Methods for Solution of Schrödinger Equation with Position Dependent Mass (PDM)

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ABSTRACT

METHODS FOR SOLUTION OF SCHRODINGER EQUATION WITH POSITION DEPENDENT MASS (PDM)

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In this study, construction of PDM Schrödinger equation has been examined starting from the kinetic energy operator approximations. In addition to this, the role and improvement of the Schrödinger type equations' solutions have been discussed.

Some of the most common methods used in order to solve Schrödinger type equations have been explained by using important articles. The potentials and the mass functions used have been emphasized. Also, the opportunity of comparing the studies have been given.

To solve PDM Schrödinger equation which has been transformed in the form of the constant mass Schrödinger equation by changing coordinate and wave function is discussed for physical acceptability. Although it was expected to have different results from both of the experiments, the same eigenvalues have been found. This situation caused the improvement of a new method without transformation. The method improved by modifying Taylor Expansion Method is called Asymptotic Taylor Expansion Method.

PDM Schrödinger equation has been solved by using Asymptotic Taylor Expansion Method for harmonic oscillator potentials. Asymptotic analyze has been done for four different Hamitonians and highly accurate energy eigenvalues and wavefunctions have been obtained. As a result of this, Asymptotic Taylor Expansion Method has been proved very useful to determine energy eigenvalues and wavefunctions in Schrödinger type equations.

Key words: PDM Schrödinger equation, Transformations, Energy eigenvalues, Wavefunctions, Asymptotic Taylor Expansion Method.

ÖZET

POZİSYONA BAĞLI KÜTLE İÇEREN SCHRÖDİNGER DENKLEMİNİN ÇÖZÜM METOTLARI

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Bu çalışmada pozisyona bağlı kütle içeren Schrödinger denkleminin oluşumu, geçmişten günümüze yapılan kinetik enerji operatörleri yaklaşımlarından başlanarak incelenmiştir. Buna ek olarak Schrödinger tipi denklemlerin çözümündeki rolü ve gelişimi irdelenmiştir.

Schrödinger tipi denklemleri çözmek için kullanılan en yaygın metotlardan bazıları önemli makaleler kullanılarak anlatılmış, kullanılan potansiyeller, kütle fonksiyonları belirtilip, yapılan çalışmaları karşılaştırma imkanı verilmiştir.

Pozisyona bağlı kütle içeren Schrödinger denklemini çözmek için sabit kütleli Schrödinger denklemine, koordinat ve dalga fonksiyonu değiştirerek çeviren dönüşüm metodu, fiziksel geçerliliği açısından değerlendirildi. İki denklemde de farklı sonuç beklenmesine rağmen aynı özdeğerlerin bulunması dönüşüm içermeyen yeni bir metot gelişimine neden oldu. Taylor seri açılımı modifiye edilerek geliştirilen bu yaklaşım metodunun adı Asimtotik Taylor Açılım Metodudur.

Pozisyona bağlı kütle içeren Schrödinger denklemi Asimtotik Taylor Açılım metotu kullanılarak harmonik osilator potansiyeli için çözüldü. Dört farklı model için asimtotik analiz yapıldı ve oldukça hassas enerji özdeğerleri ve dalga fonksiyonları bulundu. Bunun sonucunda Asimtotik Taylor Açılım Metodunun Schrödinger tipi denklemlerde enerji özdeğerleri ve dalga fonksiyonları tanımlamak için oldukça önemli olduğu ispatlandı.

Anahtar Kelimeler: Pozisyona bağlı kütle içeren Schrödinger Denklemi, Dönüşümler, Enerji özdeğerleri, Dalga fonksiyonları, Asimtotik Taylor Açılım Metotu.

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LIST OF SYMBOLS

T	Kinetic energy operator
$\hbar$	The Plank constant
$m(r)$	Mass function
∇	Gradient operator
$\vec{p}$	Momentum operator
$V(x)$	Potential function
$V(r)$	Potential function
$V_c(r)$	Conduction band edge
H	Hamiltonian
V_h	Harmonic oscillator potential
ω	Angular frequency
$\psi(r,t)$	Wavefunction
$Y(\theta,\varphi)$	Angular part of wavefunction
$R(r)$	Radial part of wavefunction
$\widehat{L^2}$	Square of angular momentum
$\Theta(\theta)$	Angular wavefunction
$\Phi(\varphi)$	Azimuthal angular wavefunction
$L_{n_l}(r)$	Laguerre polynomials

ϵ_0	Electric constant
a_0	Bohr radius
E_n	Hydrogen atom energy
n	Principle quantum number
l	Orbital quantum number
m_l	Magnetic quantum number
m^*	Effective mass
E	Energy eigenvalue
$y(x)$	Wavefunction
m_0	Constant mass
B_n	Normalizing constant
$\rho(s)$	Weight function
J^2	Casimir operator
$J_\pm$	Generators
H_{PDM}	Position dependent mass Hamiltonian
H_{eff}	Effective Hamiltonian
$U(x)$	Potential function
$Q^\pm$	Supercharges
$\sigma^\pm$	Pauli Matrices
$\Phi(x)$	Superpotential
C	Normalization constant
$A^\pm$	Supersymmetric operators

$V_{\pm}(x)$	Partner potentials
$U(r)$	Radial wavefunction
$v(\rho)$	Potential function
ε_n	Energy eigenvalues
$f^{(n)}(a)$	n^{th} derivative of the function at a
k	Iteration number

CHAPTER 1

INTRODUCTION

Position dependent mass (PDM) Hamiltonian including physical potentials has a wide range of applications, takes a crucial role in physics. In different fields of physics and material sciences, we can encounter PDM Hamiltonians, such as, semiconductors, quantum dots, wells and wires, quantum liquids, semiconductor heterostructures, graded alloys, some nuclear structures etc. Therefore, the importance of PDM is inevitable and there are many discussions about the systems [1-30].

In this thesis we review the articles about the PDM Hamiltonian. The articles can be categorized into two groups according to their topics: first group is about construction of a model Hamiltonian and second group is about development of the models to solve Schrödinger type equations. In quantum mechanics physical observables are represented in the form of the differential operators. Hamiltonian operator is the sum of kinetic energy operator and potential energy operator. It is well known that Hamiltonian gives real energy values and it should be, in general, hermitian. Unfortunately the kinetic energy operator:

$$T = -\frac{\hbar^2}{2\,m(r)}\,\nabla^2 \tag{1}$$

is non hermitian. And then, Gora and Williams [14] changed their derivation (1) to obtain correct kinetic energy operator:

$$T = -\frac{\hbar^2}{4}\left(m(r)^{-1}\nabla^2 + \nabla^2 m(r)^{-1}\right) \tag{2}$$

(2) is indeed and has also been adopted by Bastard et al [24]. van Vliet and Marshak [25] rederived (2) in addition, Zhu and Kroemer [6] postulated following kinetic energy operator:

$$T = -\hbar^2 (m(r)^{-1/2} \frac{d^2}{dr^2} m(r)^{-1/2}) \quad (3)$$

Gora and Williams, Zhu and Kroemer and other authors obtained useful kinetic energy operator for position dependent mass Hamiltonian. von Roos [1] generalized good approximations of kinetic energy operator for the movement of free carriers in semiconductors.

$$\vec{T} = \frac{1}{4}[m^{\alpha}(x)\vec{p}m^{\beta}(x)\vec{p}m^{\gamma}(x) + m^{\gamma}(x)\vec{p}m^{\beta}(x)\vec{p}m^{\alpha}(x)] \quad (4)$$

where $\vec{p}$ is momentum operator and $m(x)$ is mass function, $\alpha,\ \beta,\ \gamma$ are subject to the condition $\alpha + \beta + \gamma = -1$. Because of the noncommutativity of the momentum and (position-dependent) mass operators, maintaining hermiticity of the kinetic energy operator is not trivial [5]. Hamiltonian was written with a potential $V(x)$ and effective potential was obtained.

