organized as follows: In chapter 2, we give a review of SUSYQM extensively. In chapter 3, we introduce perturbative and semiclassical approaches based on SUSYQM as well as the Nikiforov-Uvarov (NU) method. In chapter 4, we present the important results. In the last chapter, we generally discuss the results of SUSYQM together with our results.

CHAPTER 2

BASIC FORMALISM OF SUSYQM

2.1 Review of SUSYQM

In this section, we will calculate the possible forms of the energy eigenvalues and eigenfunctions with the two partner Hamiltonians $\hat{H}_L$ and $\hat{H}_R$ respectively. Let us assume that one dimensional Schrödinger equation for the ground state wave function $\Psi_0(x)$ is

$$\hat{H}_L \Psi_0(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_L(x) \right] \Psi_0(x) = 0, \tag{2.1}$$

where we choose the ground state energy $E_0^{(L)}$ of $\hat{H}_L$ to be zero. Solving the Eq. (2.1) for $V_L(x)$, we have

$$V_L(x) = \frac{\hbar^2}{2m} \frac{\Psi_0''(x)}{\Psi_0(x)}. \tag{2.2}$$

Thus, we can globally reconstruct of $V_L(x)$ from the ground state wave function that has no nodes. Using a Hermitian positive semi-definite operator in which $\hat{\Omega}^\dagger$ is the Hermitian adjoint of the operator $\hat{\Omega}$, one can factorize the first partner Hamiltonian as

$$\hat{H}_L(x) = \hat{\Omega}^\dagger\ \hat{\Omega}, \tag{2.3}$$

where

$$\hat{\Omega}^\dagger = W(x) - \frac{i}{\sqrt{2m}}\hat{p}, \quad \hat{\Omega} = W(x) + \frac{i}{\sqrt{2m}}\hat{p}, \tag{2.4}$$

with $\hat{p} = -i\hbar\frac{d}{dx}$. In Eq. (2.4), $W(x)$ is known as the Witten superpotential. Therefore, the first partner Hamiltonian in terms of this superpotential leads to the well-known nonlinear Riccati equation:

$$V_L(x) - W^2(x) + \frac{\hbar}{\sqrt{2m}}W'(x) = 0. \tag{2.5}$$

Here, $W'(x)$ is the first order derivative of the superpotential $W(x)$. The Witten superpotential is given through the ground state wave function as

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\left(\frac{\Psi_0'}{\Psi_0}\right) = -\frac{\hbar}{\sqrt{2m}}\frac{d}{dx}\ln[\Psi_0(x)], \tag{2.6}$$

where

$$\Psi_0(x) = N\exp\left[-\frac{\sqrt{2m}}{\hbar}\int^x W(x')dx'\right]. \tag{2.7}$$

As a second step, one can construct the other partner Hamiltonian $\hat{H}_R$ for $V_R(x)$,

$$\hat{H}_R = \hat{\Omega}\hat{\Omega}^\dagger = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_R(x)\right], \tag{2.8}$$

and this yields

$$V_R(x) - W^2(x) - \frac{\hbar}{\sqrt{2m}} W'(x) = 0. \tag{2.9}$$

The potentials $V_L(x)$ and $V_R(x)$ which are connected by $W(x)$ are known as supersymmetric partner potentials. We also note that the quadratic terms $W^2(x)$ in Eqs. (2.5) and (2.9) are the average of the partner potentials $V_L(x)$ and $V_R(x)$, while $W'(x)$ is proportional with the commutators of $\hat{\Omega}$ and $\hat{\Omega}^\dagger$:

$$\begin{aligned} \frac{1}{2}[V_L(x) - V_R(x)] &= \frac{\hbar^2}{2m}\frac{d}{dx}\left(\frac{\Psi_0'}{\Psi_0}\right) \\ &= \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\ln \Psi_0(x)\right] \\ &= -\frac{\hbar}{\sqrt{2m}} W', \end{aligned} \tag{2.10}$$

and

$$\begin{aligned} \frac{1}{2}[V_L(x) + V_R(x)] &= \frac{\hbar^2}{2m}\left(\frac{\Psi_0'}{\Psi_0}\right)^2 \\ &= W^2(x), \end{aligned} \tag{2.11}$$

and also

$$[\hat{\Omega}, \hat{\Omega}^\dagger] = \sqrt{\frac{2\hbar^2}{m}} W'(x). \tag{2.12}$$

Moreover, the addition and substraction of the commutators between $[\hat{\Omega}, \hat{\Omega}^\dagger]$ and $[\hat{\Omega}^\dagger, \hat{\Omega}]$ give the significant results as

$$[\hat{\Omega}, \hat{\Omega}^\dagger] + [\hat{\Omega}, \hat{\Omega}^\dagger] = [\hat{\Omega}, \hat{\Omega}^\dagger] - [\hat{\Omega}^\dagger, \hat{\Omega}] = \frac{4\hbar}{\sqrt{2m}} W'(x), \tag{2.13}$$

and

$$[\hat{\Omega}, \hat{\Omega}^\dagger] - [\hat{\Omega}, \hat{\Omega}^\dagger] = [\hat{\Omega}, \hat{\Omega}^\dagger] + [\hat{\Omega}^\dagger, \hat{\Omega}] = 0. \tag{2.14}$$

Now, let us assume that $\Psi_n^{(L)}$ and $\Psi_n^{(R)}$ denote the eigenfunctions of the bosonic Hamiltonians $\hat{H}_L$ and $\hat{H}_R$ with the energy eigenvalues $E_n^{(L)}$ and $E_n^{(R)}$ respectively. In the wave function Ψ_n, the integer n represent the number of nodes and it takes the non-negative values greater then or equal to zero. Here, we will prove that the partner potentials V_L and V_R have identical bound-state spectra except for the ground state energy $E_0^{(L)} = 0$. In SUSYQM approach, we consider a pair of Schrödinger equations for $n > 0$ as

$$\begin{aligned} \hat{H}_L\Psi_n^{(L)} &= \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V_L(x)\right]\Psi_n^{(L)} \\ &= \hat{\Omega}^\dagger\hat{\Omega}\Psi_n^{(L)} \\ &= E_0^{(L)}\Psi_n^{(L)}. \end{aligned} \tag{2.15}$$

Similarly, one can introduce the other supersymmetric Hamiltonian by the iterating process

$$\begin{aligned} \hat{H}_R\Psi_n^{(R)} &= \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V_R(x)\right]\Psi_n^{(R)} \\ &= \hat{\Omega}\hat{\Omega}^\dagger\Psi_n^{(R)} \\ &= E_0^{(R)}\Psi_n^{(R)}, \end{aligned} \tag{2.16}$$

where $E_0^{(i)} < E_1^{(i)} < E_2^{(i)} \ldots$ for $i = L, R$. Especially, assuming that $\Psi_n^{(L)}$ is the eigenfunction of $\hat{H}_L$ with the eigenvalue $E_n^{(L)}$, then $\hat{\Omega}\Psi_n^L$ is an eigenfunction of $\hat{H}_R$ the same eigenvalue. Therefore, the Eqs. (2.15) and (2.16) yield to

$$\hat{H}_R\left[\hat{\Omega}\Psi_n^{(L)}\right] = \hat{\Omega}\hat{\Omega}^\dagger(\hat{\Omega}\Psi_n^{(L)})$$

$$\begin{aligned} &= \hat{\Omega}(\hat{H}_L\Psi_n^{(L)}) \\ &= E_n^{(L)}(\hat{\Omega}\Psi_n^{(L)}). \end{aligned} \tag{2.17}$$

Similarly, if $\Psi_n^{(R)}$ is an eigenfunction of $\hat{H}_R$ with the eigenvalue $E_n^{(R)}$, then $\hat{\Omega}^\dagger\Psi_n^{(R)}$ is also an eigenfunction of $\hat{H}_L$ with the same eigenvalue:

$$\begin{aligned} \hat{H}_L\left[\hat{\Omega}^\dagger\Psi_n^{(R)}\right] &= \hat{\Omega}^\dagger\hat{\Omega}(\hat{\Omega}^\dagger\Psi_n^{(R)}) \\ &= \hat{\Omega}^\dagger(\hat{H}_R\Psi_n^{(R)}) \\ &= E_n^{(R)}(\hat{\Omega}^\dagger\Psi_n^{(R)}). \end{aligned} \tag{2.18}$$

From the Eqs. (2.17) and (2.18), we conclude that these two supersymmetric partner Hamiltonians $\hat{H}_L$ and $\hat{H}_R$ are isospectral (or almost isospectral) and their normalized eigenfunctions are related by the following transformations:

$$\Psi_n^{(R)} = \frac{\hat{\Omega}\Psi_{n+1}^{(L)}(x)}{\sqrt{E_n^{(R)}}}, \tag{2.19}$$

and

$$\Psi_{n+1}^{(L)} = \frac{\hat{\Omega}^\dagger\Psi_n^{(R)}(x)}{\sqrt{E_{n+1}^{(L)}}}. \tag{2.20}$$

The normalized eigenfunctions of $\hat{H}_L$ and $\hat{H}_R$ are also connected by the relation as

$$\Psi_n^{(R)} = \frac{\hat{\Omega}\Psi_{n+1}^{(L)}(x)}{\sqrt{E_{n+1}^{(R)} - E_0^{(R)}}}. \tag{2.21}$$

For unbroken SUSY case in which $E_0^{(L)} = 0$ and $\hat{\Omega}\Psi_0^{(L)} = 0$, the eigenstate of $\hat{H}_R$ corresponding to $\Psi_0^{(L)}$ is not available and the relation

$$E_{n+1}^{(L)} = E_n^{(R)}, \qquad n = 0, 1, 2\ldots \tag{2.22}$$

The successive equations (2.19)-(2.21) imply that if the wave function $\Psi_{n+1}^{(L)}$ of $\hat{H}_L$ is normalizable, then $\Psi_n^{(R)}$ of $\hat{H}_R$ is also normalizable. Furthermore, when the operators $\hat{\Omega}$ and $\hat{\Omega}^\dagger$ are operated on the eigenfunctions $\hat{H}_L$ and $\hat{H}_R$ respectively, that is, they convert the eigenfunctions of $\hat{H}_L$ to that of $\hat{H}_R$ or vice versa with the same energy spectra. While $\hat{\Omega}$ destroys an extra node in the eigenfunction, the other one creates it. Due to the fact that the ground state wave function of $\hat{H}_L$ is annihilated by the operator $\hat{\Omega}$, only this state has no SUSY partner but the others are. By using the operator $\hat{\Omega}$, if we know all the eigenfunctions of $\hat{H}_L$, we can determine those of $\hat{H}_R$. In addition to that, using $\hat{\Omega}^\dagger$ we can reconstruct the eigenfunctions of $\hat{H}_L$ from those of $\hat{H}_R$ except for the ground state. This situation is illustrated in the Fig. 2.1. They are degenerate except that $V_L(x)$ has an extra energy eigenstate at zero energy $E_0^{(L)}$. The action operators $\hat{\Omega}^\dagger$ and $\hat{\Omega}$ (raising and lowering) are shown with the connected eigenfunctions.

In the case of $\hat{\Omega}\Psi_0^{(L)} \neq 0$ (broken SUSY case), all bound states including the ground state and further all the eigenstates of two Hamiltonians are paired, *e.g.*, the relations:

$$\Psi_n^{(R)}(x) = \frac{\hat{\Omega}\Psi_n^{(L)}(x)}{\sqrt{E_n^{(L)}}}, \tag{2.23}$$

and

$$\Psi_n^{(L)}(x) = \frac{\hat{\Omega}^\dagger\Psi_n^{(R)}(x)}{\sqrt{E_n^{(R)}}}, \tag{2.24}$$

and also

$$E_n^{(L)} = E_n^{(R)} > 0, \qquad n = 0, 1, 2\ldots \tag{2.25}$$

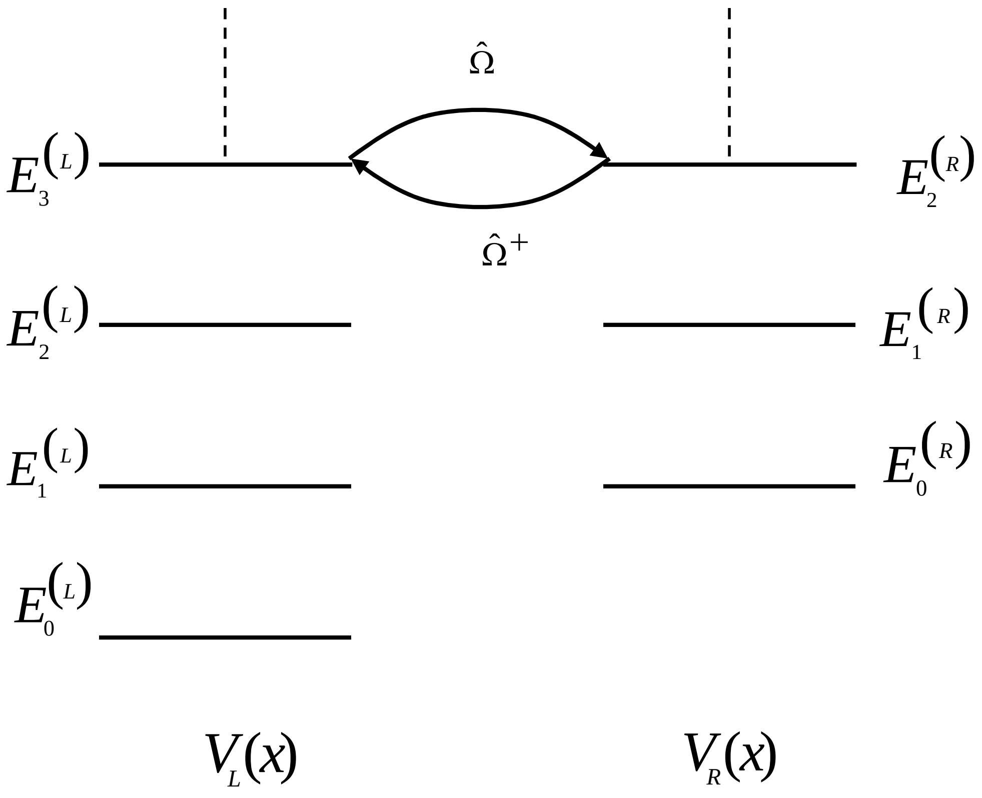


Figure 2.1: The energy levels of two supersymmetric partner potentials $V_L(x)$ and $V_R(x)$ for unbroken SUSY case.

2.2 Supersymmetric Generators

A quantum mechanical system is characterized by a self-adjoint Hamiltonian $\hat{H}$. This type of system is called as a supersymmetric one by $\hat{H}_{SUSY}$ if there exists supercharge operators, $\hat{Q}_i$ $(i = 1, 2, \ldots\ N)$, which are also self-adjoint, *i.e.*, $\hat{Q}_i = \hat{Q}_i^\dagger$. For $N = 2$, the operators $\hat{Q}_i$ and $\hat{Q}_i^\dagger$ convert a bosonic degree of freedom into fermionic ones and vice versa. Let us now introduce SUSY charge operators $\hat{Q}_i$ and $\hat{Q}_i^\dagger$ using a Hermitian positive semi-definite operator $\hat{\Omega}^\dagger$ and its adjoint $\hat{\Omega}$ in 2×2 matrix form

$$\hat{Q} = \begin{pmatrix} 0 & 0 \\ \hat{\Omega} & 0 \end{pmatrix}, \qquad \hat{Q}^\dagger = \begin{pmatrix} 0 & \hat{\Omega}^\dagger \\ 0 & 0 \end{pmatrix}. \tag{2.26}$$

To construct a supersymmetric system which has the degeneracy as $\hat{H}_L$ and $\hat{H}_R$, we consider the supersymmetric Hamiltonian, $\hat{H}_{SUSY}$

$$\begin{aligned} H_{SUSY} &= \hat{Q}\hat{Q}^\dagger + \hat{Q}^\dagger\hat{Q} \\ &= \begin{pmatrix} \hat{\Omega}^\dagger\hat{\Omega} & 0 \\ 0 & \hat{\Omega}\hat{\Omega}^\dagger \end{pmatrix} \\ &= \begin{pmatrix} \hat{H}_L & 0 \\ 0 & \hat{H}_R \end{pmatrix}. \end{aligned} \tag{2.27}$$

The SUSY Hamiltonian is a 2×2 block diagonal matrix. We also note that this Hamiltonian implies the commutation and anti-commutation relations for both bosonic and fermionic operators. They satisfy the following superalgebra as

$$[\hat{Q}, \hat{H}_{SUSY}] = [\hat{Q}^\dagger, \hat{H}_{SUSY}] = 0, \qquad \{\hat{Q}, \hat{Q}^\dagger\} = \hat{H}_{SUSY}, \tag{2.28}$$

and

$$\{\hat{Q}, \hat{Q}\} = 2\hat{Q}^2 = 0, \qquad \{\hat{Q}^\dagger, \hat{Q}^\dagger\} = 2(\hat{Q}^\dagger)^2 = 0. \tag{2.29}$$

Because of this algebra, we conclude that the spectrum of supersymmetric system has a positive semi-definite structure. For $N = 2$, supersymmetric algebra can be extended by means of the Hermitian SUSY generators

$$[\hat{Q}_i, \hat{H}_{SUSY}] = 0, \qquad \{\hat{Q}_i, \hat{Q}_j\} = \delta_{ij}\hat{H}_{SUSY}; \qquad \hat{Q}_i = \hat{Q}_i^\dagger, \tag{2.30}$$

where $(i, j = 1, 2, \ldots N)$. In these equations, $\hat{Q}_i$ and $\hat{H}_{SUSY}$ are functions of a number of bosonic and fermionic lowering and raising operators respectively denoted by $\hat{b}_i, \hat{b}_i^\dagger$ $(i = 1, 2, \ldots n_b)$ and $\hat{f}_i, \hat{f}_i^\dagger$ $(i = 1, 2, \ldots n_f)$. Here, n_b and n_f refer to boson and fermion occupation numbers. The basis vectors of bosonic and fermionic states can be described as

$$|n_b, n_f\rangle; \qquad n_b = 0, 1, 2 \ldots, \qquad n_f = 0, 1. \tag{2.31}$$

These operators $\hat{b}_i, \hat{b}_i^\dagger$ and $\hat{f}_i, \hat{f}_i^\dagger$ satisfy the following commutation and anti-commutation relations:

$$[\hat{b}_i, \hat{b}_i^\dagger] = \delta_{ij}, \qquad \{\hat{f}_i, \hat{f}_i^\dagger\} = \delta_{ij}; \qquad \hat{f}_i^2 = (\hat{f}_i^\dagger)^2 = 0, \tag{2.32}$$

and

$$[\hat{b}_i, \hat{f}_i] = [\hat{b}_i, \hat{f}_i^\dagger] = 0. \tag{2.33}$$

In Eq. (2.32), the relation $\hat{f}_i^2 = (\hat{f}_i^\dagger)^2 = 0$ is known as the property of nilpotency. For this reason, the above expressions can be computed easily.