In 1988, some authors thought about the quantization of a particle liable to a velocity dependent force and Borges et al., summarized the classical and quantum canonical treatment and they used path integral quantization method. As a result they got the Hamiltonian [7]. Csavinszky and Elabsy [10] used von Roos kinetic energy operator and wrote effective mass Hamiltonian for an abrupt heterojunctions between two crystals. In terms of $\alpha,\ \beta,\ \gamma$ parameters, they used $2\alpha + \beta = -1$, like Morrow and Browstein [19]. Galbraith and Duggan used von Roos Hamiltonian and determined that GaAs/(Al,Ga)As quantum wells [13]. Einevoll and Hemmer for inhomogenous material were obtained an effective mass Hamiltonian:

$$H = \frac{1}{2} m^{\alpha}(x) p m^{\beta}(x) p m^{\alpha}(x) + V_c(r)$$

where $2\alpha + \beta = -1$ and $V_c(r)$ is conduction band edge. They showed an exact model calculation for $\alpha = 0,\ \beta = -1$ [12]. Koc et al., used von roos kinetic energy operator and PDM Hamiltonian was written for $\alpha = \gamma$. A square well potential with a position dependent mass barrier was studied and its novel properties were obtained [16]. Li and Kuhn [18] obtained that the permutation scheme produces Ben Danial and Duke Hamiltonian and the Bastard Hamiltonian, the Zhu and Kroemer Hamiltonian and a Hamiltonian termed the redistribution in their article. Morrow and Browstein used von Roos Hamiltonian for $\alpha \neq \gamma$ and they found that the wave

function must vanish at the junction thus implying that the junctions acts as an impenetrable barrier [19]. Mustafa and Mazharimousavi studied free particles with position dependent mass d-dimensional Schrödinger equation and they used von Roos Hamiltonian for $\alpha = \gamma = 0,\ \beta = -1$ [20]. Schmidt studied Schrödinger equation with position-dependent mass inside an infinite well and revival of wave-packet was shown [22]. Tanaka generalized N-fold supersymmetry in ordinary quantum systems with position-dependent mass and used von Roos Hamiltonian [23]. From Alhaidari articles; he used this model:

$$H = \frac{1}{2}\left[\vec{P}\left(\frac{1}{m(r)}\right)\vec{P}\right] + V(r) \tag{5}$$

where $m(r)$ and $V(r)$ are real functions of the configuration space coordinates. Wavefunctions and energy spectrum were obtained for different mass functions and Morse and Coulomb potential [2-3]. Dong and Lozada-Cassou was used PDM Hamiltonian (5) and they obtained exact solutions of two dimensional Schrödinger equation with PDM for hard core potential [11].

As we mentioned before second topic of this thesis is to review the manuscript about the methods of solutions of the PDM Hamiltonian. One of the most common method is coordinate transformation and it has been used so PDM Hamiltonian was transformed in the form of constant mass Hamiltonian.

Morales et al. obtained exactly solvable potentials for the one-dimensional Schrödinger equation with a position-dependent mass and a procedure to determine their isospectral potential partners were presented. They used point canonical transformation method to covert the Schrödinger equation with a position-dependent mass problem into a Standard Schrödinger-like equation with a position-independent mass. The procedure to obtain the partner isospectral potentials that fulfill with the Schrödinger equation with a position-dependent mass involved the Darboux transform applied to the standard Schrödinger-like equation with a position-independent mass [31]. Kraenkel et al. studied exact solutions of the position-dependent effective mass Schrödinger equation by considering the new solvable nonlinear oscillator that relates to the isotonic oscillator through the method of point canonical transformations. They used physically important position-dependent mass distributions and provided the energy spectrum of the bound states and the

wavefunctions of the solvable potentials [32]. Tezcan et al. PT-symmetric solutions of Schrödinger equation were obtained for the Scarf and generalized harmonic oscillator potentials with the position-dependent mass. They used point canonical transformation by using a free parameter and three different forms of mass distributions. In that article they obtained a set of the energy eigenvalues of the bound states and corresponding wave functions for target potentials as a function of the free parameter [33]. Jia et al. used the method of point canonical transformations and choosed the Rosen-Morse-type potential as the reference potential to study exact solutions of the position-dependent effective mass Schrödinger equations. They discussed the energy spectra of the bound states and corresponding wavefunctions for the PT-symmetric potentials and the isospectrality of different Schrödinger equations with the same mass distribution or different mass distributions for different PT-symmetric potentials [34]. Mustafa et al. the *d*-dimensional generalization of the point canonical transformation for a quantum particle endowed with a position-dependent mass in the Schrödinger equation was described. They used the harmonic oscillator, Coulomb, spiked harmonic, Kratzer, Morse oscillator, Pöschl–Teller and Hulthen potentials to obtain exact energy eigenvalues and eigenfunctions at different position dependent mass settings [35]. Jiang et al. were studied the exact solutions of the PDM Schrödinger equation by using the method of point canonical transformations and they used Rosen-Morse-type potential and Scarf-type potential [15].

In literature, authors have obtained, exact solution of the Schrödinger equation with the different potentials (i.e. Rosen-Morse potential, Scarf potential, Pöschl-Teller potential, Harmonic oscillator potential, Coulomb potential, well potentials etc.) for various mass functions. Exact solutions of the Schrödinger equation can be obtained by using various methods. Some of the most common methods are Series Expansion method [28,48,49]. Nikiforov-Uvarov method [27,60-65], Lie Algebraic Techniques [67-73], Super Symmetric Quantum Mechanics [23,78-90], Coordinate transformation [15,29-44].

The Series Expansion method is useful for N dimensional PDM Schrödinger equation for finding wavefunctions, Nikiforov-Uvarov method is useful for PDM Dirac equation and Klein Gordon equation to determine energy spectrum corresponding wave functions, the Lie algebraic technique is suitable for studying the PDM Schrödinger equation, because it contains a first-derivative term. Super

Symmetric Quantum Mechanics are important for determining dynamics of quantum particle with PDM. These methods support us many useful results. On the other hand, we must find out whether these results depend on physical reality or not.

In most applications of such methods, PDM Schrödinger equation has been transformed in the form of the constant mass Schrödinger equation by changing coordinate and wave function. Obviously, this transformation generates isospectral potentials and exact solvability requirements result in constraints on the potential functions for the given mass distributions. In other words, a suitable transformation of coordinate and wave function becomes a bridge between constant mass and position dependent mass Schrödinger equation. As an example in a constant mass Schrödinger equation the choice of coordinate

$$u = \int_0^x \sqrt{m(x)}\, dx \tag{6}$$

and wave function

$$\psi(u) = [2m(x)]^{1/4}\phi(x) \tag{7}$$

provides its transformation in the form of the PDM Schrödinger equation. In this case the potential is mass dependent; i.e. harmonic oscillator potential can be expressed as

$$V_h = \frac{1}{2}m\omega^2u^2 = \frac{1}{2}m\omega^2(\int_0^x \sqrt{m(x)}\, dx)^2 \tag{8}$$

and both constant and PDM Schrödinger equations have the same eigenvalues. The origin of such an isospectrality in the constant mass scenario has not yet been studied. It will be worthwhile to discuss physical acceptability of such an isospectrality in the position dependent mass background.

The solution of the PDM Schrödinger equation has been obtained without transforming the potential into mass space. In this case the energy spectrum of the PDM Hamiltonians are not isospectral with the constant mass Hamiltonians. Therefore, it is reasonable to develop a method for solving PDM Hamiltonian without transforming the potential into the mass space. However, the fundamental question remains open: how the potential is affected when it is expressed in the mass space? To answer this question, one has to obtain a solution for the Schrödinger

equation without transforming the potential to the mass space. In this thesis, we will obtain an approximate solution of the Schrödinger equation without transforming the potential to the mass space. This is another reason, to build a realistic model for solving PDM Hamiltonian.

In the second chapter, the history of Schrödinger equation will be explained briefly and Schrödinger equation will be solved in spherical coordinate to determine quantum numbers. Kinetic energy operator for PDM will be reviewed, so useful models will be analyzed in the other part.

In the third chapter, some of the most common methods called Series Expansion method, Nikiforov-Uvarov method, Lie Algebraic Techniques, Super Symmetric Quantum Mechanics, Coordinate transformation will be determined and analyzed whether the method transforms the potential into mass space.

In the forth chapter , we will develop an approximate method Asymptotic Taylor Expansion Method (ATEM) without transforming so its formalism is determined in the first section of this chapter and by using harmonic oscillator potential PDM Hamiltonian will be solved for four different Hamiltonian and in other section asymptotic analysis will be done.

As a result, in the last chapter, what the thesis consists of will be explained briefly. Models and methods will be discussed for physical acceptability from past to the present and difference between ATEM and other methods will be analyzed about their advantages for exact solvable Hamiltonians.

CHAPTER 2

PDM SCHRÖDINGER EQUATION

In this chapter, we will introduce the importance of the Schrödinger equation and PDM Schrödinger equation in quantum physics and briefly review these equations.

The Schrödinger equation which was formulated by Erwin Schrödinger in 1927 is the most fundamental equation in non-relativistic quantum mechanics. It is well known that de Broglie showed that electron has a wave property. Schrödinger suggested a model to describe motion of electron by developing both de Broglie hypothesis and electromagnetic wave equation. This mathematical model is used to determine wave functions and quantum states of the physical systems.

Schrödinger equation explains where electrons may be present in orbital. However, we mention here that this model does not give exact information about the position or exact momentum of electrons. Accompanied by a moving particle in quantum mechanics the wave function is shown as $\psi(r,t)$. Wave function contains all the information about the quantum physical properties of the system. It is customary to define $|\psi(r,t)|^2$ whose interpretation is that the probability of finding a particle in volume element $dV = dxdydz$ at time t. Probability of wave function tells us where electrons might be mostly in orbital at a given time. Solution of the Schrödinger equation leads to the quantum numbers. For instance three quantum numbers appears in the solution of the three dimensional Schrödinger equation. These three quantum numbers are, principle n, orbital l and magnetic m quantum numbers define state of electrons. Observables are associated with operators in quantum mechanics. Hamiltonian H is the hermitian operator and equal to sum of kinetic and potential energy. $H\psi = E\psi$ this equation is the key of quantum mechanics where E is the eigenvalue of energy. Time-dependent Schrödinger equation can be written as:

$$H\psi(r,t) = i\hbar\frac{d\psi}{dt}$$

and time-independent Schrödinger equation can be written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(r)}{dr^2}+V(r)\psi(r)=E\psi(r).$$

2.1. Schrödinger Equation in Spherical Coordinate

Schrödinger equation of an electron moving in a central potential can be solved by using the method of separation of variable. For spherically symmetrical potentials (i.e Coulomb potential, Lennard-Jones potential, Yukawa potential) Schrödinger equation can be solved exactly in spherical coordinate by using separation of variables. Thus, Schrödinger equation can be written as in spherical coordinate;

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right]$$

$$+V(r)\psi=E\psi \tag{2.1}$$

using the separable wave function: $\psi=Y(\theta,\varphi)R(r)$, where $Y(\theta,\varphi)$ is angular and $R(r)$ is radial part of the wave function, Schrödinger equation , (2.1) therefore can be written as,

$$\left[\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)\frac{2m}{\hbar^2}r^2[V(r)-E]\right]=$$

$$-\frac{1}{Y}\left[\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]=l(l+1). \tag{2.2}$$

Thus, radial equation is,

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)-\frac{2m}{\hbar^2}r^2\left[V(r)-E-\frac{l(l+1)}{r^2}\right]R(r)=0 \tag{2.3}$$

and angular equation is

$$\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial Y(\theta,\varphi)}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y(\theta,\varphi)}{\partial\varphi^2}$$

$$+l(l+1)Y(\theta,\varphi)=0 \tag{2.4}$$

where $l=0,1,2,3,\ldots$ and solution of the (2.4) gives spherical harmonics $Y_{l,m}(\theta,\varphi)$.

$$\widehat{L^2} f = -\hbar^2 \left[\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial f}{\partial\theta}\right)\frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2}\right] \quad (2.5)$$

where $\widehat{L^2}$ is square of the angular momentum. If (2.5) is put into (2.4);

$$\frac{\widehat{L^2}Y(\theta,\varphi)}{-\hbar^2} + (l+1)Y(\theta,\varphi) = 0.$$

Thus

$$\widehat{L^2}Y(\theta,\varphi) = \hbar^2(l+1)Y(\theta,\varphi) \quad (2.6)$$

(2.6) is the eigenfunction operator of the square of angular momentum.

Variables are separated in the angular equation as following;

$$Y = \Theta(\theta)\Phi(\varphi)$$

$$\frac{1}{\Theta}\left[sin\theta\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\Theta}{\partial\theta}\right) + l(l+1)\sin^2\theta\right] = -\frac{1}{\Phi} + \frac{\partial^2\Phi}{\partial\varphi^2} = m^2 \quad (2.7)$$

$$sin\theta\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\Theta}{\partial\theta}\right) + [l(l+1)\sin^2\theta - m^2]\Theta = 0 \quad (2.8)$$

$$\frac{\partial^2\Phi}{\partial\varphi^2} = -m^2\Phi \quad (2.9)$$

The wave functions are equal to $\Phi = e^{im\varphi}\ and\ \Theta(\theta) = AP_l^m(cos\theta)$ where $\Theta(\theta)$ is determined by Legendre function.

If the the function R in (2.3) is arranged by

$$R = \frac{g(r)}{r};\ \frac{\partial R}{\partial r} = \frac{1}{r}\frac{\partial g(r)}{\partial r} - \frac{g(r)}{r^2},\ r^2\frac{\partial R}{\partial r} = r\frac{\partial g(r)}{\partial r} - g(r),\ \frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) = r\frac{\partial^2 g(r)}{\partial r^2}$$

it takes the form;

$$-\frac{\hbar^2}{2m}\frac{\partial^2 g(r)}{\partial r^2} + \left[V(r) + \frac{l(l+1)}{r^2}\right]g(r) = Eg(r) \quad (2.10)$$

where $V(r)$ is given by $-k\frac{Ze^2}{r}$; $k = \frac{1}{4\pi\epsilon_0}$ and the wavefunction of radial part is;

$$R(r) = Ne^{-\frac{r}{na_0}}g(r) = Ne^{-\frac{r}{na_0}}r^l L_{n_l}(r) \quad (2.11)$$

where $L_{n_l}(r)$ is called as Laguerre polynomials with the relation $n \geq l$ for integer values of n and l. Here $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ is Bohr radius and N is normalization constant. From the radial part solution for hydrogen atom energy can be written as

$$E_n = -\frac{13.6eV}{n^2}.$$

Angular wave functions $Y_{l,m}(\theta,\varphi)$ are known as spherical harmonics and its normalized form is given by:

$$Y_{l,m}(\theta,\varphi) = \varepsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}\, e^{im\varphi}P_l^m(cos\theta) \tag{2.12}$$

where $\varepsilon = \begin{cases}(-1)^m, m \geq 0\\ 1, \quad m < 0\end{cases}$.

Generally, the principle quantum number n, orbital quantum number l, and the magnetic quantum number m_l arise from the solution of the radial part $R(r)$, angular part $\Theta(\theta)$ and azimuthal angular part $\Phi(\varphi)$, respectively.

2.2. PDM Schrödinger Equation

Importance of position dependent effective mass quantum physical structures arising because of technological development which we have referred introduction part. The motion of free carries (electrons and holes) in semiconductors of non-uniform chemical composition is sometimes described by means of a Hamiltonian possessing a position dependent effective mass [1]. The first studies of position dependent effective mass was performed by von Roos and others to get better kinetic energy operator approximation.

Radial part of Schrödinger equation for homogeneous semiconductor of a uniform chemical composition, effective mass Schrödinger equation generally can be written as;

$$H = -\frac{\hbar^2}{2m^*}\frac{d^2}{dr^2}\Psi(r) + V(r)\Psi(r) - E(r)\Psi(r) \tag{2.13}$$

An extension of the Schrödinger equation to non uniform semiconductors, material possessing a position dependent varying chemical composition. $m_0 = m(r)$ we shall concentrate only on the kinetic energy term of Schrödinger equation for the envelope function Ψ. Here we briefly summarize historical process about the developments of the PDM Schrödinger equation.

In literature, some of physicist attended for finding good kinetic energy operator approximation. According to Gora and Williams [14], with the one electron approximation of many body Hamiltonian for a binary alloy of a position dependent composition [1]. The kinetic energy operator;

$$T = -\frac{\hbar^2}{2m(r)}\frac{d^2}{dr^2} \tag{2.14}$$

which is manifestly non-Hermitian. And then, Gora and Williams changed their derivation of the suitable Schrödinger equation for the envelope function Ψ and postulated;

$$T = -\frac{\hbar^2}{4}(m(r)^{-1}\frac{d^2}{dr^2} + \frac{d^2}{dr^2}m(r)^{-1}) \tag{2.15}$$

Zhu and Kroemer [6], introduced another form of PDM Kinetic energy operator;

$$T = -\hbar^2(m(r)^{-1/2}\frac{d^2}{dr^2}m(r)^{-1/2}) \tag{2.16}$$

This is also hermitian. However, solution of Schrödinger equations with these kinetic energy operators are unphysical.

In the PDM Schrödinger equation the mass and momentum operator no longer commute. The general expression for the kinetic energy operator have been introduced by von Roos [1];

$$T = -\frac{\hbar^2}{4}(m^\eta pm^\varepsilon pm^\rho + m^\rho pm^\varepsilon pm^\eta) \tag{2.17}$$

where $\eta + \varepsilon + \rho = -1$ is a constraint.