2.3 Supersymmetric Structure of the Hamiltonian

In the preceding section, we mention that supersymmetric generators $\hat{Q}_i$ send a bosonic state into a fermionic one and vice versa. An interaction between bosons and fermions can be described as the invariance of the Hamiltonian. Under supersymmetry transformations generated by the SUSY generators $\hat{Q}_i$, this is a consequence of nilpotent nature, *i.e.*, the relation $\hat{Q}_i^2 = (\hat{Q}_i^\dagger)^2 = 0$. We can define a simple supersymmetric model for the operators $\hat{Q}$ and $\hat{Q}^\dagger$ in the following way:

$$\hat{Q} = \hat{\Omega}(\hat{b}, \hat{b}^\dagger)\ \hat{f}, \qquad \hat{Q}^\dagger = \hat{\Omega}^\dagger(\hat{b}, \hat{b}^\dagger)\ \hat{f}^\dagger, \tag{2.34}$$

where $\hat{\Omega}$ and $\hat{\Omega}^\dagger$ are arbitrary functions of boson operators. These operators are adjoints of each other. Due to this property, the SUSY operators will also be adjoints of each other. Therefore, the SUSY Hamiltonian Eq. (2.27) will remain invariant as well. To construct a convenient supersymmetric structure, we choose the fermionic type wave functions, *i.e.*, two-component Pauli spinor as

$$\hat{\Phi}(x) = \begin{pmatrix} \phi_L(x) \\ \phi_R(x) \end{pmatrix}, \tag{2.35}$$

where the upper and lower components refer to fermion occupation numbers $n_F = 1$ and $n_F = 0$ respectively. The fermion raising and lowering operators $\hat{f}^\dagger$ and $\hat{f}$ are defined by 2×2 matrices:

$$\hat{f}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \hat{f} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{2.36}$$

The bosonic operators $\hat{\Omega}$ and $\hat{\Omega}^\dagger$ which are adjoints with each other are written in the form

$$\hat{\Omega}^\dagger = \hat{\Omega}_1 + i\hat{\Omega}_2, \qquad \hat{\Omega} = \hat{\Omega}_1 - i\hat{\Omega}_2, \tag{2.37}$$

where $\hat{\Omega}_1$ and $\hat{\Omega}_2$ are Hermitian operators. The supersymmetric generators $\hat{Q}_i$ for $N = 2$ system

$$\begin{aligned} \hat{Q}_1 &= \hat{\Omega}_1\sigma_1 + \hat{\Omega}_2\sigma_2 \\ &= \frac{1}{2}\left(\sigma_1\hat{p} + \sigma_2 W(x)\right), \end{aligned} \tag{2.38}$$

and

$$\begin{aligned} \hat{Q}_2 &= \hat{\Omega}_1\sigma_2 - \hat{\Omega}_2\sigma_1 \\ &= \frac{1}{2}\left(\sigma_2\hat{p} - \sigma_1 W(x)\right), \end{aligned} \tag{2.39}$$

where the σ_i are Pauli spin matrices and $W(x)$ is an arbitrary function of x. Also, these operators anti-commute each other. From the formal analogy between bosons, ($e.g., photons$) and fermions, ($e.g., electrons$) we can express the Hamiltonian

$$\begin{aligned} \hat{H} &= \hat{H}_B + \hat{H}_F \\ &= \frac{1}{2}\{\hat{\Omega}, \hat{\Omega}^\dagger\} + \frac{1}{2}[\hat{\Omega}, \hat{\Omega}^\dagger]\sigma_3, \end{aligned} \tag{2.40}$$

where σ_3 is a diagonal Pauli spin matrix for z-component. This Hamiltonian consists of two parts, *i.e.*, bosonic and fermionic parts. Although the bosonic and fermionic fields obey the commutation and anti-commutation relations respectively, our Hamiltonian reflects the difference between the boson and fermion statistics. The second part of the Hamiltonian $\hat{H}_F$ forms in diagonal which is the property of z-component of Pauli spin matrices. Further, the Hamiltonian includes a fermion degree of freedom only if $[\hat{\Omega}, \hat{\Omega}^\dagger] \neq 0$. For supersymmetric generators $\hat{Q}$ and $\hat{Q}^\dagger$, the arbitrary functions $\hat{\Omega}$ and its adjoint $\hat{\Omega}^\dagger$ are defined by the bosonic operators $\hat{b}$ and its adjoint $\hat{b}^\dagger$. While $\hat{b}$ has a kernel, *i.e.*, vacuum state, $\hat{b}^\dagger$ does not. The difference between the operators $\hat{\Omega}$ and $\hat{\Omega}^\dagger$ is important in the study of spontaneous supersymmetry breaking. By taking the Eq. (2.4) for mass $m = 1$ and substituting this equation into the Eq. (2.40), we obtain an expression for the SUSY Hamiltonian

$$\hat{H}_{SUSY} = \frac{1}{2}\left(\hat{p}^2 + W^2(x) + \hbar\sigma_3\frac{dW}{dx}\right). \tag{2.41}$$

This is the Witten's supersymmetric Hamiltonian. In the Eq. (2.41), we assume $|W(x)| \Rightarrow \infty$ as $|x| \Rightarrow \infty$ so that the spectrum of the SUSY Hamiltonian is discrete. In the Hamiltonian, while the first term represents usual free particle motion, the second and third terms represent the interaction of bosons with bosons and that of fermions with bosons. Because of this reason, we join the supersymmetric models with dynamical breaking of supersymmetry. Now, we want to rewrite the other forms of the SUSY Hamiltonian in the Fock space picture with the state $|n_B, n_F\rangle$ or in the Schrödinger picture with a matrix. The fermion occupation number n_f is either zero or one because the fermionic raising and lowering operators satisfy the anti-commutation relations. Therefore, we choose the ground state of $\hat{H}_L$ to have $n_f = 0$. The fermionic state number operator is

$$n_F = \frac{1-\sigma_3}{2} = \frac{1}{2} - \frac{[\Psi, \Psi^\dagger]}{2}. \tag{2.42}$$

the action operators $\hat{f}$ and $\hat{f}^\dagger$, Ψ and $\Psi^\dagger$ in the Fock space are

$$\hat{f}|n_b, n_f\rangle = |n_b - 1, n_f\rangle, \qquad \Psi|n_b, n_f\rangle = |n_b, n_f - 1\rangle, \tag{2.43}$$

and

$$\hat{f}^\dagger|n_b, n_f\rangle = |n_b + 1, n_f\rangle, \qquad \Psi^\dagger|n_b, n_f\rangle = |n_b, n_f + 1\rangle, \tag{2.44}$$

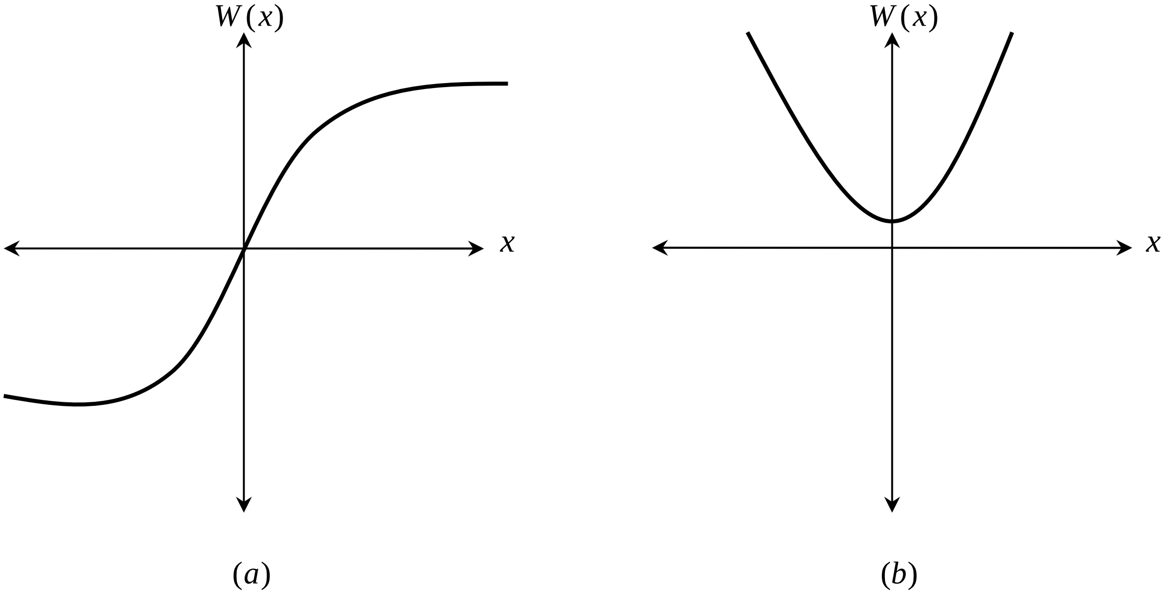
According to the boson-fermion degeneracy characteristic of the SUSY theories, the operator $\hat{Q}^\dagger = \hat{Q}\Psi^\dagger$ has the property of changing the energy state. In SUSYQM, the SUSY generators have the forms $\hat{Q} = \hat{\Omega}\Psi^\dagger$ and $\hat{Q}^\dagger = \hat{Q}^\dagger\Psi$. Hence, the general form of the SUSY Hamiltonian becomes

$$\hat{H}_{SUSY} = (-\frac{d^2}{dx^2} + W^2)\hat{I} - [\Psi, \Psi^\dagger]W'. \tag{2.45}$$

This is useful in the Lagrangian formulation of SUSYQM.

2.4 Spontaneous Breaking of Supersymmetry

Like in the usual symmetry, supersymmetry might be broken spontaneously in SUSY systems. If we know the ground state wave function of $\hat{H}_L$, then we can factorize the Hamiltonian and find a SUSY partner Hamiltonian $\hat{H}_R$. Let us now consider the case of a given superpotential $W(x)$. In this case, we have two possibilities. Using Eq. (2.4) for the operators $\hat{\Omega}$ and $\hat{\Omega}^\dagger$, we can write the



(a) (b)

Figure 2.2: (a) shows an example of the superpotential $W(x)$ for which the ground state energy is zero $E_0 = 0$ (exact SUSY), (b) corresponds to $E_0 > 0$ (unbroken SUSY case).

equations $\hat{\Omega}\Psi_0^{(L)} = 0$ and $\hat{\Omega}^\dagger\Psi_0^{(R)} = 0$ in the form

$$\left[\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + W(x)\right]\Psi_0^{(L)} = 0, \qquad \left[-\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + W(x)\right]\Psi_0^{(R)} = 0. \tag{2.46}$$

The solutions for these equations are respectively

$$\Psi_0^{(L)}(x) = N\exp\left[-\frac{\sqrt{2m}}{\hbar}\int_0^x W(x')dx'\right], \quad \int_0^x W(x')dx' \Rightarrow \infty, \quad x \Rightarrow \pm\infty, \tag{2.47}$$

and

$$\Psi_0^{(R)}(x) = N\exp\left[\frac{\sqrt{2m}}{\hbar}\int_0^x W(x')dx'\right], \quad \int_0^x W(x')dx' \Rightarrow -\infty, \quad x \Rightarrow \pm\infty, \tag{2.48}$$

where N is the normalization constant. By convention, we must choose $W(x')$ so that only one of the ground state wave functions $\Psi_0^{(L)}(x)$ and $\Psi_0^{(R)}(x)$ can be normalized. Otherwise, neither of these functions can be normalized. If a state with an energy $E = 0$ does exist, that is, the state is non-degenerate. It is implied that these ground state wave functions are normalizable. Also, we must choose $W(x)$ to be positive(negative) for large positive(negative) x. It means that the SUSY is unbroken or exact as in Fig. (2.2-a).

If there are no normalizable solutions to a state with an energy $E = 0$, it means that neither of these conditions hold. In other words, the nonnegativity of the spectrum of the SUSY Hamiltonian $\hat{H}_L$ means that the ground state has an energy $E_0 > 0$, that is the SUSY broken case as in Fig. (2.2-b).

We can generally define the distinction between spontaneous breaking of internal symmetry and supersymmetry. The Hamiltonian $\hat{H}$ is invariant under certain transformations $[\hat{H}, \Gamma] = 0$, where Γ represents the generators of the transformations but the ground state or vacuum state $|0\rangle$ is not invariant since $\Gamma|0\rangle \neq 0$. In the case of exact symmetry, without spontaneous breaking, the generators of the transformations annihilate the vacuum as $\Gamma|0\rangle = 0$. It means that the vacuum remains invariant under finite transformations of the form $\exp(i\alpha\Gamma)$, where α is a parameter.

In SUSY case, the generators of supersymmetry are the supercharge operators $\hat{Q}$ and $\hat{Q}^{\dagger}$. For unbroken SUSY case, which means exact SUSY, then we have

$$\hat{Q}|0\rangle = \hat{Q}^{\dagger}|0\rangle = 0, \tag{2.49}$$

and thus

$$\hat{H}|0\rangle = \hat{Q}^{2}|0\rangle = \hat{Q}^{\dagger^{2}}|0\rangle = 0 \tag{2.50}$$

There exists a zero energy of state. Conversely, if there is a state with a zero energy, the SUSY is exact and no spontaneous breaking is valid. The spontaneous breaking of supersymmetry is also important. We consider the supersymmetry in the field of elementary particles. It is necessary that the SUSY must be spontaneously broken. In the case of exact supersymmetry, the bosons and fermions must be in mass degenerate form.

2.5 The Witten Index

A SUSY system generates a good symmetry, *i.e.*, global symmetry. It provides us annihilation of the vacuum state by means of the supersymmetric generators $\hat{Q}$ and $\hat{Q}^{\dagger}$. Therefore, the ground state energy of the SUSY Hamiltonian must be zero. To determine whether SUSY is broken or not broken in supersymmetric field theories, Witten proposed the index

$$\Delta = Tr(-1)^{F}, \tag{2.51}$$

where the trace is taken over all bound states and continuum states of this Hamiltonian. The number of fermionic states $n_F \equiv F$ can be defined by $\frac{1}{2}(1-\sigma_3)$, where

σ_3 is the Pauli spin matrix. Using the following equation for the eigenstates of the Hamiltonian

$$\Psi_n(x) = \left(\begin{array}{c} \Psi_n^{(L)}(x) \\ \\ \Psi_n^{(R)}(x) \end{array} \right), \tag{2.52}$$

one gets the eigenvalues for ±1 of $(-1)^F$. Conventionally, the eigenvalues $(-1, +1)$ correspond to $\hat{H}_L$ and $\hat{H}_R$ respectively. The Witten index has some values as $\Delta = 0$ and $\Delta = 1$. If $\Delta = 0$ case corresponds to the broken supersymmetry. However, supersymmetry remains unbroken for non-zero Δ. In unbroken SUSY case, $\hat{Q}|0\rangle = 0$ leads to $\hat{H}|0\rangle = \hat{Q}^2|0\rangle = 0$. Moreover, if all the supersymmetries are unbroken, it is written $\sum_i \hat{Q}_i^2|0\rangle = \hat{H}|0\rangle = 0$ for any supersymmetric generator. In field theory, the Witten index needs regularizations. The determination of broken SUSY is very hard non-perturbatively. Hence, the SUSYQM gives us several different methods to understand of non-perturbative broken SUSY. In the quantum mechanical case, the breaking of SUSY is related, depending on whether having a normalizable solution or not, to the equation $\hat{Q}|0\rangle = 0|0\rangle = 0$, and it implies the Eqs. (2.47) and (2.48). These ground state wave functions do not fall off fast enough at $x = \pm\infty$. Therefore, $\hat{Q}$ does not annihilate the vacuum and the SUSY is not spontaneously broken. Using trivial calculations, the Witten index will provide the correct answer to the question of broken SUSY.