Gora and William's operator is retrieved from von Roos operator by putting $\eta = -1, \varepsilon = \rho = 0$ and for Zhu and Kroemer's $\eta = \rho = -\frac{1}{2},\ \varepsilon = 0$. Ben Danial and Duke $\eta = \rho = 0, \varepsilon = -1$, Li and Kuhn $\varepsilon = \rho = -\frac{1}{2},\ \eta = 0$ [45]. Thus, von Roos kinetic energy operator is more adequate than other we always use this operator in our PDM Schrödinger equation solutions. We can write PDM Hamiltonian generally;

$$H = \frac{1}{4}(m^\eta pm^\varepsilon pm^\rho + m^\rho pm^\varepsilon pm^\eta + V(x) \tag{2.18}$$

where $V(x)$ is potential. There are many debates for the choice of the parameters, most of the authors have been obtained solution of the PDM Schrödinger equation for the following Hamiltonians:

$$H_1 = \frac{1}{2}\left(p\frac{1}{m}p\right) + V(x);\ \ for\ \varepsilon = -1, \rho = 0, \eta = 0, \tag{2.18a}$$

$$H_2 = \frac{1}{4}\left(\frac{1}{m}p^2 + p^2\frac{1}{m}\right) + V(x);\ for\ \varepsilon = 0,\ \rho = 0,\ \eta = -1, \tag{2.18b}$$

$$H_3 = \frac{1}{2}\left(\frac{1}{\sqrt{m}}\ p^2\frac{1}{\sqrt{m}}\right) + V(x);\ for\ \ \varepsilon = -\frac{1}{2}, \rho = 0,\ \eta = -\frac{1}{2}, \tag{2.18c}$$

$$H_4 = \frac{1}{2}\left(p\frac{1}{\sqrt{m}}p\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{m}}p\left(\frac{1}{\sqrt{m}}p\right) + V(x); for\ \varepsilon = 0, \rho = -\frac{1}{2}, \eta = -\frac{1}{2}\right). \tag{2.18d}$$

Next chapter we will summarize the methods of solutions of the following Eigenvalue problems:

$$H_i\psi(x) = E\psi(x), (i = 1,2,3,4). \tag{2.19}$$

CHAPTER 3

PDM SCHRODINGER,KLEIN-GORDON AND DIRAC EQUATIONS and THEIR SOLUTIONS

In this chapter, we review the methods developed for solving PDM Schrödinger, Klein-Gordon and Dirac equations. We have analyzed almost all of the articles about the corresponding title. Our detailed analyzes shows that the following five methods come forward in order to solve concerned equations.

3.1. Series Expansion Method

It is well known that the series expansion method is one of the most common method to solve Schrödinger type equation including constant mass. This method can also be applied to solve PDM Schrödinger equation for some particular potentials and mass functions. Before reviewing solution of the PDM Schrödinger equation by power series method, we briefly summarize fundamentals of the Series Expansion Method.

Consider second order, linear, homogeneous differential equation of the form:

$$p(x)y''(x) + q(x)y'(x) + r(x)y(x) = 0 \tag{3.1}$$

where the functions $q(x)/p(x), and\ r(x)/p(x)$ are analytic at $x = x_0$, then every solution, $y(x)$, is analytic at $x = x_0$ and it can be represented by a power series in powers of $x = x_0$. Therefore, we have a power series solution of the form given by,

$$y(x) = \sum_{m=0}^{\infty} a_m\,(x - x_0)^{m+r}. \tag{3.2}$$

This is referred to as an extended power series with r chosen such that $a_0 \neq 0$. A second independent solution may contain a logarithmic term if the roots are repeated or if they differ by an integer. A function written in the form of a power series can be differentiated term by term. In the derivatives of expression (3.2), has are given by

$$y'(x) = \sum_{m=0}^{\infty} a_m\,(m + r)(x - x_0)^{m+r-1} \tag{3.3}$$

$$y''(x) = \sum_{m=0}^{\infty} a_m\,(m + r)(m + r - 1)(x - x_0)^{m+r-2} \tag{3.4}$$

Substitute (3.2), (3.3) and (3.4) in to (3.1) we obtain:

$$p(x)\sum_{m=0}^{\infty} a_m\,(m+r)(m+r-1)(x-x_0)^{m+r-2} + q(x)\sum_{m=0}^{\infty} a_m\,(m+r)(x-x_0)^{m+r-1} + r(x)\sum_{m=0}^{\infty} a_m\,(x-x_0)^{m+r} = 0 \quad (3.5)$$

Then, using the standard procedure given in any differential equation text book [47], one can obtain a solution for the differential equation (3.1).

In literature, approximate solution of the N-dimensional PDM Schrödinger equation can be obtained by using series method [48,49].

The model Hamiltonian of N-dimensional position-dependent mass Schrödinger equation is given by

$$\nabla\left(\frac{1}{m}\,\nabla\psi(r)\right) + 2[E - V(r)]\psi(r) = 0$$

where $m = m(r)\ and\ \nabla$ is the N-dimensional gradient operator. For N-dimensional spherical symmetry, the wave functions given an angular momentum L are given by [50-57]

$$\psi(r) = r^{-\frac{N-1}{2}} R(r) Y^{L}_{L_{N-2\ldots L^1}}(\phi,\theta) \quad (3.6)$$

Thus,

$$\nabla\frac{1}{m}\,\nabla\psi(r) = \left(\nabla\frac{1}{m}\right).[\nabla\psi(r)] + \frac{1}{m}\nabla^2\psi(r) \quad (3.7)$$

and (3.6) we can obtain the following N-dimensional radial position-dependent mass Schrödinger equation

$$\left\{\frac{d^2}{dr^2} + \frac{m'}{m}\left(\frac{N-1}{2}\frac{1}{r} - \frac{d}{dr}\right) - \frac{L(L+N-2)+\frac{(N-1)(N-3)}{4}}{r^2} + 2m[E - V(r)]\right\}R(r) = 0 \quad (3.8)$$

where $m' = \frac{dm(r)}{dr}$. It is obvious that, for$N = 1\ then\ L = 1$, (3.8) turns into the one-dimensional position-dependent mass Schrödinger equation [58]

$$\left\{\frac{d^2}{dr^2} + \frac{m'}{m}\frac{d}{dr} + 2m[E - V(r)]\right\}R(r) = 0. \quad (3.9)$$

It is convenient to change the function $R(r)$ in the (3.8), such that:

$$R(r) = r^{L+\frac{N-1}{2}} e^{-Br} F(r) \quad , \quad B = \sqrt{-2m_0 E}. \quad (3.10)$$

Substitute $R(r)$ into the (3.8) we obtain:

$$[(2L+N-1)\frac{d}{dr} - (2L+N-1)B - \frac{m'}{m}L]F(r) + [\frac{d^2}{dr^2} - 2B\left(\frac{m'}{m}\right)\frac{d}{dr} + \frac{m'}{m}B + 2E(m-m_0) - 2mV(r)]rF(r) = 0 \quad (3.11)$$

In (3.11) if three functions $V(r), m(r)\ and\ m'(r)/m(r)$ are given in the power series form, then method of series solution can be applied to solve the PDM Schrödinger equation. Let us consider the following potential, and mass functions:

$$V(r) = A\sum_{l=0}^{\infty} c_l r^l \tag{3.12}$$

$$m(r) = A\sum_{v=0}^{\infty} b_v r^v = m_0 + \sum_{v=1}^{\infty} b_v r^v \tag{3.13}$$

In principle, m'/m can be written as

$$\frac{m'}{m} = \sum_{v=0}^{\infty} b'_v r^v \tag{3.14}$$

for simplicity $b_0 = m_0$ and the standard series $F(r)$ is:

$$F(r) = \sum_{k=0}^{\infty} a_k r^k \quad , \quad a \neq 0 \tag{3.15}$$

if use Eq.(3.10) into Eq. (3.8)

$$\begin{aligned}
&(2L+N-1)\sum_{k=0}^{\infty} k a_k\, r^{r-1} - (2L+N-1)\sum_{k=0}^{\infty} a_k r^k \\
&- L\sum_{k=0}^{\infty}\sum_{v=0}^{\infty} a_k b'_v r^{v+k} + \sum_{k=0}^{\infty} k(k-1) a_k r^{k-1} - 2B\sum_{k=0}^{\infty} k a_k\, r^k \\
&- \sum_{k=0}^{\infty}\sum_{v=0}^{\infty} k a_k b'_v r^{v+k} + B\sum_{k=0}^{\infty}\sum_{v=0}^{\infty} a_k b'_v r^{v+k+1} \\
&+ 2E\sum_{k=0}^{\infty}\sum_{v=0}^{\infty} a_k b'_v r^{v+k+1} + -2Em_0\sum_{k=0}^{\infty} a_k r^{k+1} \\
&- 2A\sum_{k=0}^{\infty}\sum_{v=0}^{\infty}\sum_{l=0}^{\infty} a_k b_v c_l r^{k+v+l+1} = 0
\end{aligned} \tag{3.16}$$

Assuming the coefficients of the power of $r^n\ (n = k+v+l+1)$ to zero, one yields the following recursion relation of energy spectrum [48]:

$$\begin{aligned}
&(2L+N-1)(n+1)a_{n+1} + n(n+1)a_{n+1} - (2L+N-1)Ba_n - LM'_n - 2B_n a_n - \\
&+BM'_{n-1} + 2EM_{n-1} - 2Em_0 a_{n-1} - 2AS_{n-1} = 0
\end{aligned} \tag{3.17}$$

where

$$S_n = \sum_{i,v,l=0}^{i+v+l=n} a_i b_v c_l,\ M_n = \sum_{i,v=0}^{i+v=n} a_i b_v,$$

$$M'_n = \sum_{i,v=0}^{i+v=n} a_i b'_v, \qquad T_n = \sum_{i,v=0}^{i+v=n} i a_i b'_v.$$

The final wave functions can be written:

$$R(r) = r^{L+\frac{N-1}{2}} e^{-Br} \sum_{k=0}^{\infty} a_k r^k \quad , \quad a_0 \neq 0 \tag{3.18}$$

It has been shown that only if the potential and mass can be expanded about the origin the series form for example Morse potential and $m(r) = m_0 e^{\lambda r}$ this type mass functions, the series solutions of the N-dimensional position-dependent mass Schrödinger equation with physical potentials would be obtained [48]. In addition, Chen et al.,[28] studied *N*-dimensional Schrödinger equation with position-dependent effective mass for the position dependent mass by series expansion method. The special cases of the Coulomb potential and the harmonic oscillator were discussed. Series expansion method do not include any transformations of coordinate and wavefunction.

3.2 Nikiforov-Uvarov Method

The Nikiforov-Uvarov (NU) Method [59] have been applied to solve PDM Klein Gordon equation and Dirac equation besides PDM Schrödinger equation. Arda et.al., solved by using the Nikiforov-Uvarov method the effective mass Klein-Gordon equation for the Woods-Saxon potential. Energy eigenvalues and the corresponding eigenfunctions were computed. Results were also given for the constant mass case [60]. Arda et.al., solved analytically the Klein Gordon equation for the q parameter Pöschl-Teller potential in one-dimension in the case of mass dependent formalism (they used an exponentially mass distribution function). They obtained an energy eigenvalue and studied the energy spectra for the case that mass is constant and potential vanishes [61]. Ikhdair [27] obtained the analytic solutions of the spatially-dependent mass Schrödinger equation of diatomic molecules by using NU method. In that article, mass function was $m(r) = \frac{m_0}{\left(1-\delta e^{-a(r-r_e)}\right)^2}$, $0 \leq \delta < 1$, where a and r_e are the range of the potential and the equilibrium position of the nuclei. The energy eigenvalues and the corresponding normalized radial wave functions were calculated.

Before the review the solved these equations we briefly summarize the NU Method. This technique depends on solving the second-order linear differential equations. In this method, for a given potential, the Schrödinger equation in one dimension is reduced to a generalized equation of hypergeometric type with an appropriate coordinate transformation and it can be written in the following form [62]:

$$\Psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0 \qquad (3.19)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Hence, from the (3.19) the Schrödinger equation and the Schrödinger-like equations can be solved by means of the special potentials or some quantum mechanics problems. To find particular solution of (3.19) by separation of variables, if one deals with the transformation:

$$\Psi(s) = \varphi(s)y(s) \tag{3.20}$$

it reduces to an equation of hypergeometric type:

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0 \tag{3.21}$$

and $\varphi(s)$ is defined as a logarithmic derivative:

$$\frac{\varphi(s)}{\varphi'(s)} = \frac{\pi(s)}{\sigma(s)} \tag{3.22}$$

The other part $y(s)$ is the hypergeometric type function whose polynomial solutions are given by Rodrigues relation:

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma^n(s)\rho(s)] \tag{3.23}$$

where B_n is a normalizing constant and the weight function $\rho(s)$ must satisfy the condition:

$$(\sigma(s)\rho(s))' = \tau(s)\rho(s) \tag{3.24}$$

The function π and λ the parameter required for this method are defined as follows;

$$\pi(s) = \left(\frac{\sigma'-\tilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma'-\tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \tag{3.25}$$

$$\lambda = k + \pi' \tag{3.26}$$

On the other hand, in order to find the value of k, the expression inside the square root must be square of polynomial. Thus, a new eigenvalue equation for the Schrödinger equation becomes:

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'' \tag{3.27}$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \tag{3.28}$$

and its derivative is negative. To obtain the energy eigenvalues, (3.26) and (3.27) are compared.

In the relativistic quantum mechanics, for a spinless particle, the time-independent Klein-Gordon equation with position-dependent mass in one dimension is written as follows [65]:

$$\left\{h^2c^2\frac{d^2}{dx^2}+[E-V(x)]^2-[m(x)c^2+S(x)]^2\right\}u(x)=0 \tag{3.29}$$

where E denotes the energy of the particle, and $V(x)$ and $S(x)$ are vector and scalar potentials, respectively. From equation (3.29), we have

$$\frac{d^2u(x)}{dx^2}+\left(\frac{E^2-m^2c^4-2mSc^2-2EV+V^2-S^2}{h^2c^2}\right)u(x)=0 \tag{3.30}$$

Dai et.al.[64] consider the case when the scalar potential is equal to the vector potential, which is inversely proportional to the absolute value of the coordinate:

$$S(x)=V(x)=-\frac{hcq}{|x|} \tag{3.31}$$

where the coupling constant q is a dimensionless real parameter and the following mass distribution was taken

$$m(x)=m_0\left(1+\frac{\lambda b}{|x|}\right) \tag{3.32}$$

where m_0 and are the rest mass of a spinless particle and the Compton-like wavelength, respectively; b is a dimensionless real parameter. Defining the quantity $z=|x|$ and letting

$$\varepsilon^2=\frac{m_0^2c^4-E}{h^2c^2},\ \beta=\frac{2\left(bm_0c^2-qm_0c^2-qE\right)}{hc},\ \gamma=b(b-2q) \tag{3.33}$$

and substituting these expressions in (3.30), one obtains:

$$\frac{d^2u(z)}{dz^2}-\frac{\varepsilon^2z^2+\beta z+\gamma}{z^2}u(z)=0 \tag{3.34}$$

If the NU method is applied in the present case by comparing (3.33) and (3.19), the following expressions are obtained:

$$\tilde{\tau}=0,\ \sigma=z,\ \tilde{\sigma}=-(\varepsilon^2z^2+\beta z-\gamma) \tag{3.35}$$

Substituting the above expression into (3.25), the function

$$\pi(z)=-\frac{1}{2}\pm\sqrt{\frac{1}{4}\varepsilon^2z^2+\beta z+\gamma+kz} \tag{3.36}$$

According to the NU method, the expression in the square root must be the square of the polynomial. Then the solution of (3.36) gives two roots of k individually

$$k_{1,2}=-\beta\pm\varepsilon\sqrt{1+4\gamma} \tag{3.37}$$

Then the function π for each k can be expressed as:

$$\pi=\left\{\frac{1}{2}\pm\left[\varepsilon z+\frac{1}{2}\sqrt{1+4\gamma}\right]\right\},\qquad for\ k_1=-\beta+\varepsilon\sqrt{1+4\gamma} \tag{3.38}$$

$$\pi=\left\{\frac{1}{2}\pm\left[\varepsilon z-\frac{1}{2}\sqrt{1+4\gamma}\right]\right\},\qquad for\ k_2=-\beta-\varepsilon\sqrt{1+4\gamma} \tag{3.39}$$

where k is determined by the polynomial $\tau=\tilde{\tau}+2\pi$ and has a negative derivative.

The most suitable form of $\pi(x)$ is selected as:

$$\pi(z) = -\varepsilon z + \frac{1}{2}\left[1 + \sqrt{1+4\gamma}\right], \qquad for\ k_2 = -\beta - \varepsilon\sqrt{1+4\gamma} \tag{3.40}$$

Thus,

$$\tau(x) = -2\varepsilon z + \left[1 + \sqrt{1+4\gamma}\right], \quad \tilde{\tau}'(z) = -2\varepsilon < 0 \tag{3.41}$$

According to (3.26) and (3.27)

$$\lambda = -\beta - \varepsilon\left[1 + \sqrt{1+4\gamma}\right], \ \lambda_n = 2n\varepsilon \tag{3.42}$$

Letting $\lambda = \lambda_n$ the relation of the values n and the constant ε can be obtained as:

$$\varepsilon = -\frac{\beta}{2n+1+\sqrt{1+4\gamma}} \tag{3.43}$$

Substituting the (3.30) into the (3.43), the exact energy eigenvalues of the Klein-Gordon equation for this system are derived as:

$$E = \frac{-A \pm B\sqrt{B^2-\gamma}}{q^2+B^2} m_0 c^2, \qquad A = q(q-b), \qquad B = n + \frac{1}{2} + \sqrt{\gamma + \frac{1}{4}}.$$

Therefore we have shown that (3.19) can exactly be solved. Thus, Nikiforov-Uvarov Method is useful for solving PDM Klein-Gordon Equation. In literature, beside PDM Klein-Gordon equation, Dirac equation Schrödinger equation have been also solved by using Nikiforov-Uvarov Method [60-65].