2.6 Reflection and Transmission Coefficients

Supersymmetry provides us an understanding of the relationship between the reflection $R(k)$ and transmission $T(k)$ coefficients in the case of two partner potentials $\hat{H}_L$ and $\hat{H}_R$ having continuous spectra in scattering concept. Let us now consider an incident plane wave e^{ikx} with energy E at $x \Rightarrow -\infty$. Because of having the scattering concept and the partner potentials $V_L(x)$ and $V_R(x)$, one can obtain transmitted waves $T_{L,R}(k)\ e^{ik'x}$and reflection waves $R_{L,R}(k)\ e^{-ikx}$. The total wave functions are written as

$$\Psi^{(L,R)}(k, x \Rightarrow -\infty) \longrightarrow e^{ikx} + R_{L,R}(k)\ e^{-ikx}, \tag{2.53}$$

and

$$\Psi^{(L,R)}(k', x \Rightarrow \infty) \longrightarrow T_{L,R}(k)\ e^{ik'x}. \tag{2.54}$$

Here, k and k' are defined by

$$k = \sqrt{E - W_-^2}, \qquad k' = \sqrt{E + W_-^2}, \tag{2.55}$$

where we use the definition $W(x \to \pm\infty) \equiv W_\pm$ and the partner potentials are equal to $V_L(x) = W_+^2$ as $x \Rightarrow \infty$ and $V_R(x) = W_-^2$ as $x \Rightarrow -\infty$. The wave functions of $\hat{H}_L$ and $\hat{H}_R$ are continuous in SUSY. Analogously, the question of energy spectrum in discrete levels is important. Using the Eqs. (2.19) and (2.20), we can write

$$e^{ikx} + R_L(k)\ e^{-ikx} \quad = \quad N\left[(-ik + W_-)e^{ikx} + (ik + W_-)e^{-ikx} R_R\right]$$

$$T_L(k)\ e^{ik'x} \;=\; N\left[(-ik'+W_+)e^{ik'x}T_R\right], \tag{2.56}$$

where N the normalization constant. From these two equations, we can eliminate N by comparing term-by-term and get the following results

$$\frac{R_L(k)}{R_R(k)} = \left(\frac{W_- + ik}{W_- - ik}\right), \qquad \frac{T_L(k)}{T_R(k)} = \left(\frac{W_+ - ik'}{W_- - ik'}\right). \tag{2.57}$$

A few remarks can be arranged about these two coefficients. The partner potentials have identical probabilities of reflection and transmission since they are $|R_L|^2 = |R_R|^2$ and $|T_L|^2 = |T_R|^2$. With the exception of an additional pole of $R_L(T_L)$ at $k = -iW_-$, $R_L(T_L)$ and $R_R(T_R)$ have the same poles in complex plane. The pole at $k = -iW_-$ is on the positive imaginary axis only if $W_- < 0$, corresponds to the zero energy bound state. If we choose $W_+ = W_-$ and $k = k'$, we have $T_L(k) = T_R(k)$. Moreover, when $W_- = 0$ is chosen, then one gets $R_L(k) + R_R(k) = 0$. Furthermore, if, say, $W_+ = -W_-$ and $k = k'$, we have the relationship between these coefficients as $R_L(k)/R_R(k) = T_L(k)/T_R(k)$.

2.7 Hierarchy of Hamiltonian

In order to construct a hierarchy of non-relativistic Hamiltonians, a systematic procedure is followed with the adjacent members of supersymmetric partner potentials. This procedure, known as the factorization method, is also related to the factorization of the Hamiltonian. In this approach, the solution of the second-order Schrödinger equation for a given potential reduces to the first-order

Riccati equation involving the superpotential $W(x)$. The method was proposed by Darboux in a first time, and later was provided for the derivation of exact spectra of hydrogen atom problem by Schrödinger in the framework of quantum mechanics. Infeld and Hull [53] developed this technique for solving second-order differential equations in six different types of factorization. In this section, we want to show how to factorize a Hamiltonian in details.

Let us start by calling $\hat{H}_L$ as $\hat{H}_1$ and $\hat{H}_R$ as $\hat{H}_2$, and suitably changing the other subscripts. If we know the ground state wave function of a Hamiltonian $\hat{H}_1$, we can find the superpotential $W_1(x)$ via the Eq. (2.6). The positive semi-definite operator $\hat{\Omega}_1$ and its adjoint $\hat{\Omega}_1^\dagger$ are used to factorize the Hamiltonian $\hat{H}_1$. This time, we can also determine the other partner Hamiltonian $\hat{H}_2$ by means of the semi-definite operators. This Hamiltonian is refactorizable in terms of $W_2(x)$. This refactorization process provides us to get the another partner Hamiltonian $\hat{H}_3$. It is repeated that until the number of bound states is exhausted. Therefore, if the potential problem for $\hat{H}_1$ is exactly solvable, one can get the energy eigenvalue spectra and corresponding wave functions by repeating the refactorization procedure. However, once the ground state wave functions for all partner Hamiltonians $\hat{H}_1, \hat{H}_2, \ldots$ are known, we can reconstruct the solution of the original problem. Any Hamiltonian with the choice of ground state wave function

$\Psi_0^{(1)}$ can be written as

$$\begin{aligned}\hat{H}_1\Psi_0^{(1)} &= \left[-\frac{d^2}{dx^2} + V_1(x)\right]\Psi_0^{(1)} \\ &= \left[\hat{\Omega}_1^\dagger\hat{\Omega}_1 + E_0^{(1)}\right]\Psi_0^{(1)} \\ &= E_0^{(1)}\Psi_0^{(1)}, \qquad (2.58)\end{aligned}$$

where we set $\hbar = 2m = 1$ for simplicity and have

$$\hat{\Omega}_1 = \frac{d}{dx} + W_1(x), \quad \hat{\Omega}_1^\dagger = -\frac{d}{dx} + W_1(x), \quad W_1(x) = -\frac{d}{dx}\ln\Psi_0^{(1)}(x). \qquad (2.59)$$

Then, the supersymmetric partner one is given as

$$\begin{aligned}\hat{H}_2 &= \left[-\frac{d^2}{dx^2} + V_2(x)\right] \\ &= \left[\hat{\Omega}_1\hat{\Omega}_1^\dagger + E_0^{(1)}\right]. \qquad (2.60)\end{aligned}$$

Hence, the SUSY relations between the SUSY partner potentials $V_1(x)$ and $V_2(x)$

$$\begin{aligned}V_2(x) &= W_1^2 + W_1' + E_1^{(0)} \\ &= V_1(x) + 2W_1' \\ &= V_1(x) - 2\frac{d^2}{dx^2}\ln\Psi_0^{(1)}, \qquad (2.61)\end{aligned}$$

are obtained. The energy spectra and corresponding eigenfunctions of two SUSY Hamiltonians are related as

$$E_n^{(2)} = E_{n+1}^{(1)}, \qquad \hat{\Omega}_1\Psi_{n+1}^{(1)} = \sqrt{E_{n+1}^{(1)} - E_0^{(1)}}\Psi_n^{(2)}. \qquad (2.62)$$

Let us now construct a third partner Hamiltonian $\hat{H}_3$ with respect to a SUSY partner $\hat{H}_2$. By choosing the ground state energy of $\hat{H}_2$ as $E_0^{(2)} = E_1^{(1)}$, we can factorize $\hat{H}_2$ in terms of the ground state wave function $\Psi_0^{(2)}$

$$\begin{aligned} \hat{H}_2 &= \hat{\Omega}_1 \hat{\Omega}_1^\dagger + E_0^{(1)} \\ &= \hat{\Omega}_2^\dagger \hat{\Omega}_2 + E_1^{(1)}, \end{aligned} \tag{2.63}$$

where we have

$$\hat{\Omega}_2 = \frac{d}{dx} + W_2(x), \quad \hat{\Omega}_2^\dagger = -\frac{d}{dx} + W_2(x), \quad W_2(x) = -\frac{d}{dx} \ln \Psi_0^{(2)}(x). \tag{2.64}$$

As a result, the SUSY partner Hamiltonian $\hat{H}_3$ of $\hat{H}_2$ is written

$$\begin{aligned} \hat{H}_3 &= -\frac{d^2}{dx^2} + V_3(x) \\ &= \hat{\Omega}_2 \hat{\Omega}_2^\dagger + E_1^{(1)}. \end{aligned} \tag{2.65}$$

The energy eigenvalues and wave functions are respectively

$$E_n^{(3)} = E_{n+1}^{(2)} = E_{n+2}^{(1)}, \tag{2.66}$$

and

$$\begin{aligned} \Psi_n^{(3)} &= \frac{1}{\sqrt{E_{n+1}^{(2)} - E_0^{(2)}}} \hat{\Omega}_2 \Psi_{n+1}^{(2)} \\ &= \frac{1}{\sqrt{[E_{n+2}^{(1)} - E_0^{(1)}][E_{n+2}^{(1)} - E_1^{(1)}]}} \hat{\Omega}_2 \hat{\Omega}_1 \Psi_{n+2}^{(1)}. \end{aligned} \tag{2.67}$$

By repeated application of the same procedure for a finite number, M, of bound states leads to the generation of a hierarchy of Hamiltonians as

$$\begin{aligned} \hat{H}_n &= -\frac{d^2}{dx^2} + V_n(x) \\ &= \hat{\Omega}_n^\dagger \hat{\Omega}_n + E_0^{(n)} \\ &= \hat{\Omega}_{n-1} \hat{\Omega}_{n-1}^\dagger + E_0^{(n-1)}, \end{aligned} \tag{2.68}$$

where $n = 2, 3, \ldots, M$. We also have

$$\hat{\Omega}_n = \frac{d}{dx} + W_n(x), \quad \hat{\Omega}_n^\dagger = -\frac{d}{dx} + W_n(x), \quad W_n(x) = -\frac{d}{dx} \ln \Psi_0^{(n)}(x). \tag{2.69}$$

The energy eigenvalues and corresponding wave functions satisfy the following relations:

$$E_n^{(m)} = E_{n-1}^{(m+1)} = \ldots = E_1^{(n+m-1)}, \tag{2.70}$$

and

$$\Psi_n^{(m)} = \frac{1}{\sqrt{[E_{n+m-1}^{(1)} - E_{m-2}^{(1)}] \ldots [E_{n+m-1}^{(1)} - E_0^{(1)}]}} \hat{\Omega}_{n-1} \ldots \hat{\Omega}_1 \Psi_{n+m-1}^{(1)}, \tag{2.71}$$

and also

$$\begin{aligned} V_n(x) &= V_{n-1}(x) - 2\frac{d^2}{dx^2} \ln[\Psi_0^{(n-1)}] \\ &= V_1(x) - 2\frac{d^2}{dx^2} \ln[\Psi_0^{(1)} \Psi_0^{(2)} \ldots \Psi_0^{(n-1)}], \end{aligned} \tag{2.72}$$

where $n = 2, 3, \ldots, M$ and $m = 0, 1, 2, \ldots, M - n$. We note that the $n - th$ member of the hierarchy has the same eigenvalue spectrum as $\hat{H}_1$ except for the missing of the first $(n - 1)$ eigenvalues of $\hat{H}_1$. Moreover, the energy eigenvalue of the $(n - 1) - th$ excited state of $\hat{H}_1$ is degenerate with the ground state of $\hat{H}_n$. We can further construct the $n - th$ member wave function and the successive SUSY partner potentials with the use of $\hat{\Omega}_i$ $(i = 1, 2, \ldots, n - 1)$ and $\Psi_{n+m-1}^{(1)}$ as well as the $(n - 1) - th$ excited state wave functions respectively.

2.8 Various Aspects of SUSYQM

2.8.1 Concepts of Exactly Solvability, Shape Invariance and Self-Similarity

In recent studies of supersymmetric quantum mechanics, several conditions are proposed for determining the complete spectrum of the Hamiltonians $\hat{H}_1$ and $\hat{H}_2$. The exactly solvability condition of any given potential, means exactly solvable potentials, is obtained through the concept of "*shape*" or "$form - invariance$" introduced by Gendenshtein. If the pair of SUSY partner potentials $V_1(x)$ and $V_2(x)$ are similar in shape and differ only in parameters, then, these potentials are in shape invariant form. The spectra for these class of potentials can be obtained exactly. The Schrödinger equation for a given potential is transformed to a hypergeometric or confluent hypergeometric form. There are a number of exactly solvable potential problems in nonrelativistic quantum mechanics for which all the energy spectra and corresponding the eigenfunctions are known explicitly, such as harmonic oscillator, Coulomb, Morse, Eckart and Pöschl-Teller potentials. Let us define shape invariance requirement for the partner potentials as

$$V_2(x, a_1) = V_1(x, a_2) + \Re(a_1), \tag{2.73}$$

where a_1 is a set of parameters, a_2 is a function of a_1 and the remainder term $\Re(a_1)$ is independent of x. Hence, the new partner potentials for parameters a_1 and a_2 are called as shape invariant. This requirement is also an integrability condition. Using the Eq. (2.73), and the Hamiltonian Hierarchy method, one obtains the energy eigenvalues and eigenfunctions of any shape invariant potential (SIP) for unbroken case. Let us start from the definition of integrability condition for SUSY partner Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ as

$$\Psi_0^{(1)}(x, a_1) = N \exp\left[-\int_0^x W_1(y, a_1)\, dy\right], \quad E_0^{(1)}(a_1) = 0. \tag{2.74}$$

Using the shape invariance condition (2.73), the entire spectrum of partner potential $\hat{H}_1$ can be obtained. In order to do this, we construct a series of Hamiltonians $\hat{H}_1, \hat{H}_2, \ldots, \hat{H}_k$. By repeating the shape invariance procedure, we have

$$\hat{H}_k = -\frac{d^2}{dx^2} + V_1(x; a_k) + \sum_{i=1}^{k-1} \Re(a_i), \tag{2.75}$$

where $a_k = f^{k-1}(a_1)$, f^{k-1} means that the function f is applied $k-1$ times. If we put $k \Rightarrow k+1$ in the Eq. (2.75), one can get

$$\begin{aligned} \hat{H}_k &= -\frac{d^2}{dx^2} + V_1(x; a_{k+1}) + \sum_{i=1}^{k} \Re(a_i) \\ &= -\frac{d^2}{dx^2} + V_2(x; a_k) + \sum_{i=1}^{k-1} \Re(a_i). \end{aligned} \tag{2.76}$$

Here, $\hat{H}_k$ and $\hat{H}_{k+1}$ are SUSY partner Hamiltonians and they must have the same spectrum except for the ground state of $\hat{H}_k$ whose energy is

$$E_0^{(k)} = \sum_{i=1}^{k-1} \Re(a_i). \tag{2.77}$$

By following the Eq. (2.75) and using $E_0^{(1)}$, we can generalize this to the Hamiltonian $\hat{H}_n$. Therefore, the complete energy eigenvalues of $\hat{H}_1$ are given by

$$E_n^{(1)}(a_1) = \sum_{i=1}^{n} \Re(a_i), \qquad E_0^{(1)}(a_1) = 0. \tag{2.78}$$

Let us now determine the bound state wave function $\Psi_n^{(1)}(x, a_1)$ for any shape invariant potential, $V_1(x, a_1)$ using the ground state wave function $\Psi_0^{(1)}(x, a_1)$. The operators $\hat{\Omega}$ and $\hat{\Omega}^\dagger$ are connected by the eigenfunctions for supersymmetric Hamiltonians. If we take $\hat{H}_1 \to \hat{H}_2 \to \hat{H}_{k-1} \to \hat{H}_k$ and use the Eq. (2.20), one can find the excited wave function for the original Hamiltonian $\hat{H}_1(x; a_1)$ as

$$\Psi_n^{(1)}(x; a_1) \propto \hat{\Omega}^\dagger(x; a_1)\hat{\Omega}^\dagger(x; a_2)\ldots\hat{\Omega}^\dagger(x; a_n)\Psi_0^{(1)}(x; a_{n+1}). \tag{2.79}$$

It is more convenient to use the relation

$$\Psi_n^{(1)}(x; a_1) = \hat{\Omega}^\dagger(x; a_1)\Psi_{n-1}^{(1)}(x; a_{n+1}). \tag{2.80}$$

Using the Eqs. (2.19) and (2.20), we can finally obtain the relationships between the scattering amplitudes with respect to the shape invariance requirement

$$R_1(k; a_1) = \left[\frac{W_-(a_1) + ik}{W_-(a_1) - ik}\right] R_1(k; a_2), \quad T_1(k; a_1) = \left[\frac{W_+(a_1) - ik'}{W_-(a_1) - ik}\right] T_1(k; a_2), \tag{2.81}$$

where $a_2 = f(a_1)$. The other important concept used in the determination of the complete energy spectrum of partner Hamiltonians is the self-similarity. Shabat and Spiridonov discussed the form of the self-similar potentials. In fact, the result obtained from the shape invariance and self-similarity are entirely equivalent to each other. Moreover, the Shabat-Spiridonov self-similarity condition (SS) turns out to be a special case of the shape invariance one. However, it is necessary to emphasize that the shape invariance is a much more general concept than self-similarity.