3.3 Lie Algebraic Technique

Exact solvability of the partial differential equations depends on its symmetry properties. Continuous group theory, Lie algebras and differential geometry are used to understand the structure of linear and nonlinear partial differential equations for generating integrable equations [66]. Kerimov, suggested a generalized procedure to obtain exactly solvable position dependent mass Hamiltonians in one dimension. The second-order Casimir invariant of the regular representation of a non-compact semi-simple Lie group *G*, the spectral properties of which are well known, was used to introduce exactly solvable Hamiltonians [67]. Roy et.al., used the $su(1,1)$ algebra, both as a spectrum generating algebra and as a potential algebra, to obtain exact solutions of effective mass Schrödinger equations corresponding to a number of potentials [68].

This method can also be applied to solve PDM Schrödinger equation this algebra with three operators are used $su(2),\ and\ su(1,1)$ for solving PDM Schrödinger equation.

The Lie algebraic technique is suitable for studying the PDM Schrödinger equation, because it contains a first-derivative term. The $su(1,1)$ Lie algebra is described by the commutation relations,

$$[J_+, J_-] = 2J_0\ ,\ \ [J_0, J_\pm] = \pm J_\pm \tag{3.44}$$

The Casimir operator of this structure is given by,

$$J^2 = -J_\pm J_\mp + J_0^2 \mp J_0 \tag{3.45}$$

The eigenstate of J^2 and J_0 can be denoted by $|jN\rangle$ where

$$J^2|jN\rangle = j(j+1)|jN\rangle \quad , \quad J_0|jN\rangle = -N|jN\rangle \tag{3.46}$$

while the allowed values of N are

$$N = -j, j+1, -j+2, \ldots = (-j+n) \tag{3.47}$$

where n is a positive integer. We consider the most general form of the generators of the algebra which was introduced by Sukumar [69]

$$J_\pm = e^{\pm i\varphi}\left(\pm h(x)\frac{\partial}{\partial x} \pm g(x) + f(x)J_0 + c(x)\right) \quad , \quad J_0 = -i\frac{\partial}{\partial \varphi} \tag{3.48}$$

The commutation relations (3.44) are satisfied when the functions $h(x), f(x)$ and $c(x)$ take the forms

$$h(x) = \frac{r}{r'} \quad f(x) = \frac{1+ar^2}{1-ar^2} \quad c(x) = -\frac{br}{1-ar^2} \tag{3.49}$$

where $r = r(x)$ and a and b are constants. The differential realization (3.48) can be used to derive the second order differential equations of the orthogonal polynomials. The differential equations of these polynomials can be expressed in terms of Casimir operator J^2:

$$H = J^2 \quad , \quad H|jN\rangle = j(j+1)|jN\rangle \tag{3.50}$$

Let us consider the basis function,

$$|jN\rangle = e^{iN\varphi}\Re_{jN}(x) \tag{3.51}$$

In terms of the realizations (3.48) and with the basis (3.51), the Hamiltonian (3.50) takes the form

$$H = \frac{r^2}{r'^2}\frac{d^2}{dx^2} + \frac{r}{r'}\left(2g - \frac{2ar^2}{1-ar^2} - \frac{rr''}{r'^2}\right)\frac{d}{dx} + g^2 + g + \frac{rg'}{r'} - \frac{2g}{1-ar^2} - \frac{r(2N+br)(2aNr+b)}{(1-ar^2)^2} \tag{3.52}$$

Let us now turn our attention to the PDM Schrödinger equation which can be written as

$$H_{PDM} = T + V(x) \qquad H_{PDM}\psi(x) = E\psi(x) \tag{3.53}$$

where $V(x)$ is the potential of the physical system and $\psi(x)$ and E are eigenstates

and eigenvalues of the PDM Schrödinger equation. Introducing the eigenfunction and momentum operator p,

$$\psi(x) = -\frac{2mr^2}{r'^2}\Re(x) \qquad , \qquad p = -i\frac{d}{dx} \tag{3.54}$$

respectively, the position dependent mass Hamiltonian takes the form

$$\begin{aligned} H_{PDM} = {} & \frac{r^2}{r'^2}\frac{d^2}{dx^2} + \frac{r}{r'}\left(4 - \frac{4rr''}{r'^2} + \frac{rm'}{r'm}\right)\frac{d}{dx} + 2 + \frac{2r}{r'^2}\left(\frac{3rr''^2}{r'^2} - \frac{rr'''}{r'} - 3r''\right) \\ & + \frac{m'r^2}{mr'^2}\left(\frac{(1+\eta)(\varepsilon+\eta)}{m} + \frac{(1+\varepsilon)m''}{2m'} + \frac{2(r'^2 - rr'')}{rr'}\right) \\ & - \frac{2mr^2}{r'^2}V(x) \end{aligned} \tag{3.55}$$

This PDM Hamiltonian can be solved for different potentials i.e (Coulomb, harmonic oscillator and Morse family potentials) [70]. Therefore, in literature, PDM Schrödinger equation, Klein Gordon, Dirac equation have been also solved with using Lie Algebraic Technique [67-73].

3.4 Supersymmetric Quantum Mechanics (SUSYQM)

Supersymmetric Quantum Mechanics (SUSYQM) [74,75] includes pairs of Hamiltonians which share a particular mathematical relationship, which are called partner Hamiltonians. (The potential energy terms which occur in the Hamiltonians are then called partner potentials.) SUSYQM explain that, to every eigenstate of one Hamiltonian, its partner Hamiltonian has a suitable eigenstate with the same energy. This method can be applied to solve PDM Schrödinger, Dirac equation. For example, Jia et.al., consider a case for which the mass distribution combines linear and inversely linear forms, the Dirac problem with a *PT*-symmetric potential is mapped into the exactly solvable Schrödinger-like equation problem with the isotonic oscillator by using the local scaling of the wavefunction and they took a mass distribution with smooth step shape, the Dirac problem with a non-*PT*-symmetric imaginary potential was mapped into the exactly solvable Schrödinger-like equation problem with the Rosen–Morse potential. The real relativistic energy levels and corresponding wavefunctions for the bound states were obtained in terms of the supersymmetric quantum mechanics approach and the function analysis method [76].

Using the restricted Hamiltonian from the $\eta = \rho$ constraint, we can write,

$$H = \frac{1}{2}\left(m^{-\frac{1}{2}(\varepsilon+1)} p m^{\varepsilon} p m^{-\frac{1}{2}(\varepsilon+1)}\right) \tag{3.56}$$

Before going further we derive a general effective Hamiltonian for the case of position-dependent mass. Let us turn our attention to the Hamiltonian (2.18). Using the commutation relation; $[p, m^a] = -i\hbar a m^{a-1}$

one can put the momenta to the right, the Hamiltonian (2.18) takes the form

$$H = H_{eff} + V(x) \tag{3.57}$$

The effective Hamiltonian H_{eff} is given by,

$$H_{eff} = \frac{p^2}{2m} - \frac{i\hbar m'}{2m^2} p - U(x) \tag{3.58}$$

where

$$U(x) = -\frac{\hbar^2}{4m^3}(2(\varepsilon + \eta + \varepsilon\eta + \eta^2 + 1)m'^2 - (\varepsilon + 1)mm''). \tag{3.59}$$

Note that the effective potential term $U(x)$ can be eliminated by imposing the constraints over the parameters such that $\varepsilon = -1$ and $\eta = 0$. In this case the Schrödinger equation will not depend on the parameters. The solution of the Hamiltonian (3.56) in the framework of SUSYQM. Let us take a look at the SUSYQM for the standard Schrödinger equation. The algebra of SUSYQM satisfies the following commutation relations:

$$\{Q^+, Q^-\} = H, \quad [Q^{\pm}, H] = 0, \quad \{Q^{\pm}, Q^{\pm}\} = 0 \tag{3.60}$$

The supercharges $Q^{\pm}$ are defined as

$$Q^{\pm} = B^{\mp}\sigma^{\pm}, \quad B^{\mp} = \frac{1}{\sqrt{2}}\left(\pm\frac{d}{dx} + \Phi(x)\right) \tag{3.61}$$

where $\sigma^{\pm}$ are Pauli matrices and $\Phi(x)$ is a superpotential. We may construct a supersymmetric quantum mechanical system by defining the Hamiltonians such that the relations in (3.60) holds,

$$H_{\pm} = B^{\mp}B^{\pm} = -\frac{1}{2}\frac{d^2}{dx^2} + V_{\pm}(x) \tag{3.62}$$