2.8.2 Coordinate Transformations

In the previous section, we have shown that the idea of SUSY and the concept of shape invariance leads to the solution of exactly solvable potentials. Moreover, by following certain strategies, *i.e.*, translation and scaling of parameters etc., we get the complete energy spectrum for solvable potentials. There is another useful approach for these potentials. The most general solvable potentials are reduced to either hypergeometric or confluent hypergeometric equation for Schrödinger equation introduced by Natanzon in 1971 [105]. However, some potentials are not shape invariant. Furthermore, the energy eigenvalues and corresponding eigenfunctions of these potentials are known implicitly rather than explicitly. Finding the solutions of these problem is important as those of the shape invariant potentials. To do this, we first consider a SIP for a Schrödinger equation which is exactly solvable. Under point canonical coordinate transformations (PCCT), the Schrödinger equation is mapped into another form. In the nature of coordinate transformation, several restrictions on this equation exist. This transformation satisfying the restrictions allows us to obtain new solvable problems. If we have an implicit relationship between the coordinates, we can determine the new solutions implicitly. However, when the relationship is explicit, new solvable potentials obtained by the transformation, are shape invariant as well. The coordinate transformation idea is applied on the $d-$dimensional Coulomb and harmonic oscillator problems. Let us first consider the one-dimensional Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + (V(x) - E_n)\right] \Psi_n(x) = 0. \tag{2.82}$$

The suitable coordinate transformation $x \to z$ is,

$$f(z) = \frac{dz}{dx}, \qquad \frac{d}{dx} = f\frac{d}{dz}. \tag{2.83}$$

Substituting the transformation into the Eq. (2.82) and rearranging it, we have

$$\left[-\frac{d^2}{dz^2} - \frac{f'}{f}\frac{d}{dz} + \frac{1}{f^2}\left(V(x) - E_n\right)\right] \Psi_n = 0. \tag{2.84}$$

In order to eliminate the second term, one can rescale the wave function as

$$\Psi_n = \frac{1}{\sqrt{f}}\ \phi_n. \tag{2.85}$$

Also, when we add a term $\varepsilon_n \phi_n$ for both sides of the Eq. (2.83), it yields

$$\left\{-\frac{d^2}{dz^2} + \left[\widetilde{V}(E_n) + \varepsilon_n\right]\right\} \phi_n(x) = \varepsilon_n \phi_n, \tag{2.86}$$

where

$$\widetilde{V}(E_n) = \frac{1}{f^2}(V(x) - E_n) - \left[\frac{f'^2}{4f^2} - \frac{f''}{2f}\right]. \tag{2.87}$$

This potential $\widetilde{V}(E_n) + \varepsilon_n$ must be independent of n so that Schrödinger equation is reasonable. For this, we define the quantity as

$$G = V - E_n + \varepsilon_n\ f^2. \tag{2.88}$$

Now, we need to satisfy this condition. There is one way to have f^2 and G, which have the same functional dependence on $x(z)$ as the original potential

V. It requires that the new potential $\widetilde{V}$ is independent of n. Therefore, the parameters of V have to be changed with n, and the wave function corresponding to the $n-th$ member energy level of the new Hamiltonian is related to a wave function of the old Hamiltonian with parameters, depending on n. We finally note that all shape invariant potentials are inter-related by point canonical coordinate transformations.

2.8.3 Parametrization of SUSY Potentials

Let us now consider an interesting problem: How to classify the various solutions to the shape invariance requirement (2.73)? When the classification problem is available, the new shape invariant potentials (SIPs) are then discovered by algebraic methods [56].

Two classes of solutions have been found so far. In the first case, the parameters a_1 and a_2 are connected to each other by a translation ansatz as $a_2 = a_1 + \alpha$. All standard problems discussed in nonrelativistic quantum mechanics, which are analytically solvable, belong to this class. In the second case, these parameters are connected to each other by using a scaling ansatz as $a_2 = qa_1$. We are going to discuss these two types of classes.

We first consider the translation ansatz case $a_2 = a_1 + \alpha$. The structure of $n-th$ member eigenvalue of the Schrödinger equation for any SIP can be expected to be of the form

$$E_n \sim \sum_\alpha C_\alpha n^\alpha, \qquad -2 \leq \alpha \leq 2, \tag{2.89}$$

where the upper bound is satisfied by the inverse square well potential, *i.e.*, Bn^2, though the lower bound is satisfied by the Coulomb potential *i.e.*, $\frac{A}{n^2}$. Therefore, the structure of the complete eigenvalue spectrum for any SIP can be given as the Eq. (2.78), then it follows

$$\Re(a_k) \sim \sum_\beta k^\beta, \qquad -3 \leq \beta \leq 1, \tag{2.90}$$

where we translate a_i with a_k in Eq. (2.78). The important question is how to implement the $\beta-$constraint on the remainder $\Re(a_k)$. The general factorizable form of a new ansatz superpotential $W(x;a_1)$ for the $k-$dependent remainder $\Re(a_k)$ is defined as

$$W(x;a_1) = \sum_{i=1}^{n} \left[(k_i + c_i) g_i(x) + \frac{1}{(k_i + c_i)} h_i(x) + f_i(x) \right], \tag{2.91}$$

where the translation parameters are

$$a_1 = (k_1, k_2, \ldots), \qquad a_2 = (k_2 + \alpha, k_2 + \beta \ldots), \tag{2.92}$$

with α, β and C_i as constants. All of the potentials which contain fractional power of n are excluded by this ansatz equation. We can use the ansatz for W in the shape invariance condition (2.73) as

$$V_2(x, a_1) \;\; = \;\; W^2(x, a_1) + W'(x, a_1)$$

$$
\begin{aligned}
&= W^2(x,a_2) - W'(x,a_2) + \Re(a_2) \\
&= V_1(x,a_2) + \Re(a_2). \qquad (2.93)
\end{aligned}
$$

From Eq. (2.91), we get the conditions satisfied by the functions $g_i(x)$, $h_i(x)$ and $f_i(x)$. One condition is that the superpotentials W are admissible to give a square integrable ground state wave function. Therefore, the shape invariance condition is in a simple form by choosing a rescaled set of parameters $m = m_1, m_2, \ldots, m_n$. The SI condition (2.73) is connected by translation with an integer m as well

$$V_2(x,m) = V_1(x,m-1) + \Re(m-1). \qquad (2.94)$$

We note that under re-parametrization of this procedure, the functional differential equation (2.93) is converted to the differential-difference equation

$$W^2(x,m+1) - W^2(x,m) + W'(x,m+1) + W'(x,m) = \Re(m), \qquad (2.95)$$

where $\Re(m) = L(m) - L(m+1)$. By substituting the ansatz equation (2.91) into the Eq. (2.95) and using the Eq. (2.93) as well, we get various admissible solutions: The first simplest case is

$$W(x;a_1) = (k+c)g_1(x) + \frac{1}{(k+c)}h_1(x) + f_1(x). \qquad (2.96)$$

Using the Eqs. (2.92) and (2.95) in Eq. (2.93), we can find the complete energy spectrum for various potentials, such as harmonic oscillator, Morse and Pöschl-Teller ones *etc.* Moreover, we can write the more complicated case

$$W(x;a_1) = (k_1+c_1)g_1(x) + \frac{1}{(k_2+c_2)}g_2(x) + f_1(x). \qquad (2.97)$$

When we substitute the Eqs. (2.92) and (2.95) in the Eq. (2.93), we can find the conditions for the functions $g_1(x)$, g_2 and $f_1(x)$. Hence, these conditions lead to the various acceptable solutions for Pöschl-Teller I and II potentials. Several expressions are given for the various SIPs, that is, $V_1(x)$ and its partner $V_2(x)$ with the parameters a_1 and a_2 [56].

Let us now consider the second class of shape invariant potentials. The parameters a_1 and a_2 are connected by scaling as $(a_2 = qa_1)$. These type of potentials are reflectionless and have an infinite number of bound states. Also, they can be obtained in a series form. Suppose we have an expansion of the superpotential as

$$W(x; a_1) = \sum_{j=0}^{\infty} g_j(x) a_1^j, \tag{2.98}$$

with the scaling ansatz

$$a_2 = qa_1, \qquad 0 < q < 1. \tag{2.99}$$

By expanding the Eq. (2.98) for the Eq. (2.95) and solving the set of first-order differential equation, one can get the complete energy spectrum. It is important here to note that the self-similarity condition introduced by Shabat and Spiridonov is considered for this class. It is a special case of the shape-invariance requirement (2.73). In shape invariant potentials which are not contained the self-similar ansatz, we must choose $r_n = R_n/(1-q^n)$ as non-zero. For example, if $r_n = 0$ for $n \geq 3$, we obtain the symmetric partner potentials $V_{1,2}(x)$. This corresponds to the unbroken SUSY case.

For shape invariant potentials, there is another classification of solutions except for scaling and translation. To obtain a new type of shape invariant potentials, there are several possibilities. One of them is $a_2 = qa_1^p$ with $p = 2, 3, \ldots$; $a_2 = qa_1/(1 + pa_1)$. For $p = 2$, we consider the new first type as $a_2 = qa_1^2$. Following the same procedure as in the scaling part, we get complete energy spectrum.

The other possibility for obtaining the shape invariant potentials (SIPs) is the cyclic case. In this case, the SUSY partner Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ refer to a series of SIPs that repeat after a cycle of p iterations as $f^p(a_1) = a_1$, where $a_2 = f(a_1)$ and $a_3 = f^2(a_1)$ *etc.* These types of potentials have an infinite number of periodically spaced eigenvalues.. Also, the potentials are in a closed form except for $p = 2$.

CHAPTER 3

METHODS IN SUSYQM

3.1 Perturbative and Semiclassical Methods

In the framework of SUSYQM, various methods have been used for calculating the energy eigenvalues and corresponding eigenfunctions, *i.e.*, supersymmetric WKB method, variational approach, $\delta-$expansion method, $1/N$ expansion technique. The superymmetric WKB (SWKB) method known as the semiclassical approach is a very useful approximation technique for obtaining the energy eigenvalues and computing barrier tunneling probabilities of quantum mechanical systems. There are numerous applications of the method in many branches of physics and mathematics. The analytic properties of the WKB approximation method have been studied from a purely mathematical point of view. By comparison, the accuracy of this method can be tested with both analytic and numerical results. The new aspect of the semiclassical approach is described by the inspiration of supersymmetry called the supersymmetric WKB (SWKB) method. We point out that this method gives better accuracy than the usual WKB method for quantum mechanical problems. In fact, the lowest order SWKB approximation produces exact energy eigenvalues for all simple shape invariant potentials (SIPs). Let us now give some general comments on WKB method. There are two remarkable aspects of this method. The first one is to determine the energy eigenvalues accurately, while the second one is the ability of describing the tunneling rate. These are not totally independent so that the spectrum is related to an analytic continuation of the scattering amplitude. One can define the well-known WKB quantization condition as

$$\int_{x_L}^{x_R} \sqrt{2m\left(E-V(x)\right)}\, dx = \left(n+\frac{1}{2}\right)\hbar\pi, \quad n=0,1,\ldots \tag{3.1}$$

where n refers to the number of nodes of the WKB function between the turning points x_L and x_R. If n is large compared to unity or the turning points are several wave lengths, the WKB theory shall give good results. For additional accuracy, it is necessary to consider second and higher order corrections in $\hbar$.

The other remarkable application of the WKB approximation method is an exact computation of the tunneling probability. In the classical limit ($\hbar \Rightarrow 0, T \Rightarrow 0$), there is indeed no barrier penetration. For the transmission and reflection probabilities, there is an expected relation $|R|^2 + |T|^2 = 1$, as given by $|T|^2 = 1/\left(1+e^{2K}\right)$, $|R|^2 = e^{2K}/\left(1+e^{2K}\right)$, where $K = \frac{1}{\hbar}\int_{x_L}^{x_R} \sqrt{2m\left(E-V(x)\right)}\, dx$. Let us now consider combining the ideas of SUSY with the lowest order WKB method. The lowest order SWKB quantization condition for unbroken SUSY case was obtained by Bandrauk and Campbell [104]. They showed that it yields the energy eigenvalues which are not only accurate for large quantum numbers n but they are also exact for the ground state ($n = 0$). For the partner potential, corresponding to the superpotential $W(x)$, the lowest order WKB quantization condition (3.1) takes the form

$$\int_{x_L}^{x_R} \sqrt{2m\left[E_n^{(1)} - W^2(x) + \frac{\hbar}{\sqrt{2m}} W'\right]}\, dx = \left(n + \frac{1}{2}\right)\hbar\pi. \tag{3.2}$$

By expanding the left hand side in powers of $\hbar$ and integrating over the turning points, one gets the SWKB quantization conditions (3.2) for unbroken SUSY case

$$\int_a^b \sqrt{2m\left[E_n^{(1)} - W^2(x)\right]}\, dx = n\hbar\pi, \qquad n = 1, 2, 3, \ldots. \tag{3.3}$$

By following the same procedure, the SWKB quantization condition for the partner potential $V_2(x)$ takes

$$\int_a^b \sqrt{2m\left[E_n^{(1)} - W^2(x)\right]}\, dx = (n+1)\hbar\pi, \qquad n = 0, 1, 2, \ldots. \tag{3.4}$$

The lowest order SWKB condition gives the exact eigenvalues for all shape invariant potentials with translation. By recalling the shape invariance condition (2.73) and using the general expression for the $k-th$ Hamiltonian given by the Eq. (2.75), we have an expression for the exactness of the bound state spectrum given by the Eq. (2.78). As a result, the SWKB quantization condition can be defined

$$\int \sqrt{2m\left[E_n^{(k)} - \sum_{i=1}^{k-1} R(a_i) - W^2(a_k; x)\right]}\, dx = n\hbar\pi. \tag{3.5}$$

Let us now discuss the SWKB quantization condition for broken SUSY. As in the case of unbroken SUSY, the same derivation applies until one examines the

$O(\hbar)$ term. For this case, one has

$$W(a) = W(b) = \sqrt{E_n^{(1)}}. \tag{3.6}$$

The leading order in $\hbar$, the SWKB quantization condition for broken SUSY (BSWKB) is

$$\int_a^b \sqrt{2m\left[E_n^{(1)} - W^2(x)\right]}\, dx = (n+\frac{1}{2})\hbar\pi, \qquad n = 0, 1, 2, \ldots. \tag{3.7}$$

As in the unbroken SUSY case, the lowest order BSWKB quantization condition reproduces the exact spectra for SIPs with a translation parameters.

The variational method is very useful for estimating the ground state energy E_0 when such exact solutions are not available. In this method, we propose an ansatz, *i.e.*, a normalized trial wave function to estimate the ground state energy. Suppose we have a normalizable trial function ϕ and define $E[\phi]$ as

$$\begin{aligned} E[\phi] &= \frac{\langle\phi|\hat{H}|\phi\rangle}{\langle\phi|\phi\rangle} \\ &= \frac{\int \phi^*\ \hat{H}\ \phi\ d^3r}{\int \phi^*\ \phi\ d^3r}, \end{aligned} \tag{3.8}$$

where the integration is over all space coordinates. By considering various ϕ, we can obtain an upper bound to the ground state energy E_0

$$E[\phi] \geq E_0. \tag{3.9}$$

It means that the minimum of the function $E[\phi]$ corresponds to the ground state energy. To apply this method, we characterize the trial wave function by one or more parameters $\lambda_1, \lambda_2, \ldots$, and compute $E[\phi]$ as a function of these parameters. Then, $E[\phi]$ is minimized by setting the derivative with respect to the parameters to zero, namely,

$$\frac{\partial E[\phi]}{\partial \lambda_1} = 0, \quad \frac{\partial E[\phi]}{\partial \lambda_2} = 0, \ldots . \tag{3.10}$$

Also, we determine the optimum values of $\lambda_1, \lambda_2, \ldots$ and substitute them back to the expression for $E[\phi]$. By using this method, the true ground state energy function $E[\phi]$ is obtained if the trial wave function has a functional form of the exact ground energy function. Following the SUSYQM procedures, we can find the energy difference between the ground state and the first excited state of a given potential. This result is compared with the exact numerical values. It is necessary to extend the number of variational parameters to obtain a better accuracy. Then, by constructing the energy functional $E[\phi]$ and requiring Eq. (3.10), we can minimize this functional for a given potential.

Let us now discuss the $\delta-$expansion method. In this method, we introduce a perturbation parameter δ. This describes the degree of nonlinearity of a given potential. By following the ideas of perturbation theory, both the ground state energy and the superpotential $W(x)$ have an expansion in the perturbation parameter. The Riccati equation takes the form with a perturbation parameter

$$V_1(x) = V(x, \delta) - C(\delta) = W^2(x, \delta) - W', \tag{3.11}$$

where C is the ground state energy of a given potential. To determine the superpotential $W(x)$, we use the Taylor series expansion for both $W(x)$ and $V_1(x)$ in δ. Using the expression

$$V_1(x) = \sum_{n=0}^{\infty} \delta^n W_{(n)}(x), \tag{3.12}$$

and inserting these into Eq. (3.11), we match terms order by order. For the zero-th and first order, we obtain differential equations for $W_0, W_1, \ldots, W_n$. The solution of these equations gives us the ground state energy in δ expansion. If we want to get more accuracy for the ground state energy, we must do the calculation up to the order of δ^2. Thus, we can continue in δ using Padé approximation analytically. To calculate all excited states of a given potential in a δ expansion, the standard SUSY methods are used. Moreover, this method can be extended to perturbing about any shape invariant potential. The determination of energy levels of a given potential in variational method is simpler and more accurate than the $\delta-$expansion method.