The partner potentials $V_{\pm}(x)$ are related to the superpotential $\Phi(x)$ by

$$V_{\pm}(x) = \frac{1}{2}(\Phi^2(x) \pm \Phi'(x)). \tag{3.63}$$

The Hamiltonian H_+ and H_- possess the same eigenvalues except for the zero energy ground state. The zero-energy eigenstate belongs to the H_- ,and supersymmetry of quantum system is said to be good SUSY if the ground state energy of H_- (or H_+) vanishes. In the other case SUSY is said to be broken. For good SUSY the ground state of H_- is given by

$$\psi_0(x) = Cexp(-\int \Phi(x)dx) \tag{3.64}$$

where C is normalization constant. The potentials are shape invariant [77], that is $V_+(x)$ has the same functional form as $V_-(x)$ but different parameters except for an additive constant:

$$V_+(x;a_0) = R(a_0) + V_-(x;a_1) \tag{3.65}$$

where a_0 and a_1 stand for the potential parameters in the supersymmetric partner potentials, and $R(a_0)$ is a constant. This property permits an immediate analytical determination of eigenvalues and eigenfunctions. The eigenvalues and eigenfunctions of the Hamiltonians H_+ and H_- are related by

$$E_0^- = 0, \quad E_1^- = R(a_0), \quad E_{n+1}^- = E_n^+, \quad E_n^- = \sum_{k=0}^{n-1} R(a_k) \tag{3.66}$$

$$\psi_n^-(x;a_0) = B^+(x;a_0) + \psi_{n-1}^-(x;a_1). \tag{3.67}$$

In the following we shall modify the standard SUSY technique to the systems with position-dependent mass. Since the mass is a function of the position, the supersymmetric operators include mass term. It will be shown that the following form of the operators are appropriate to study the Hamiltonian (3.56),

$$A^+ = -\frac{1}{\sqrt{2}}\left[m^{-\left(\frac{1}{2}\right)(\varepsilon+1)}\frac{d}{dx}m^{\frac{\varepsilon}{2}}\right] + \frac{W(x)}{\sqrt{2m}}, \tag{3.68}$$

$$A^- = \frac{1}{\sqrt{2}}\left[m^{\frac{\varepsilon}{2}}\frac{d}{dx}m^{-\left(\frac{1}{2}\right)(\varepsilon+1)}\right] + \frac{W(x)}{\sqrt{2m}} \tag{3.69}$$

where $W(x)$ is the superpotential and m depends on the position. It can be checked that the supersymmetry relations in (3.60) and (3.61) are satisfied when $B^{\pm}$ are replaced by $A^{\pm}$. Note that the operator $\frac{d}{dx}m^a$ read as follows:

$$\frac{d}{dx}m^a = m^a\frac{d}{dx} + am^{a-1}\frac{dm}{dx} \tag{3.70}$$

We assume that, for good SUSY the ground state wave function belongs to H_- and is given by

$$\psi_0^-(x) = m^{\left(\frac{1}{2}\right)(\varepsilon+1)}exp(-\int W(x)dx) \tag{3.71}$$

One can easily check that $A^-\psi_0^-(x) = 0$. The Hamiltonians of quantum systems with position-dependent mass take the form

$$H_- = A^+A^- = -\frac{1}{2}\left(m^{-\left(\frac{1}{2}\right)(\varepsilon+1)}\frac{d}{dx}m^{\varepsilon}\frac{d}{dx}m^{-\left(\frac{1}{2}\right)(\varepsilon+1)}\right) + V_-(x), \tag{3.72}$$

$$H_+ = A^-A^+ = -\frac{1}{2}\left(\frac{d}{dx}\,m^{-(\varepsilon+1)}\frac{d}{dx}m^{\frac{\varepsilon}{2}}\right) + V_+(x). \tag{3.73}$$

where the partner potentials are given by

$$V_-(x) = \frac{1}{2m}\left(W^2(x) - W'\left(x - \frac{\varepsilon m'}{m}W(x)\right)\right), \tag{3.74}$$

$$V_{+}(x)=\frac{1}{2m}\left(W^{2}(x)-W'\left(x-\frac{(\varepsilon+1)m'}{m}W(x)\right)\right)+\frac{2(\varepsilon+1)}{2m}+\left(\frac{3}{8}\frac{m'^{2}}{m^{2}}-\frac{1}{4}\frac{m''}{m}\right). \quad (3.75)$$

It is obvious that the kinetic energy terms of the effective mass Hamiltonian (3.56) and H_{-} are not identical. Therefore the shape-invariance condition (3.60) does not satisfy for the position-dependent mass system. If mass is constant it is easy to check that the physical quantities of the position-dependent mass system reduce to the physical quantities of the standard system.

If mass function is $m=\left(\frac{\delta+x^{2}}{1+x^{2}}\right)^{2}$ and suitable potentials [78] (i.e. harmonic oscillator, Coulomb and Morse potential) is used PDM Schrödinger equation can be solved. In literature, beside PDM Schrödinger equation, Klein Gordon equation, Dirac equation have been also solved with using SUSYQM [23,78-90].

3.5 Transformations

Solution of the differential equations go easy by a suitable transformations. In literature, PDM Schrödinger Equations have been solved by using Coordinate transformation, Point Canonical transformation, Darboux transform, Liouville--Green transformation, Form-Preserving transformation. In most applications of such methods, PDM Schrödinger equation has been transformed in the form of the constant mass Schrödinger equation by changing coordinate and wave function. There is an example about Coordinate transformation from CAI Chang-Ying, REN Zhong-Zhou, and JU Guo-Xing article [91] in this part.

Now we analyse solution of the PDM Schrödinger Equations by using coordinate transformation. Consider Levy-Leblod [92] kinetic energy operator, for PDM Hamiltonian:

$$H=\vec{P}\frac{1}{2M(\vec{r})}\vec{P}+V(\vec{r})=-\frac{\hbar^{2}}{2m_{0}}\left[\vec{\nabla}\frac{1}{m(\vec{r})}\vec{\nabla}\right]U(r)+V(\vec{r})U(r). \quad (3.76)$$

We know that in 3-dimensions Schrödinger equation $V(\vec{r})$ and $m(\vec{r})$ are dependent on radial coordianate in the spherical coordinate system. Where units of $m_{0}=\hbar=1$ so we can write the radial part of the Schrödinger equation for the (3.76),

$$\left\{\frac{d^{2}}{dr^{2}}-\frac{l(l+1)}{r^{2}}+\frac{m'}{m}\left(\frac{1}{r}-\frac{d}{dr}\right)-2m[V(r)-E]\right\}\varphi(r)=0 \quad (3.77)$$

where $U(r)=\frac{\varphi(r)}{r}$ which is radial wavefunction, E is eigenvalue of energy and l is angular momentum quantum number. The radial part of the Schrödinger equation with constant mass and angular momentum L can be written as;

$$\left\{\frac{d^2}{d\rho^2}-\frac{L(L+1)}{\rho^2}-2m[v(\rho)-\varepsilon]\right\}\psi(\rho)=0 \tag{3.78}$$

where $v(\rho)$ is the potential function and ε is eigenvalue of energy. Thus, the following transformation is made [91] to (3.78),

$$\rho=q(r)\ \ ,\quad \psi(\rho)=g(r)\varphi(r) \tag{3.79}$$

If (3.79) into (3.78) are substituted. Therefore;

$$\left.\begin{matrix}\frac{d^2}{dr^2}+\left(2\frac{g'}{g}-\frac{q''}{q'}\right)\frac{d}{dr}+\left(\frac{g''}{g}-\frac{q''}{q'}\frac{g'}{g}\right)\\ -L(L+1)\left(\frac{q'}{q}\right)^2-2(q')^2\left[v\left(q(r)\right)-\varepsilon\right]\end{matrix}\right\}\varphi(r)=0 \tag{3.80}$$