The large-N expansion method is also a powerful technique for analytically determining the energy eigenstates of the Schrödinger equation even for potentials which have no coupling constant. N denotes the number of spatial dimensions. By using the ideas of SUSYQM, the convergence rate of shifted $1/N$ expansion is improved. In this method, the solution of the Schrödinger equation in N spatial dimensions can be considered by taking N to be large and the expansion parameter $1/N$ for perturbation theory. The supersymmetry concept has played an important role in making for a better expansion.

3.2 The Nikiforov-Uvarov Method

Many physical processes lead to differential, integral, or integro-differential equations. One needs to simplify the original problem in order to clarify its most important qualitative features and to understand the relative roles played by various factors. If a problem is simplified, the solution of the problem can be obtained in an explicit mathematical form. Thus, we can easily analyse the results and obtain a qualitative picture. Also, the behavior of the solution can be analysed depending on the parameters of the problem. Moreover, a knowledge of special functions is essential for understanding many important problems of physics such as harmonic oscillator, hydrogen atom problems, in solving the Schrödinger, Dirac and Klein-Gordon, Bethe-Salpeter equations *etc.* The most commonly encountered special functions are also known as the classical orthogonal polynomials (Jacobi, Laguerre, Hermite), spherical harmonics and the Bessel and hypergeometric functions. The main interest in the study of problems is that discrete energy spectra and corresponding wave functions can be determined by means of the classical orthogonal polynomials.

Let us introduce the Nikiforov-Uvarov (NU) method [68]. In this method, a differential equation is reduced to the hypergeometric type by an appropriate coordinate transformation, $x = x(z)$ as

$$\frac{d^2\Psi(z)}{dz^2} + \frac{\tilde{\tau}(z)}{\sigma(z)}\frac{d\Psi(z)}{dz} + \frac{\tilde{\sigma}(z)}{\sigma^2(z)}\Psi(z) = 0 \tag{3.13}$$

where $\sigma(z)$ and $\tilde{\sigma}(z)$ are polynomials having at most second degree, and $\tilde{\tau}(z)$ is a polynomial having at most first degree. If we take the following factorization

$$\Psi(z) = \phi(z)\ y(z), \tag{3.14}$$

the Eq. (3.13) becomes as

$$\sigma(z)\frac{d^2y(z)}{dz^2} + \tau(z)\frac{dy(z)}{dz} + \Lambda y(z) = 0, \tag{3.15}$$

where

$$\sigma(z) = \pi(z)\frac{d}{dz}(\ln\phi(z)), \tag{3.16}$$

and

$$\tau(z) = \tilde{\tau}(z) + 2\pi(z). \tag{3.17}$$

Also, Λ is given

$$\Lambda_n + n\tau' + \frac{[n(n-1)\sigma'']}{2} = 0, \quad n = 0, 1, 2, \ldots \tag{3.18}$$

The energy eigenvalues can be calculated from the above equation. We first have to determine $\pi(s)$ and Λ by defining

$$k = \Lambda - \pi'(z). \tag{3.19}$$

Solving the quadratic equation for $\pi(s)$ with the Eq. (3.19), we get

$$\pi(z) = \frac{(\sigma' - \tau')}{2} \pm \sqrt{\left[\frac{\sigma' - \tau'}{2}\right]^2 - \tilde{\sigma} + k\sigma}. \qquad (3.20)$$

Here, $\pi(z)$ is a polynomial with the parameter z and primes denote the derivatives at first degree. The determination of k is the essential point in the calculation of $\pi(z)$. It is simply defined as the value that sets the discriminant of the polynomials inside square root to zero. Therefore, we obtain a general quadratic equation for k. The determination of the wave function is now in order. We consider the Eq. (3.16) and the Rodriguez relation

$$y_n(z) = \frac{C_n}{\rho(z)} \frac{d^n}{dz^n} \left[\sigma^n(z)\ \rho(z)\right], \qquad (3.21)$$

where C_n is a normalization constant and the weight function $\rho(z)$ satisfy the following relation

$$\frac{d}{dz}\left[\sigma(z)\ \rho(z)\right] = \tau(z)\ \rho(z). \qquad (3.22)$$

The Eq. (3.21) gives the classical orthogonal polynomials that have many important properties especially orthogonality relation can be defined as

$$\int_a^b y_n(z) y_m(z) \rho(z)\ dz = 0, \quad m \neq n. \qquad (3.23)$$

In Table 3.1, we give the relationships between the orthogonal polynomials and hypergeometric type functions.

Table 3.1: Relationship between the polynomial $\sigma(z)$ and corresponding orthogonal and hypergeometric functions with their weight functions.

$\sigma(z)$	*Orthogonal Polynomials*	*Hypergeometric Functions*	*Weight Function*
1	$H_n(z)$, *Hermite*	${}_1F_1(a,b,z)$, *confluent*	e^{-z^2}
z	$L_n^\alpha(z)$, *Laguerre*	${}_1F_1(a,b,z)$, *confluent*	$z^\beta\ e^{-\alpha z}$
$(1-z^2)$	$P_n^{(\alpha,\beta)}(z)$, *Jacobi*	${}_2F_1(a,b,c,z)$, *hypergeometric*	$(1-z)^\alpha(1+z)^\beta$
z^2	$J_n(z)$, *Bessel*	${}_1F_1(a,b,z)$, *confluent*	$e^{-2/z}$

CHAPTER 4

APPLICATIONS

4.1 The Basic Structure of Diatomic Molecules

In this section, we shall discuss the basic structure of diatomic molecules. Their wave functions are necessary for understanding the meaning and significance of the term symbols used for these type of molecules [73]. A simple application model for quantum mechanical systems is the harmonic oscillator problem. The unperturbed energy of the system is given by $\varepsilon_n = (n + 1/2)h\nu$ with $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$, where k and μ are the constant of force and the reduced mass, respectively. A molecule consisting of two atoms bonded together by forces. The wave solution for any but the simplest molecules is very difficult. The simplest molecules is known as the hydrogen molecules ion. However, the empirical results of molecular spectroscopy show that the energy of the molecule (aside from translational energy) consist of three parts. They are called the electronic energy, vibrational energy and the rotational energy. The energy levels fall into widely separated groups. They corresponds to different electronic states of the molecule. For a given electronic state , the levels are again divided into groups, which follow one another at nearly equal intervals. These correspond to successive states of vibration of the nuclei. There is also the fine structure due to the different states of rotation of the molecule. The successive rotational energy levels are being separated by larger and larger intervals with increasing rotational energy. The simple structure of the energy levels suggest a method of approximate solution of the wave equation involving three separable equations. The first one deals with the motion of the electrons, the second deals with the vibrational motion of the nuclei, the last one is related to the rotational motion of the nuclei. Let us discuss these approaches respectively. Just for an atomic system, the Hamiltonian H for a diatomic or polyatomic molecule is the sum of the kinetic energy T and the potential energy V. For a molecule, the kinetic energy consists of two parts. The contributions to the energy are T_e and T_n from the motions of the electrons and nuclei respectively. The potential energy comprises three terms, V_{ee}, V_{nn} and V_{en}. The first and second ones are due to Coulombic attraction between the electrons and between the nuclei and the third one is the repulsions among the electrons and the nuclei. It is a fact that the mass of every atomic nucleus is several thousand times as great as the mass of an electron. This approximation was proposed by Born-Oppenheimer in 1927. It is also assumed that a vibrating nuclei move so slowly compared to the electrons, when the electrons adjust instantaneously to any nuclear motion. In this case, the Born-Oppenheimer approximation is valid. Following this treatment, the approximate solution $\Psi_{n,\mu}(x, \lambda)$ to the Schrödinger equation for nuclear motion is

$$\Psi_{n,\mu}(x,\lambda) = \Psi_n(x,\lambda)\Psi_{n,\mu}(\lambda). \tag{4.1}$$

Here, the wave functions $\Psi_n(x,\lambda)$ and $\Psi_{n,\mu}(\lambda)$ known as the electronic wave functions correspond to different sets of values of the electronic quantum numbers n and nuclear wave functions, respectively. On the other hand, each of the wave functions is a function of the nuclear coordinates λ and the electronic coordinates x. These wave functions can be obtained by solving the Schrödinger wave equation for electrons only by the assumption of the fixed nuclei. The electronic wave equation is an ordinary wave equation for the s electrons. The nuclear wave functions are the acceptable solutions of a wave equation in the nuclear coordinates λ. We now consider the vibrational and rotational parts. It is important here to note that the solution of nuclear wave equation correspond to the vibrational and rotational energy levels of the diatomic molecule. This wave function can also be factorized into vibrational and rotational parts. By using the separation of variables, the wave equation for the rotation and vibration of a diatomic molecule is identical with the wave equation of the hydrogen atom. In cartesian coordinates, the wave equation can be separated into two equations which denote the translational and internal motions of the molecule. For hydrogen atom, the wave function $\Psi(r,\vartheta,\varphi)$ is factorized into the radial $R_{n,\ell}$ and angular parts $Y_{\ell,m}(\vartheta,\varphi)$ respectively. It may also note that if the atoms are very far ($r \Rightarrow \infty$) from each other, the potential energy is just the sum of the energies of the two individual atoms. Conversely, if the atoms approach one another, a slight attraction will appear. A stable molecules has a minimum value at the equilibrium position. For $(r \Rightarrow 0)$, this corresponds to the high repulsion of atoms.

As a result, the total wave function $\Psi_{n,\mu}(x,\lambda)$ and the energy of the diatomic molecules are written as

$$\Psi_{n,\mu}(x,\lambda) = \Psi_n \Psi_{vib} \Psi_{rot}, \tag{4.2}$$

and

$$E_{\nu,\kappa} = \left(\nu + \frac{1}{2}\right) h\nu_e + \frac{h^2}{8\pi^2 I_e}\kappa(\kappa+1) - \frac{\left[\kappa(\kappa+1)h^2\right]^2}{128\pi^6 \nu_e^2 I_e^3}, \tag{4.3}$$

where ν_e, I_e and κ are the reduced mass of the molecule, the equilibrium moment of inertia of the molecule and the angular momentum due to the rotation of the molecule, respectively. In addition, the first term refers to the vibrational energy of the molecule which is similar to the harmonic oscillator energy. The second term refers to the rotational energy of the molecule which is similar to the energy of rigid rotator. The last term is the correction for non-rigid molecules due to the rotation. Furthermore, molecules can absorb, or emit radiation not only as a result of changes in their rotational and vibrational energies but also changes in electronic energy [74]. The energy changes involved in a transition from one electronic state of a molecule to another are very large. They correspond to radiation in visible or ultraviolet regions. Diatomic molecules exhibit many different excited electronic states. The energy of these states is deduced from electronic transitions. In fact, in the analysis of electronic bands of diatomic molecules, the vibrational and rotational structures are considered. These bands contain a large amount of fine structure. The analysis of the electronic spectra of diatomic molecules can be generalized to a study of electronic spectra of polyatomic molecules like benzene or ions. For the above reasons, we will concentrate on the solution of the ring-shaped potential in our studies. This potential is used in quantum chemistry and nuclear physics for describing the ring-shaped molecules like benzene and interactions between the deformed nuclei, respectively.

4.1.1 Ring-Shaped Potential

One of the exactly solvable potentials is the deformed ring-shaped potential introduced by Hartmann [75]. This potential involves an attractive Coulomb potential with a repulsive inverse square potential one. In spherical coordinates it can be expressed as

$$V(r,\theta) = \left[\frac{2}{r} - \ q\delta\frac{a_0}{r^2 sin^2\theta}\right]\delta\sigma^2 a_0\epsilon_0, \tag{4.4}$$

where a_0 and ϵ_0 denote the Bohr radius and the ground state energy of the hydrogen atom, respectively. δ and σ are dimensionless positive real parameters as well. They take values in the range 1 to 10. This potential can be used in quantum chemistry and nuclear physics to describe ring-shaped molecules like benzene and interactions between deformed pairs of nuclei. We point out that the potential takes the form of the Coulomb potential in the limiting case $\delta\sigma^2 = Z$

and $q = 0$ for hydrogen-like atoms. The energy eigenvalues of the potential has been calculated before by using various methods such as a non-bijective canonical transformation, namely, Kustaanheimo-Stiefel (KS) transformation, dynamical group method, path integral and SUSYQM method etc. [76-90]. Moreover, this potential can be defined as a Coulomb plus Aharonov-Bohm potential by defining the parameters as $-ee' = 2a_0\epsilon_0\delta\sigma^2$, $-A/2\mu = q\epsilon_0 a_0^2\delta^2\sigma^2$ and $B = 0$. [91, 92, 93]. In the present work, we will obtain an exact solution of the Schrödinger equation with the q-deformed ring shaped potential by using the Nikiforov-Uvarov (NU) method in both parabolic and spherical coordinates. The Schrödinger equation in spherical coordinates becomes

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\left[E - V(r,\theta)\right]\Psi = 0. \tag{4.5}$$

4.1.1.1 Parabolic Coordinates

First, we are going to study the solution of the problem using parabolic coordinates. One can write the second-type parabolic coordinates as [77, 78, 95]

$$x = \xi\eta\ cos\varphi, \quad y = \xi\eta\ sin\varphi \quad and \quad z = \frac{1}{2}\left(\eta^2 - \xi^2\right), \tag{4.6}$$

and

$$\xi\ \eta = r\ sin\theta \quad and \quad r = \frac{1}{2}\left(\eta^2 + \xi^2\right). \tag{4.7}$$

If we write trial wave function in the following form [78]

$$\Psi(\xi,\eta,\varphi) = \frac{1}{\sqrt{\xi\eta}}\ u(\xi)\ v(\eta)\ e^{im'\varphi}, \tag{4.8}$$

one can get the following differential equations

$$\frac{d^2u}{d\xi^2} - \frac{(\Upsilon^2 - \frac{1}{4})}{\xi^2}u + (\frac{2mE}{\hbar^2})\xi^2 u - (\frac{2m}{\hbar^2})\mu_1 u = 0, \tag{4.9}$$

and

$$\frac{d^2v}{d\eta^2} - \frac{(\Upsilon^2 - \frac{1}{4})}{\eta^2}v + (\frac{2mE}{\hbar^2})\eta^2 v - (\frac{2m}{\hbar^2})\mu_2 v = 0, \tag{4.10}$$

where $\Upsilon = \sqrt{m'^2 + \ q\delta^2\sigma^2}$ and $\mu_1 = \mu_2 = 2\sigma^2 \ \delta \ a_0 \ \epsilon_0$. We will first solve the Eq. (4.9) and then easily get the other one. By using the transformation $s = \xi^2$, the Eq. (4.9) can be converted into an equation of hypergeometric type. Hence, we have

$$u''(s) + \frac{1}{2s}u'(s) + \frac{1}{4s^2}\left[-\varepsilon^2 s^2 - \alpha_1^2 s - \beta^2\right]u(s) = 0, \tag{4.11}$$

where $\varepsilon^2 = \frac{2mE}{\hbar^2}$, $\alpha_1^2 = \frac{2m}{\hbar^2}\mu_1$ and $\beta^2 = (\Upsilon^2 - \frac{1}{4})$. Comparing the Eq. (4.11) with the Eq. (3.13), we get

$$\sigma(s) = 2s, \quad \tilde{\tau}(s) = 1 \quad and \quad \tilde{\sigma}(s) = \left(-\varepsilon^2 s^2 - \alpha_1^2 s - \beta^2\right). \tag{4.12}$$

Substituting these into the Eq. (3.20), we write

$$\pi(s) = \frac{1}{2} \pm \frac{1}{2}\sqrt{4\varepsilon^2 s^2 + (8k + 4\alpha_1^2)s + 4\beta^2}. \tag{4.13}$$

The constant k can be determined from the condition that the discriminant of the square root must be zero, so that

$$k_{1,2} = -\frac{1}{2}\alpha_1^2 \pm \varepsilon\beta. \tag{4.14}$$

Hence the final result for Eq. (4.13) can be written as

$$\pi(s) = \frac{1}{2} \pm \begin{cases} (\varepsilon s - \beta), & for \quad k = -\frac{1}{2}\alpha_1^2 - \varepsilon\beta \\ \\ (\varepsilon s + \beta), & for \quad k = -\frac{1}{2}\alpha_1^2 + \varepsilon\beta. \end{cases} \tag{4.15}$$

A proper value for $\pi(s)$ is chosen, so that the function

$$\tau(s) = 2(1 \pm \beta) - 2\varepsilon s, \tag{4.16}$$

must have a negative derivative [68]. Two solutions are acceptable for Eq. (4.16) since it has a negative derivative. Here, we choose as a solution with plus so that the result becomes physical. From the Eq. (3.18), we can obtain

$$\begin{aligned} \Lambda_n &= -\frac{1}{2}\alpha_1^2 - \varepsilon - \beta\varepsilon \\ &= 2n\varepsilon. \end{aligned} \tag{4.17}$$

Following the same procedure again one gets for Eq. (4.10) as

$$\begin{aligned} \Lambda_{n'} &= -\frac{1}{2}\alpha_2^2 - \varepsilon - \beta\varepsilon \\ &= 2n'\varepsilon. \end{aligned} \tag{4.18}$$

By combining each side of the Eqs. (4.17) and (4.18), we obtain energy eigenvalues

$$E_{n,n'} = -\left[\frac{\delta^2 \ \sigma^4}{(n + n' + 1 + \beta)^2}\right]\epsilon_0. \qquad n, n' = 0, 1, 2\ldots \tag{4.19}$$

This solution is identical for $\beta \simeq \Upsilon^2$ with the ones obtained before [77, 78, 80, 81, 82, 83, 87]. Now, we are going to determine the wave function. Using the Eq. (3.16), we get

$$\phi(s) = s^{\nu/4}\ e^{-\frac{\varepsilon}{2}s}, \tag{4.20}$$

where $\nu = 1 + 2\beta$. From the Eqs. (4.22) and (4.21), we obtain

$$y_n(s) = \frac{C_n}{\rho(s)} \frac{d^n}{ds^n} \left[s^n\ \rho(s) \right], \tag{4.21}$$

with $\rho(s) = s^{(\nu-1)/2}\ e^{-\varepsilon s}$. The Eq. (4.21) stands for the associated Laguerre polynomials. That is

$$y_n(s) \equiv L_n^{\beta}(s), \tag{4.22}$$

Hence we have found the wave function that belongs to the Eq. (4.9) as

$$u_n(\xi) = C_n\ s^{\nu/4}\ e^{-\frac{\varepsilon}{2}s}\ L_n^{\beta}(s), \tag{4.23}$$

with $s = \xi^2$. Similarly, we can also write the wave function for Eq. (4.10)

$$v_n(\eta) = C_{n'}\ s^{\nu/4}\ e^{-\frac{\varepsilon}{2}s}\ L_{n'}^{\beta}(s), \tag{4.24}$$

with $s = \eta^2$. Therefore, the total wave function becomes

$$\Psi_{n,n',m'}(\xi, \eta, \varphi) = \frac{1}{\sqrt{\xi\ \eta}}\ C_{n,n'}\ s^{\nu/2}\ e^{-\varepsilon s}\ L_n^{\beta}(s)\ L_{n'}^{\beta}(s)\ e^{im'\varphi}, \tag{4.25}$$

where the normalization constant $C_{n,n'}$ can be found from the Eq. (3.23) as

$$C_{n,n'} = \sqrt{\frac{4(n!)(n')!}{(n+\beta)!\ (n'+\beta)!}}, \qquad n,\ n' = 0, 1, 2 \ldots \tag{4.26}$$

One can easily see that in the case of $rsin\theta = \xi\eta$, the problem reduces to harmonic oscillator plus inverse square potential case. This problem also reduces to the molecular Kratzer potential case as Coulomb plus inverse square. Now, we are dealing with this problem.

4.1.1.2 Spherical Coordinates

Let us now consider the problem in spherical coordinates. Considering the Eq. (4.8), we can write the total wave function as

$$\Psi(r,\theta,\varphi) = \frac{U(r)}{r}\ \Theta(\theta)\ \Phi(\varphi), \tag{4.27}$$

with the well-known azimuthal angle solution

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}}\ e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \ldots \tag{4.28}$$

Thus, we get as

$$\frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta}{d\theta}\right) + \left(\kappa - \frac{(m^2+b')}{sin^2\theta}\right)\Theta = 0, \tag{4.29}$$

and

$$\frac{d^2U}{dr^2} + \frac{2}{\gamma}\left(-E' - \frac{a'}{r} - \frac{\kappa}{r^2}\right)U = 0, \tag{4.30}$$

where $E' = \frac{2mE}{\hbar^2}$, $a' = \frac{2ma}{\hbar^2}$ and $b' = \frac{2mb}{\hbar^2}$, κ and m^2 are also separation constants. Using the NU-method, we are going to solve them. By defining $m' = \sqrt{m^2+b}$ in Eq. (4.29) and taking $x = cos\theta$, it will have a form of hypergeometric type

$$\frac{d^2\Theta}{dx^2} - \frac{2x}{(1-x^2)}\frac{d\Theta}{dx} + \frac{1}{(1-x^2)^2}\left[\kappa(1-x^2) - m'^2\right]\Theta(x) = 0. \tag{4.31}$$

Comparing this with the Eq. (3.13), we get

$$\sigma(x) = x, \quad \tilde{\tau}(x) = -2x \quad and \quad \tilde{\sigma}(x) = \kappa(1 - x^2) - m'^2. \tag{4.32}$$

Substituting these into the Eq. (3.20), we get

$$\pi(x) = \pm\sqrt{-(k + \kappa)(1 - x^2) + m'^2}. \tag{4.33}$$

The constant k is determined from the condition that the discriminant of the square root must be zero. Thus, we find

$$\pi(x) = \begin{cases} \pm\ m', & for \quad k = \kappa \\ \\ \pm\ m'\ x, & for \quad k = \kappa - m'^2. \end{cases} \tag{4.34}$$

A proper value for $\pi(x)$ can be chosen, so that the function

$$\tau(x) = -2(m' + 1)\ x, \tag{4.35}$$

has a negative derivative. From the Eq. (3.18) we can obtain

$$\begin{aligned} \Lambda_n &= \kappa - m'(m' + 1) \\ &= 2n\ (m' + 1) + n\ (n - 1). \end{aligned} \tag{4.36}$$

Solving for κ, we have

$$\kappa = \kappa_n = \ell'(\ell' + 1), \tag{4.37}$$

where $\ell' = n + m'$. Now we are going to determine the wave function. From the Eqs. (3.22) and (3.21), we can write

$$y_n(x) = \frac{B_n}{\rho(x)} \frac{d^n}{dx^n} \left[(1-x^2)^{n+m'} \right], \tag{4.38}$$

with $\rho(x) = (1-x^2)^{m'}$. Therefore the Eq. (4.38) stands for Jacobi polynomial as

$$y_n \equiv \; P_n^{(m',m')}(x), \tag{4.39}$$

where $n = l' - m'$. The wave function becomes

$$\begin{aligned} \Theta(x) &= \Theta_{l',m'} \\ &= C_{l',m'} \; (1-x^2)^{m'/2} \; P_{l'-m'}^{(m',m')}(x), \end{aligned} \tag{4.40}$$

with $x = cos\theta$ ($x \in [-1,1]$). Using the Eq. (3.23), we get

$$C_{\ell',m'} = \frac{1}{2^{m'}(\ell'+1)} \sqrt{\frac{2\ell'+1}{2} (\ell'-m')!(\ell'+m')!}. \tag{4.41}$$

Let us now consider the Eq. (4.30)

$$u''(r) + \frac{1}{r^2} \left[-E'r^2 - a'r - \kappa \right] u(r) = 0, \tag{4.42}$$

Comparing this equation with the Eq. (3.13), we obtain

$$\sigma(r) = r, \quad \tilde{\tau}(r) = 0 \quad and \quad \tilde{\sigma}(r) = -E'r^2 - a'r - \kappa. \tag{4.43}$$

If we insert these into the Eq. (3.20), one gets

$$\pi(r) = \frac{1}{2} \pm \sqrt{4E'r^2 + 4(k+a')r + (1+4\kappa)}. \tag{4.44}$$

We can determine the constant k by using the condition that discriminant of the square root is zero, that is

$$k_{1,2} = -a' \pm \sqrt{E' \; (1+4\kappa)}. \tag{4.45}$$

Hence the final form of the Eq. (4.44) for each value of k becomes

$$\pi(r)=\frac{1}{2}\pm\frac{1}{2}\begin{cases}[2\sqrt{E'}r+\sqrt{1+4\kappa}], & for \quad k=-a'+\sqrt{E'(1+4\kappa)}\\ \\ [2\sqrt{E'}r-\sqrt{1+4\kappa}], & for \quad k=-a'-\sqrt{E'(1+4\kappa)}.\end{cases} \tag{4.46}$$

A proper value for $\pi(r)$ is taken, so that the function

$$\tau(r)=(1+\sqrt{1+4\kappa})-2\sqrt{E'}r, \tag{4.47}$$

has a negative derivative. From the Eq. (3.18), we can write

$$\begin{aligned}\Lambda_n &= -a'-\sqrt{E'(1+4\kappa)}-\sqrt{E'}\\ &= 2n\,\sqrt{E'}.\end{aligned} \tag{4.48}$$

Therefore, it gives us the energy eigenvalues of the radial equation with the deformed ring-shaped potential

$$E=\left[-\left(\frac{\delta^2\,\sigma^4}{n_r+\ell'+1}\right)^2\epsilon_0\right], \quad n_r=0,1,2,\ldots \tag{4.49}$$

where n_r denotes the radial quantum number which belongs to the Eq. (4.30). To determine the wave function, we consider the Eqs. (3.14) and (3.16) for obtaining

$$\phi(r)=\ e^{-\sqrt{E'}\ r}\ r^{(\nu-1)/2}, \tag{4.50}$$

where $\nu=1+2\sqrt{1+4\kappa}$. Thus from the Eqs. (3.22) and (3.21) we have

$$y_n(r)=\frac{B_n}{\rho(r)}\frac{d^n}{dr^n}\left[\sigma^n(r)\ \rho(r)\right], \tag{4.51}$$

with $\rho(r) = e^{-\sqrt{E'}r}\ r^{(1-\nu)/2}$. The Eq. (4.51) stands for associated Laguerre polynomials, that is

$$y_n(r) = L_n^{\bar{k}}(r), \tag{4.52}$$

where $\bar{k} = (\nu - 1)/2$. The radial part wave function is written as

$$U_n(r) = C_n\ e^{-\sqrt{E'}r}\ r^{\bar{k}}\ L_n^{\bar{k}}(r). \tag{4.53}$$

By using the orthogonality condition, we can determine the coefficient as

$$C_{n,\bar{k}} = \sqrt{\frac{n!}{2(n+\bar{k})(n+\bar{k})!}}, \tag{4.54}$$

with $\kappa = \ell'(\ell'+1)$. Hence, the total wave function takes the form

$$\begin{aligned}\Psi(r,\theta,\varphi) &= \frac{1}{\sqrt{2\pi}}\ C_{n,\bar{k}}\ C_{\ell',m'}\left[e^{-\sqrt{E'}r}\ r^{\bar{k}}\ (Sin\theta)^{m'}\right. \\ &\times \left. P_n^{(m',m')}(cos\theta)\ L_n^{\bar{k}}(r)\ e^{im\varphi}\right]. \end{aligned} \tag{4.55}$$

As a conclusion, we have obtained the exact eigenfunctions and corresponding energy eigenvalues of the Schrödinger equation with the deformed ring-shaped potential in both second type parabolic and also spherical coordinates by using the Nikiforov-Uvarov method. At first our problem reduces to the harmonic oscillator plus inverse square potential, it also reduces to the problem that molecular Kratzer (Coulomb plus inverse square) one in second case. Results obtained in two different coordinate systems are identical by following the conditions $\beta \simeq \Upsilon^2$ in Eq. (4.19) and $\ell' = n + m'$ in Eq. (4.49). Some numerical values of energy for a hydrogen-like atom due to the attractive Coulomb potential are presented in tabular form. The total wave functions, in both coordinates, are physical. They behave asymptotically. The agreement of our analytic and numerical results is good.

4.2 SUSYQM and Central Confining Potentials

In this section, we present the exact supersymmetric solutions of the hypergeometric form of Schrödinger equation with the Morse, Pöschl-Teller and Hulthén potentials by using the Nikiforov-Uvarov (NU) method.

4.2.1 Morse Potential

The Morse potential is

$$V_M(r) = D\left(e^{-2ax} - 2e^{-ax}\right), \tag{4.56}$$

with $x = (r - r_0)/r_0$ [95]. Here, D denotes the dissociation energy parameter and r_0 is the equilibrium distance between nucleus. Its supersymmetric form becomes [56]

$$W(x) = A - Be^{-ax}. \tag{4.57}$$

Thus, we first get the superpartner potentials as

$$V_{\pm}(x, A, B) = A^2 + B^2 e^{-2ax} - 2B\left(A \mp \frac{\hbar a}{\sqrt{8m}}\right) e^{-ax}. \tag{4.58}$$

From the Eqs. (2.1) and (2.8), the Schrödinger equation can be written as [96]

$$H_{\pm}\Psi = E_{\pm}\Psi \tag{4.59}$$

or explicitly

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}\left[E_{-} - V_{-}\right]\Psi = 0. \tag{4.60}$$

Using the Eq. (4.58) for V_{-}, we get

$$\Psi''(x) + \frac{2m}{\hbar^2}\left[\bar{E} - \bar{B}e^{-2ax} + \bar{C}e^{-ax}\right]\Psi(x) = 0, \tag{4.61}$$

where $\bar{E} = E_{-} - A^2$, $\bar{B} = B^2$ and $\bar{C} = 2B\left(A + \frac{\hbar\ a}{\sqrt{8m}}\right)$. By introducing a transformation

$$-s = e^{-ax}, \tag{4.62}$$

the Eq. (4.61) takes the form

$$\Psi''(s) + \frac{1}{s}\Psi'(s) + \frac{1}{s^2}\left[\beta^2 - \gamma^2 s - \alpha^2 s^2\right]\Psi(s) = 0, \tag{4.63}$$

where

$$\alpha^2 = \frac{2m\bar{B}}{a^2\hbar^2}, \quad \beta^2 = \frac{2m\bar{E}}{a^2\hbar^2}\left(E^{'} < 0\right) \quad and \quad \gamma^2 = \frac{2m\bar{C}}{a^2\hbar^2}. \tag{4.64}$$

Comparing the Eq. (4.63) with the Eq. (3.13), we obtain

$$\sigma(s) = s, \quad \tilde{\tau}(s) = 1 \quad and \quad \tilde{\sigma}(s) = \left(-\beta^2 - \gamma^2 s - \alpha^2 s^2\right). \tag{4.65}$$

Substituting these polynomials into the Eq. (3.20), we get

$$\pi(s) = \pm\sqrt{\alpha^2 s^2 + (k + \gamma^2)s + \beta^2}. \tag{4.66}$$

The constant k is determined as

$$k_{1,\,2} = -\gamma^2 \pm 2\alpha\beta, \tag{4.67}$$

and we have

$$\pi(s) = \begin{cases} \pm(\alpha s - \beta), & for \quad k = -\gamma^2 - 2\alpha\beta \\ \\ \pm(\alpha s + \beta), & for \quad k = -\gamma^2 + 2\alpha\beta. \end{cases} \tag{4.68}$$

A proper value for $\pi(s)$ is chosen, so that the function

$$\tau(s) = (1 \pm 2\beta) - 2\alpha s, \tag{4.69}$$

has a negative derivative [68]. Two solutions are acceptable for $\tau(s)$. Here, we choose the solution with plus which is physical. By using the Eq. (3.18), we can find

$$\begin{aligned} \Lambda &= -\gamma^2 - 2\alpha\beta - \alpha \\ &= 2\alpha n. \end{aligned} \tag{4.70}$$

Thus, we simply get the energy eigenvalues as

$$\bar{E}_{n,\,\ell=0} = \frac{a^2\hbar^2}{2m}\left[\bar{D} - (n + \frac{1}{2})\right]^2, \tag{4.71}$$

where $\bar{D} = \gamma^2/2\alpha$. By setting $\alpha = 1$, this equation reduces to the Eq. (10) as [98] for $s - states$. For Eq. (4.71), the square term refers to the anharmonic oscillator correction and the other one corresponds to the harmonic oscillator solution. Now, we are going to determine the eigenfunctions for this potential.

By considering the Eq. (3.14) and using the Eq. (3.16), we obtain

$$\phi(s) = s^{\beta}\ e^{-\alpha s}. \tag{4.72}$$

By using the Eqs. (3.22) and (3.21), we obtain

$$y_n(s) = \frac{C_n}{\rho(s)} \frac{d^n}{ds^n} \left[s^n \rho(s)\right], \tag{4.73}$$

where $\rho(s) = s^{2\beta}\ e^{-2\alpha s}$. The Eq. (4.73) stands for the associated Laguerre polynomials, that is

$$y_n(s) \equiv L_n^t(s), \tag{4.74}$$

where $t = 2\beta$. Hence, we can write the wave function in the final form

$$\Psi_n(x) = C_n\ s^{\beta}\ e^{-\eta s}\ L_n^t(s), \tag{4.75}$$

with $s = -e^{ax}$. It is normalizable. Using the Eq. (3.23), the normalization constant can be found as

$$C_n = \sqrt{\frac{n!}{(n+\beta+\frac{1}{2})(n+2\beta)!}}, \quad n = 0, 1, 2\ldots \tag{4.76}$$

4.2.2 Pöschl-Teller Potential

Let us now consider the Pöschl-Teller potential

$$V_{PT}(x) = -\frac{U_0}{\cosh^2 \alpha x}, \tag{4.77}$$

where $U_0 = \lambda\ (\lambda - 1) > 0$ [68]. Also, its superpotential potential is [56]

$$W(x) = A \tanh \alpha x. \tag{4.78}$$

By means of the Eqs. (2.5) and (2.9), we get its superpartners

$$V_{\pm}(x, A) = A^2 - A\left(A \mp \frac{\alpha\hbar}{\sqrt{2m}}\right)\frac{1}{\cosh^2 \alpha x}. \tag{4.79}$$

Thus, we can write the Schrödinger equation as

$$\Psi''(x) + \frac{2m}{\hbar^2}\left[\widetilde{E} - \frac{\kappa}{\cosh^2 \alpha x}\right]\Psi(x) = 0, \tag{4.80}$$

where $\widetilde{E} = E_{-} - A^2$ and $\kappa = A\left(A + \frac{\alpha\hbar}{\sqrt{2m}}\right)$. Introducing a transformation

$$s = \tanh \alpha x, \tag{4.81}$$

we rewrite the Eq. (4.80)

$$\Psi''(s) + \frac{-2s}{(1-s^2)}\Psi'(s) + \frac{1}{(1-s^2)^2}\left[-\beta^2 + \gamma^2(1-s^2)\right]\Psi(s) = 0, \tag{4.82}$$

where

$$\beta^2 = \frac{2m\widetilde{E}}{\alpha^2\hbar^2}\ (\widetilde{E} < 0) \quad \textit{and} \quad \gamma^2 = \frac{2m\kappa}{\alpha^2\hbar^2}. \tag{4.83}$$

By comparing the Eq. (4.82) with the Eq. (3.13), we determine polynomials as

$$\sigma(s) = (1-s^2), \quad \tilde{\tau}(s) = -2s \quad \textit{and} \quad \tilde{\sigma}(s) = -\beta^2 + \gamma^2(1-s^2). \tag{4.84}$$

Substituting them into the Eq. (3.20), we obtain

$$\pi(s) = \pm\sqrt{\beta^2 - \gamma^2(1-s^2) + k(1-s^2)}. \tag{4.85}$$

The constant k is determined in the same way. Therefore, we get

$$\pi(s) = \begin{cases} \pm\beta, & for \quad k = \gamma^2 \\ \\ \pm\beta s, & for \quad k = \gamma^2 - \beta^2. \end{cases} \tag{4.86}$$

Here we choose the proper value, so that

$$\tau(s) = -2(1+\beta)s, \tag{4.87}$$

has a negative derivative. From the Eq. (3.18), we can calculate

$$\begin{aligned} \Lambda &= \gamma^2 - \beta^2 - \beta \\ &= n^2 + n + 2n\beta. \end{aligned} \tag{4.88}$$

Hence, the energy eigenvalues are found as

$$\widetilde{E}_n = A^2 - \frac{\hbar^2\alpha^2}{2m}\left[-(n+\frac{1}{2}) + \frac{1}{2}\sqrt{1+4\gamma^2}\right]^2. \tag{4.89}$$

The wave function $\Psi_n(x)$ is obtained from the Eq. (3.14) by taking $\pi(s) = -\beta s$ as follows. We first get

$$\phi(s) = (1-s^2)^{\beta/2}, \tag{4.90}$$

and using the Eqs. (3.22) and (3.21), we find

$$y_n(s) = \frac{C_n}{\rho(s)}\frac{d^n}{ds^n}\left[(1-s^2)^n\rho(s)\right], \tag{4.91}$$

where $\rho(s) = (1-s^2)^\beta$. The Eq. (4.91) stands for the Jacobi polynomials as

$$y_n \equiv P_n^{(\beta,\,\beta)}(s). \tag{4.92}$$

Hence, $\Psi_n(x)$ can be written in the following form

$$\Psi_n(x) = C_n \ (1-s^2)^{\beta/2} \ P_n^{(\beta,\ \beta)}(s), \tag{4.93}$$

with $s = \tanh \alpha \ x$. Considering the Eq. (3.23), the normalization constant is obtained as

$$C_n = \frac{1}{2^\beta \ (n+\beta)!}\sqrt{\frac{(2n+2\beta+1)}{2} n!(2n+\beta)!}. \tag{4.94}$$

where $n, \ \beta \geq 0$.

4.2.3 Hulthén Potential

Now, we consider the Hulthén potential. This potential is given by

$$V_0^H = -V_0 \frac{e^{-\delta x}}{(1-e^{-\delta x})}, \tag{4.95}$$

where $\delta = 1/a$, is the screening parameter. We get the supersymmetric form the potential for $s-states$ [99]

$$W_1 = \bar{a} + \bar{b}\frac{e^{-\delta x}}{(1-e^{-\delta x})}. \tag{4.96}$$

Here, $\bar{a}$ and $\bar{b}$ are arbitrary constants. We can also write the supersymmetric partner of the potential as [100]

$$V_1^H = V_0^H + \frac{V_0^2 \ e^{-\delta x}}{(1-e^{-\delta x})^2}. \tag{4.97}$$

The second term in the Eq. (4.97) behaves like centrifugal barrier [95]. The

Schrödinger equation has the form

$$\Psi''(x) + \frac{2m}{\hbar^2}\left[\overline{E} - V_1^H(x)\right]\Psi(x) = 0. \tag{4.98}$$

Using the transformation

$$s = e^{-\delta x}, \tag{4.99}$$

we rewrite

$$\Psi''(s) + \frac{(1-s)}{[s(1-s)]}\Psi'(s) + \frac{1}{[s(1-s)]^2}\left[-(\varepsilon^2+\beta^2)s^2 + (2\varepsilon^2+\beta^2-\gamma^2)s - \varepsilon^2\right]\Psi(s) = 0, \tag{4.100}$$

where

$$\varepsilon^2 = \frac{2m\overline{E}}{\delta^2\hbar^2}(\overline{E} > 0), \quad \beta^2 = \frac{2mV_0}{\delta^2\hbar^2} \quad and \quad \gamma^2 = \frac{2mV_0^2}{\delta^2\hbar^2}. \tag{4.101}$$

By comparing the Eq. (4.100) with the Eq. (3.13), we get

$$\sigma(s) = s(1-s), \quad \tilde{\tau}(s) = 1-s \quad and \quad \tilde{\sigma}(s) = -(\varepsilon^2+\beta^2)s^2 + (2\varepsilon^2+\beta^2-\gamma^2)s - \varepsilon^2. \tag{4.102}$$

Substituting them into the Eq. (3.20), we obtain

$$\pi(s) = -\frac{1}{2}s \pm \frac{1}{2}\sqrt{4\left(\varepsilon^2+\beta^2-k+\frac{1}{4}\right)s^2 - 4\left(2\varepsilon^2+\beta^2-\gamma^2-k\right)s + 4\varepsilon^2}. \tag{4.103}$$

From the Eq. (4.103), k is determined as

$$k_{1,\,2} = -\gamma^2 + \beta^2 \pm \varepsilon\sqrt{1+4\gamma^2}. \tag{4.104}$$

Following the same procedure, we get

$$\pi(s) = -\frac{1}{2}s \pm \frac{1}{2}\left[\left(2\varepsilon + \sqrt{1+4\gamma^2}\right)s - 2\varepsilon\right], \tag{4.105}$$

and the energy eigenvalues for the supersymmetric Hulthén potential becomes

$$\overline{E}_{\bar{n},\ \ell=0} = -V_0\left[\frac{\beta^2 - \bar{n}^2}{2\ \bar{n}\ \beta}\right]^2, \quad \bar{n} = 1, 2, \ldots \tag{4.106}$$

Here, $\beta^2 = 2V_0/\delta^2$ with $(\hbar = m = 1)$ and $\bar{n} = \left[(n+\frac{1}{2}) - \frac{1}{2}\sqrt{1+4\gamma^2}\right]$. If the limit $\gamma \to 0$ is chosen, the energy eigenvalue reduces to the form obtained from the usual solution of the Hulthén potential.

The wave functions can now be obtained similarly from the Eq. (3.14). Using the Eq. (3.16), we have

$$\phi(s) = s^{\varepsilon}\ (1-s)^{\mu/2}, \tag{4.107}$$

where $\mu = 1 + \sqrt{1+4\gamma^2}$. Thus, the Eqs. (3.22) and (3.21) lead to

$$y_n(s) = \frac{C_n}{\rho(s)}\frac{d^n}{ds^n}\left[s^n(1-s)^n\rho(s)\right]. \tag{4.108}$$

Here, $\rho(s) = s^{2\varepsilon}\ (1-s)^{\mu-1}$. It stands for the Jacobi polynomials as [97]

$$y_n(s) \simeq P_n^{(2\varepsilon,\ \mu-1)}(1-2s). \tag{4.109}$$

Thus, the final form of the wave function can also be written in terms of the Jacobi polynomials resulting

$$\Psi_n(x) = C_n\ s^{\varepsilon}\ (1-s)^{\mu/2}\ P_n^{(2\varepsilon,\ \mu-1)}(1-2s), \tag{4.110}$$

with $s = e^{-\delta x}$, and also the normalization constant C_n.

In this study, we have applied the NU-method to obtain the exact energy eigenvalues and the corresponding eigenfunctions of the three well-known shape invariant potentials, i.e. Morse, Pöschl-Teller and Hulthén. Using with the SUSYQM together, the Schrödinger equation can be solved analytically. All wave functions of the three potentials are physical. They are finite everywhere as well.

4.3 SUSYQM and PT-Symmetric Quantum Mechanics with their Applications

Recently, PT-symmetric quantum mechanics has focused on the study of the spectral properties of various non-Hermitian PT-symmetric Hamiltonians. In the formalism of PT-symmetric quantum mechanics, the Hamiltonian is required to be invariant under the simultaneous action of the parity P, $(x \Rightarrow -x)$ and the time reversal T, $(i \Rightarrow -i)$ operations. Also, it is based on the CPT theorem, $(C - \mathit{charge\ conjugation\ operator})$, that follows from the axiomatic quantum field theory. One may obtain the general field theory by replacing the axiom of the Hermiticity of the Hamiltonian by means of $CPT-$symmetry. The simplest nonrelativistic examples of such theories is the PT-symmetric quantum mechanics. Bender and his collaborates [64] suggested that certain non-Hermitian Hamiltonians possess real spectra. These type of Hamiltonians are invariant under PT-symmetric transformations so that their spectral properties are associated to their PT-symmetry. However, the eigenvalues of every PT-symmetric Hamiltonians are real or complex. If the PT-symmetry is exact, the spectrum of the

Hamiltonian is real. Otherwise, the eigenvalues are complex conjugate pairs and spontaneous breaking of PT-symmetry exists. Mostafazadeh has suggested that another version of the non-Hermitian Hamiltonian, termed pseudo-Hermitian concept, that also gives rise to real eigenvalues [65]. Certain class of Hamiltonians satisfy

$$\hat{H}^{\dagger} = \eta \hat{H} \eta^{-1}, \tag{4.111}$$

where $\hat{H}^{\dagger}$ denotes the adjoint of the corresponding Hamiltonian operator and η is a Hermitian invertible linear operator. Pseudo-Hermiticity of a Hamiltonian implies the existence of an antilinear symmetry. PT-symmetric Hamiltonians also satisfy

$$[\hat{H}, PT] = 0. \tag{4.112}$$

Moreover, an eigenvalue of $\hat{H}$ is real provided that the corresponding eigenstate is invariant under the action of PT and

$$\hat{H}^{\dagger}|E\rangle = \varepsilon|E\rangle, \qquad PT|E\rangle = |E\rangle, \tag{4.113}$$

imply $\varepsilon \in \mathbf{R}$.

Furthermore, pseudo-Hermiticity is a necessary condition for having a real spectrum, but it is not sufficient. PT-symmetric Hamiltonians admit a complete set of bi-orthonormal eigenvectors $\{|\Psi_n, a\rangle, \ |\phi_n, a\rangle\}$. These Hamiltonians are also diagonalizable and have a discrete spectrum. There are many applications of non-Hermitian PT-invariant Hamiltonians in physics. All the Hermitian as well as the non-Hermitian Hamiltonians are used in ionization optics, the study of dissipative systems and resonant states, two-component formulation of the quantum cosmology. The spectral properties of the PT-symmetric Hamiltonians can also be obtained by using numerical methods. Further, using perturbation and semiclassical approaches, various PT-invariant potentials have been analysed. In particular, non-Hermitian Hamiltonians obtained by the addition of an imaginary external field have been recently introduced to study delocalization transitions in condensed matter physics. The Lagrangian

$$\mathcal{L} = (\nabla\phi)^2 + m^2\phi^2 - g(i\phi)^{\mathcal{N}}, \quad \mathcal{N} \in \mathcal{R} \tag{4.114}$$

possesses PT-invariance. One can calculate the real, positive Higgs mass in a renormalizable theory such as $-g\phi^4$ or $ig\phi^3$ in which symmetry breaking occurs naturally by using the Schwinger-Dyson equations. If we replace conventional $g\phi^4$ or $g\phi^3$ theories by $-g\phi^4$ or $ig\phi^3$ theories, it has the effect of reversing signs in $\beta-$function. For example, PT-symmetric massless electrodynamics has a nontrivial stable critical value of the fine structure constant α. Supersymmetric non-Hermitian, PT invariant Lagrangians have also been examined. The breaking of parity symmetry does not include a breaking of the apparently robust global symmetry. The strong coupling constant limit of non-Hermitian PT-symmetric Hamiltonians has been investigated in quantum field theories. There have been many applications in constructing non-Hermitian PT-symmetric Hamiltonians within the context of SUSYQM. In these studies, a straightforward generalization of supersymmetric quantum mechanics is developed for pseudo-Hermitian Hamiltonians.

4.3.1 Morse Potential and Hierarchy of Hamiltonian

Supersymmetric solution of PT-/non-PT-symmetric and non-Hermitian Morse potential is studied to get real and complex-valued energy eigenvalues and corresponding wave functions. Hamiltonian Hierarchy method is used in the calculations.

4.3.1.1 The General q-deformed Morse Potential

Let us first consider the generalized Morse potential as [101]

$$V_M(x) = V_1\ e^{-2ax} - V_2\ e^{-ax}. \tag{4.115}$$

where V_1 and V_2 are real parameters. By comparing this potential with the Eq. (4.56), we conclude $V_1 = D$ and $V_2 = 2qD$. Thus, one can construct the hierarchy of Hamiltonians for Schrödinger equation with $\ell = 0$,

$$\left[-\frac{d^2\Psi}{dx^2} + \mu^2(e^{-2ax} - 2qe^{-ax})\right]\Psi(x) = \varepsilon\Psi(x), \tag{4.116}$$

where $\mu^2 = \frac{2mV_1}{a^2\hbar^2}$ and $E = \varepsilon\frac{a^2\hbar^2}{2m}$. We can also write the Riccati equation as

$$W_1^2 - W_1' + \varepsilon_0^{(1)} = V_1(x). \tag{4.117}$$

Here $V_1(x)$ is the superpartner of the superpotential $W_1(x)$. Following by ansatz equation, we have

$$W_1(x) = -\mu\ e^{-ax} + q\ \delta, \tag{4.118}$$

and inserting this into the Eq. (4.117), we get

$$\delta = (\mu - \frac{a}{2q}), \tag{4.119}$$

with the first ground state energy

$$\varepsilon_0^{(1)} = -q^2(\mu - \frac{a}{2q})^2. \tag{4.120}$$

In order to construct the other superpartner potential $V_2(x)$, we will solve the equation

$$W_1^2 + W_1' + \varepsilon_0^{(1)} = V_2(x). \tag{4.121}$$

Then, we can find the second member superpotential as

$$W_2(x) = -\mu\ e^{-ax} + q\ \kappa. \tag{4.122}$$

Now, putting this ansatz into the Eq. (4.117), we get

$$\kappa = (\mu - \frac{3a}{2q}), \tag{4.123}$$

with

$$\varepsilon_0^{(2)} = -q^2(\mu - \frac{3a}{2q})^2. \tag{4.124}$$

By similar iterations, one can get the general results

$$W_{n+1}(x) = -\mu\ e^{-ax} + q\left[\mu - \frac{a}{q}(n+\frac{1}{2})\right], \tag{4.125}$$

$$V_{n+1}(x) = \mu^2(e^{-2ax} - 2qe^{-ax}) + 2na\mu\ e^{-ax}, \tag{4.126}$$

$$E_{n+1}^{(\ell=0)} = -q^2\left[\mu - \frac{a}{q}(n+\frac{1}{2})\right]^2, \tag{4.127}$$

and ground state wave function

$$\Psi_0(x) = N\ \exp\{-\widetilde{\mu}e^{-ax} + q\left[\mu - \frac{a}{q}(n+\frac{1}{2})\right]x\}. \tag{4.128}$$

where we choose $\widetilde{\mu} = a\mu$ and set ($\hbar = 2m = 1$) in Eq. (4.127).

4.3.1.2 Non-PT-symmetric and Non-Hermitian Morse Case

Now, we will concentrate on the non-PT-symmetric and non-Hermitian Morse case. Let us now consider the Eq. (4.115) with respect to $V_1 \rightarrow\ D$ as real and $V_2 \rightarrow\ 2iqD$ as complex parameters. Hence we construct the hierarchy of Hamiltonian of the Schrödinger equation for the complexified Morse potential as

$$\left[-\frac{d^2\Psi}{dx^2} + \mu^2(e^{-2ax} - 2iqe^{-ax})\right]\Psi(x) = \varepsilon\Psi(x), \tag{4.129}$$

where $\mu^2 = \frac{2mV_1}{a^2\hbar^2}$ and $E = \varepsilon\frac{a^2\hbar^2}{2m}$. Applying the hierarchy of Hamiltonians as in the previous section, the $(n+1)$-th member results will be

$$W_{n+1}(x) = -\mu\ e^{-ax} + q\left[i\mu - \frac{a}{q}(n+\frac{1}{2})\right], \tag{4.130}$$

$$V_{n+1}(x) = \mu^2(e^{-2ax} - 2qe^{-ax}) + 2na\mu\ e^{-ax}, \tag{4.131}$$

$$E_{n+1}^{(\ell=0)} = -q^2\left[i\mu - \frac{a}{q}(n+\frac{1}{2})\right]^2, \tag{4.132}$$

with

$$\Psi_0(x) = N \ \exp \ \{-\widetilde{\mu} e^{-ax} + q \left[i\mu - \frac{a}{q}(n + \frac{1}{2}) \right] x\}, \tag{4.133}$$

where $\widetilde{\mu} = a\mu$.

4.3.1.3 PT-symmetric and Non-Hermitian Morse case

Now, let us consider the PT-symmetric and non-Hermitian Morse case. We assume the potential parameters $V_1 = (\alpha + i\beta)^2$ and $V_2 = (2\gamma + 1)(\alpha + i\beta)$ in the Eq. (4.115). Here we choose α and β and $\gamma = -\frac{1}{2} + q(\alpha + i\beta)$. When $a \Rightarrow ia$ in Eq. (4.115) and choosing V_1 and V_2, the potential form will be

$$V_M(x) = (\alpha + i\beta)^2 (e^{-2iax} - 2q e^{-iax}). \tag{4.134}$$

The ansatz equation is

$$W_1(x) = \xi \ e^{-iax} + iq \ \delta. \tag{4.135}$$

As a result the Schrödinger equation can be written by using the Eq. (4.116) for $\mu^2 = \frac{2m(\alpha+i\beta)^2}{a^2\hbar^2}$ and $E = \varepsilon \frac{a^2\hbar^2}{2m}$ $(if E < 0)$. Applying the same procedure again, one can get

$$W_{n+1}(x) = \xi \ e^{-iax} + iq \left[i\xi - \frac{a}{q}(n + \frac{1}{2}) \right], \tag{4.136}$$

$$V_{n+1}(x) = \mu^2 (e^{-2iax} - 2q e^{-iax}) + 2in\xi \ a \ e^{-iax}, \tag{4.137}$$

$$E_{n+1}^{(\ell=0)} = -q^2 \left[i\xi - \frac{a}{q}(n + \frac{1}{2}) \right]^2, \tag{4.138}$$

with

$$\Psi_0(x) = N \ \exp \ \{-\widetilde{\xi} e^{-iax} + iq \left[i\xi - \frac{a}{q}(n + \frac{1}{2}) \right] x\}, \tag{4.139}$$

where $\widetilde{\mu} = ia\mu$. In this study, we have used the PT-symmetric formulation developed recently within non-relativistic quantum mechanics to a more general Morse potential. We have solved the Schrödinger equation in one dimension by applying Hamiltonian hierarchy method within the framework of SUSYQM. We discussed many different complex forms of this potential. Energy eigenvalues and corresponding eigenfunctions are obtained exactly. We also point out that the exact results obtained for the complexified Morse potential may increase the number of interesting applications in the study of different quantum mechanical systems. In the case of $\beta = 0$ in Eq. (4.138), there is only real spectra, when $\alpha = 0$, otherwise there exists a complex-valued energy spectra. This implies that broken PT-symmetry doesn't occur spontaneously. Moreover, PT-/non-PT-symmetric non-Hermitian solutions have the same spectra. We also note that both the real and imaginary parts of the energy eigenvalues correspond to the anharmonic and harmonic oscillator solutions. The $(n+1)-th$ member superpotential, its superpartner and also corresponding ground state eigenfunctions of PT-symmetric non-Hermitian potentials satisfy the condition of PT-invariance though the others do not.

4.3.2 SUSYQM and Woods-Saxon Potential

Supersymmetric solution of PT-/non-PT-symmetric and non-Hermitian form of the general q-deformed Woods-Saxon potential is investigated. The real and complex-valued energy eigenvalues and corresponding eigenfunctions are obtained. Hamiltonian hierarchy method within the framework of SUSYQM is used. By taking appropriate values for the parameter q, similar results are obtained for Hulthén and exponential type screened potentials.

4.3.2.1 The General q-deformed Woods-Saxon Potential

Let us consider the three-parameter Woods-Saxon potential

$$V_0^{WS}(r) = -V_0 \, \frac{e^{-\delta r}}{1 + q \; e^{-\delta r}}. \tag{4.140}$$

Here, $\delta = 1/a$ is screening parameter. To determine the superpartner of WS potential we propose an ansatz for the ground state wavefunction as

$$\Psi_0 \sim \; e^{-Ar} \; \left(1 + q e^{-\delta r}\right), \tag{4.141}$$

where $A = (\beta^2 - 1) \; \delta/2$ and $\beta = \sqrt{V_0}/\delta > 0$ [100]. The superpartner potential $V_1^{WS}(r)$ of Hamiltonian H_1 is

$$V_1^{WS}(r) = V_0^{WS}(r) - q \; \delta^2 \frac{e^{-\delta r}}{(1 + q \; e^{-\delta r})^2} \tag{4.142}$$

Let us now construct the other superpartner potential $V_2^{WS}(r)$ through the approximate $p - state$ solution for WS potential. The solution is given as [100]

$$\Psi_1^{(0)}(r) \sim \; \hat{\Omega} \; \Psi_0^{(1)}. \tag{4.143}$$

By using the Hermitian operator $\hat{\Omega}$

$$\hat{\Omega} = -\frac{d}{dr} - q \; \delta \frac{e^{-\delta r}}{1 + q \; e^{-\delta r}} - A, \tag{4.144}$$

and

$$\Psi_0^{(1)} \sim \; e^{-Br}\; (1 + q\; e^{-\delta r})\; (1 - \lambda\; e^{-\delta r}), \tag{4.145}$$

in the Eq. (2.7), we get

$$\Psi_1^{(0)} \sim \; -\, \lambda'\; e^{-Br}\; (1 + q\; e^{-\delta r})^2. \tag{4.146}$$

In these equations, the constants are defined as $B = (\beta^2 - 4/4\delta)$, $\lambda = [(\beta^2 + 2)/(\beta^2 - 2)]$ and $\lambda' = \lambda\; [(\beta^2 - 4)/4a]$ respectively. Then, we substitute the Eq. (4.146) into the Eq. (4) [100] to obtain the other superpartner potential

$$V_2^{WS}(r) = V_0^{WS}(r) - 3q\; \delta^2 \frac{e^{-\delta r}}{(1 + q\; e^{-\delta r})^2}. \tag{4.147}$$

Similarly, the $(n+1) - th$ member of superpartner potential for iterating process of supersymmetric partner Hamiltonians takes

$$V_{n+1}^{WS}(r) = V_0^{WS}(r) - 2q\; \delta^2 \left(n + \frac{1}{2}\right) \frac{e^{-\delta r}}{(1 + q\; e^{-\delta r})^2}, \tag{4.148}$$

where $n = 0, 1, 2, \ldots$, and $-1 \leq \; q \leq \; 1$.

4.3.2.2 PT-/Non-PT-symmetric and Non-Hermitian of the Woods-Saxon potential

Now, we consider the PT-symmetric form of WS Potential. To obtain this potential, we take $\delta \Rightarrow i\delta$ in the Eq. (4.140). The ansatz equation for this potential is

$$\Psi_0 \sim \; e^{-Ar}\; \left(1 + qe^{-i\delta r}\right). \tag{4.149}$$

Following the same procedure again as in the previous section, we have

$$V_1^{WS}(r) = V_0^{WS}(r) + q\ \delta^2 \frac{e^{-i\delta r}}{(1+q\ e^{-i\delta r})^2}. \tag{4.150}$$

If we use the definition of approximate $p-state$ wave function for PT-symmetric WS potential as in the Eq. (4.143), one gets

$$V_2^{WS}(r) = V_0^{WS}(r) + 3q\ \delta^2 \frac{e^{-i\delta r}}{(1+q\ e^{-i\delta r})^2}. \tag{4.151}$$

Consequently, the iterating process gives us a general $(n+1)-th$ member PT-symmetric superpartner potentials as

$$V_{n+1}^{WS}(r) = V_0^{WS}(r) + 2q\ \delta^2 \left(n+\frac{1}{2}\right) \frac{e^{-i\delta r}}{(1+q\ e^{-i\delta r})^2}. \tag{4.152}$$

This holds for only $n = 0, 1, 2, \ldots$, and $-1 \leq\ q \leq\ 1$.

4.3.2.3 Energy Eigenvalue Characteristics

The energy eigenvalue characteristics of these type potentials are in the following: To get the energy eigenvalues for the general q-deformed WS potential, we suggest an ansatz superpotential in the Eq. (4) as [102]

$$W(r) = \frac{a}{e^{\delta r}+q} + b, \tag{4.153}$$

where a and b are real parameters. Using the Eqs. (2.5), (2.6) and (2.9) for $(\hbar = 2m = 1)$, one can get

$$W(r) = \frac{-q\delta}{e^{\delta r}+q} + A. \tag{4.154}$$

Comparing the Eqs. (4.153) and (4.154) term-by-term, we have

$$a = -q\delta, \tag{4.155}$$

and

$$b = A = \frac{V_0}{2\delta} - \frac{\delta}{2}. \tag{4.156}$$

The partner potentials $V_1(r;\ a_0)$ and $V_2(r;\ a_1)$ must satisfy the shape invariant requirement

$$V_1(r; a_0) = V_2(r; a_1) + \Re(a_1). \tag{4.157}$$

Thus, we choose $a_0 = a$ and $a_1 = a - q\delta$. The remainder term $\Re(a_1)$ can also be easily determined as

$$\Re(a_1) = \left(\frac{V_0}{2a_0} - \frac{a_0}{2q}\right) - \left(\frac{V_0}{2a_1} - \frac{a_1}{2q}\right)^2. \tag{4.158}$$

The energy eigenvalues are obtained for partner Hamiltonian $\hat{H}_1$

$$E_n^{(1)} = \sum_{k=1}^{n} \Re(a_k) = \left(\frac{V_0}{2a_0} - \frac{a_0}{2q}\right)^2 - \left(\frac{V_0}{2a_n} - \frac{a_n}{2q}\right)^2, \tag{4.159}$$

where $a_n = a - nq\delta$. For unbroken SUSY case, the ground state energy $E_0^{(1)}$ is zero. Finally, the most general energy eigenvalue becomes

$$E_n = -\left\{\frac{1}{2}\left[\frac{V_0/a}{(n+1)} - \frac{a}{q}(n+1)\right]\right\}^2. \tag{4.160}$$

This holds for $n \geq 0$.

In non-PT-symmetric and non-Hermitian WS case, we consider the coefficient $V_0 \rightarrow\ V_0 + iV_I$ in Eq. (17) as in [103]. It corresponds to the non-PT-symmetric case. Hence, we determine the parameters a and b from the ansatz superpotential (4.153) as $a = -iq\delta$ and $b = A = \frac{V_0}{2\delta} - \frac{\delta}{2}$. By means of analogy, the energy eigenvalue can be written in a compact form as

$$E_n = -\left\{\frac{1}{2}\left[\frac{a}{q}(n+1) - \frac{V_0/a}{(n+1)}\right]\right\}^2, \tag{4.161}$$

for $n \geq 0$.

In the case of PT-symmetric and non-Hermitian WS potential, we use $\delta \Rightarrow i\delta$ in Eqs. (4.140) and (4.141) so that the potential must be PT-symmetric. Then, the parameters of superpotential in Eq. (4.153) are obtained as $a = -iq\delta$ and $b = A = \frac{V_0}{2\delta} - \frac{\delta}{2}$, respectively. One can also write the energy eigenvalues of the potential in a compact form

$$E_n = -\left\{\frac{1}{2}\left[\frac{a}{q}(n+1) - \frac{V_0/a}{(n+1)}\right]\right\}^2, \tag{4.162}$$

with $n \geq 0$.

In this section, using the Hamiltonian hierarchy method within the context of SUSYQM, we have constructed the $(n+1) - th$ member superpartner potentials and determined the characteristics of energy eigenvalue spectra of both the general q-deformed Woods-Saxon potential and its PT-symmetric form. The approximate $p - state$ solution for WS potential leads to constructing of the $(n+1) - th$ member partner potentials. All results obtained by the method for cases $q \geq 1$, $q = 0$ and $q \leq -1$ refer to the solutions of Woods-Saxon, exponential and Hulthén potentials respectively. By taking $\delta \Rightarrow i\delta$, the $(n+1) - th$ member superpartner potential of WS potential reduces to the $(n+1)-th$ member PT-symmetric superpartner potential one. However, this statement is not true for vice versa. We have also shown that Woods-Saxon and Hulthén potentials have similar characteristics. Because of having real eigenvalue spectra, PT-symmetry is exact for these two potentials. We also conclude that PT-symmetry is unbroken spontaneously.

CHAPTER 5

CONCLUSIONS AND REMARKS

Supersymmetry is a key model for understanding the basic structures of quantum mechanical systems. Many results are acquired in the work of SUSYQM. One of the most important properties of supersymmetry is that it collects the continuous $(e.g., translations)$ and discrete transformations $(e.g., reflections)$. The fermionic and bosonic type systems can be defined by SUSYQM, that is, the SUSYQM algebra is the result of these systems. A study of supersymmetry in quantum mechanics is worthwhile for two reasons: Supersymmetry provides a new point of view for solving of the quantum mechanical problems, which are widely used in a variety of branches of physics. The second reason is that this model is useful for developing supersymmetric theories. Because these theories include a number of concepts which are accumulated in research on the problems of quantum mechanics. For a SUSY quantum mechanical system, if the ground state wave function $\Psi_0(x)$ is known, the superpotential $W(x)$ is obtained by using the Eq. (2.7). Instead, if the superpotential is obtained for a given potential, the ground state wave function can be found by means of the Eq. (2.6). One of the other important results is that if we have an exactly solvable potential with at least one bound state, then we can always construct its SUSY partner which is also exactly solvable. In addition to this, shape invariance requirement is a sufficient but not a necessary condition for exactly solvability. For instance, the energy eigenvalues and corresponding eigenfunctions of Natanzon potentials are obtained implicitly. There are a large number of shape invariant potentials (SIPs) which satisfy the shape invariance condition. The whole spectrum of these type of potentials can be obtained algebraically by means of the Hamiltonian Hierarchy method. The classification of solvable potentials is an important problem in SUSYQM. In order to classify the potentials, certain parametrization techniques (translation, scaling, etc) are introduced. In SUSYQM framework, the other important concept is spontaneous breaking of supersymmetry. If we have a quantum system with unbroken supersymmetry, means exact, then we have a state with a zero ground state energy as $E_0^{(1)} = 0$. The converse is also true. If there is a supersymmetry in the field of elementary particles, the spontaneous breaking of supersymmetry is needed. In the case of exact supersymmetry, the bosons and fermions would have to be mass degenerate. Another advantage of the SUSYQM is that new solvable/exactly solvable potentials can be constructed such as self-isospectral, phase equivalent ones etc. Moreover, some useful methods are used in SUSYQM. For example, supersymmetric WKB (SWKB), $\delta-$expansion methods are well-known ones. There is no doubt that the SWKB method gives a better result than the usual WKB method in the case the ground state wave function and hence the superpotential W is known.

In the present thesis, we have studied on some well-known problems within the framework of SUSYQM and the Nikiforov-Uvarov (NU) method. In the first study, exact supersymmetric solution of Schrödinger equation with the Morse, Pöschl-Teller and Hulthén potentials is obtained by using the Nikiforov-Uvarov method. Eigenfunctions and corresponding eigenvalues are also calculated for these potentials [69]. In the second study, exact solution of Schrödinger equation with the deformed ring-shaped potential is presented both in parabolic and spherical coordinates. These type of potentials are used in quantum chemistry and nuclear physics to describe the ring-shaped molecules like benzene and interactions between deformed pair of nuclei respectively. The energy eigenvalues of the potential are calculated by means of the NU method [70]. In the third study, we use the Hamiltonian Hierarchy method to get supersymmetric solution of PT/non-PT-symmetric and non-Hermitian Morse potential. In addition, the real and complex-valued energy eigenvalues and eigenfunctions are obtained for the potential [71]. In the last study, we deal with supersymmetric solution of q-deformed and PT/non-PT-symmetric version of Woods-Saxon potentials via the Hamiltonian Hierarchy method. Furthermore, we construct the $(n+1)-$th member superpartner potentials and eigenvalue spectra for both type of potentials [72].

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