If we compare (3.80) and (3.77),

$$g(r)=\left(\frac{q'}{m}\right)^{\frac{1}{2}}, \tag{3.81}$$

$$V(r)-E=\frac{(q')^2}{m}[v(q)-\varepsilon]+\frac{L(L+1)}{2m}\left(\frac{q'}{q}\right)^2-\frac{l(l+1)}{2mr^2}+\frac{m'}{2m^2r}$$
$$+\frac{1}{4m}[F(m)-F(q')] \tag{3.82}$$

where $F(z)=\frac{z''}{z}-\frac{3}{2}\left(\frac{z'}{z}\right)^2$ The linear relation between the quantum numbers l and L can be written as;

$$L=al+b \tag{3.83}$$

Thus,

$$L(L+1)=cl(l+1)+d \tag{3.84}$$

where a , b and c , d are real constants. Mass function is taken,

$$m(r)=e^{-\beta r} \tag{3.85}$$

where $\beta>0$ and Coulomb potential has the following potential function, energy spectra, and wave functions, respectively [93]

$$v(\rho)=-\frac{Z}{\rho} \tag{3.86}$$

$$\varepsilon_n=-\frac{Z^2}{2(n+L+1)^2} \tag{3.87}$$

$$\psi_n(\rho)=a_n\rho^{L+1}\,e^{-\frac{Z\rho}{n+L+1}}\ \times F\left(-n,2L+2,\frac{2Z\rho}{n+L+1}\right) \tag{3.88}$$

where $n=0,1,2,\ldots$ denotes the radial quantum number and a_n, Z and $F(a,c,x)$ are the normalization coefficient ,the particle's charge number, and the confluent hypergeometric function. The transformation function is;

$$q(r)=\gamma e^{vr} \tag{3.90}$$

where $\gamma > 0$ and v is nonzero real parameter. Adding (3.85), (3.87) and (3.90) into (3.82), and (3.81) and (3.88) into (3.79). Therefore, there are two solutions for γ and v the first one is;

When $\gamma = (n + L + 1)/Z$ and $v = -\beta$, the potential function, energy eigenvalues and eigenfunctions are;

$$V(r) = \frac{\beta^2}{2} e^{-\beta r} + \frac{1}{2}\left[C - \frac{\beta}{r} - \frac{l(l+1)}{r^2}\right] e^{\beta r}, \tag{3.91}$$

$$E_n = \beta^2(n + L + 1), \tag{3.92}$$

$$\varphi(r) = A_n e^{-\beta(L+1)r} exp - e^{-\beta r} \times F\left(-n, 2L + 2, 2e^{-\beta r}\right). \tag{3.93}$$

where $C = \beta^2(L^2 + L)$, A_n is the normalization coefficient, and $L(l)$ is defined by (3.83)

The second solution is; When $\gamma = 2/Z$ and $v = -\beta/2$ so the potential function, energy eigenvalues and eigenfunctions are;

$$V(r) = -\frac{\beta^2}{2} e^{\frac{\beta r}{2}} + \frac{1}{2}\left[C - \frac{\beta}{r} - \frac{l(l+1)}{r^2}\right] e^{\beta r}, \tag{3.94}$$

$$E_n = -\frac{\beta^2}{2(n+L+1)^2}, \tag{3.95}$$

$$\varphi(r) = A_n e^{-\frac{(2L+3)\beta r}{4}} exp\left(-(\xi_n e^r)^{-\frac{\beta}{2}}\right) \times F\left(-n, 2L + 2, 2(\xi_n e^r)^{-\frac{\beta}{2}}\right). \tag{3.96}$$

where $C = \frac{1}{16}(4L^2 + 4L - 3)\beta^2$, $\xi_n = \left(\frac{2}{N+L+1}\right)^{-\frac{2}{\beta}}$.

The exact solution of the three-dimensional Schrödinger equation by using coordinate transformation method has been studied for an exponentially position-dependent mass with Coulomb potential. Exact results of energy eigenvalues and eigenfunctions have been obtained. We can see that in this example transformation function must be satisfy some conditions to obtain explicit results.

In literature, there are good examples about transformations. Some of articles have been discussed in introduction part. In addition of these, Quesne's article [29] is very important. Constant-mass Schrödinger equation was transformed into a PDM Schrödinger equation by using point canonical transformation. Wavefunctions were obtained for Pöschl–Teller potential and Morse potential. The changes of variable, potentials, PDM wavefunctions were listed in that article. Tezcan et al. [30], Exact solutions of the Schrödinger equation were obtained for the Rosen–Morse and Scarf potentials with the position-dependent effective mass by applying a general point canonical transformation. Different types of mass functions were used:

$$m(x) = \frac{a^2}{q + x^2}\ , m(x) = \frac{a^2}{(b + x^2)^2}\ , m(x) = e^{-ax}.$$

As result, energy eigenvalues and wavefunctions were obtained in that article.

CHAPTER 4

ASYMPTOTIC TAYLOR EXPANSION METHOD (ATEM)

In this chapter, we suggested a new method to solving PDM Hamiltonian, it is named Asymptotic Taylor Expansion Method (ATEM) [26]. This chapter is planned as follows. In the first section Taylor series expansion of a function is reformulated for solving second order differential equations. Section 2 is devoted to the application of the main result for solving Schrödinger equation including various potentials. With using harmonic oscillator potential PDM Hamiltonian is solved for four different Hamiltonian and asymptotic analyze is done.

4.1 Formalism of ATEM

In this section, we show the solution of the Schrödinger type equation for a quite ample class of potentials, by modifying Taylor series expansion by means of a finite sequence instead of an infinite sequence and its termination possessing the property of quantum mechanical wave function. Let us consider Taylor series expansion [94] of a function $f(x)$ about the point a :

$$f(x) = f(a) + (x-a)f'(a) + \left(\frac{1}{2}\right)(x-a)^2 f''(a) + \left(\frac{1}{6}\right)(x-a)^3 f^{(3)}(a) + \ldots$$
$$= \sum \frac{(x-a)^n}{n!} \; f^{(n)}(a) \tag{4.1}$$

where $f^{(n)}(a)$ is the n^{th} derivative of the function at a . Taylor series specifies the value of a function at one point, in terms of the value of the function and its derivatives at a reference point a. Expansion of the function $f(x)$ about the origin $(a = 0)$, is known as Maclaurin's series and it is given by,

$$f(x) = f(0) + xf'(0) + \left(\frac{1}{2}\right)x^2 f''(0) + \left(\frac{1}{6}\right)x^3 f^{(3)}(0) + \ldots$$
$$\sum_{n=0}^{\infty} \frac{x^n}{n!} f^{(n)}(0). \tag{4.2}$$

Here we develop a method to solve a second order linear differential equation of the form:

$$f''(x) = p_0(x)f'(x) + q_0(x)f(x) \tag{4.3}$$

It is obvious that the higher order derivatives of the $f(x)$ can be obtained in terms

of the $f(x)$ and $f'(x)$ by differentiating (4.3). Then, higher order derivatives of $f(x)$ are given by

$$f^{(n+2)}(x) = p_n(x)f'(x) + q_n(x)f(x) \tag{4.4}$$

where

$$p_n(x) = p_0(x)p_{n-1}(x) + p'_{n-1}(x) + q_{n-1}(x), \qquad and$$
$$q_n(x) = q_0(x)p_{n-1}(x) + q'_{n-1}(x). \tag{4.5}$$

Of course, the last result shows there are a formal relation between asymptotic iteration method (AIM) [95] and ATEM. We have observed that eigenfunction of the Schrödinger type equations can efficiently be determined by using ATEM. It is clear that the recurrence relations (4.5) allow us algebraic exact or approximate analytical expression for the solution of (4.3) under some certain conditions. Let us substitute (4.5) into the (4.1) to obtain

$$f(x) = f(0)\left(1 + \sum_{n-2}^{m} q_{n-2}(0)\frac{x^n}{n!}\right) + f'(0)\left(1 + \sum_{n-2}^{m} p_{n-2}(0)\frac{x^n}{n!}\right) \tag{4.6}$$

After all, we have obtained useful formalism of the Taylor expansion method. In the solution of the eigenvalue problems, truncation of the asymptotic expansion to a finite number of terms is useful. If the series optimally truncated at the smallest term then the asymptotic expansion of series is known as superasymptotic [96], and it leads to the determination of eigenvalues with minimum error. Then boundary conditions can be applied as follows. When only odd or even power of x collected as coefficients of $f(0)$ or $f'(0)$ and vice verse, the series is truncated at $n = m$ then an immediate practical consequence of these condition for $q_{m-2}(0) = 0$ or $p_{m-2}(0) = 0$. In this way, one of the parameter in the $q_{m-2}(0)$ and/or $p_{m-2}(0)$ belongs to the spectrum of the Schrödinger equation. Therefore eigenfunction of the equation becomes a polynomial of degree m. Otherwise the spectrum of the system can be obtained as follows: In a quantum mechanical system eigenfunction of the system is discrete. Therefore in order to terminate the eigenfunction $f(x)$ we can concisely write that

$$q_m(0)f(0) + p_m(0)f'(0) = 0$$
$$q_{m-1}(0)f(0) + p_{m-1}(0)f'(0) = 0 \tag{4.7}$$

eliminating $f(0)$ and $f'(0)$ we obtain

$$q_m(0)p_{m-1}(0) - p_m(0)q_{m-1}(0) = 0 \tag{4.8}$$

again one of the parameter in the equation related to the eigenvalues of the problem.

In quantum mechanics bound state energy of the atom is quantized and eigenvalues are discrete and for each eigenvalues there exist one or more eigenfunctions. When we are dealing with the solution of the Schrödinger equation, we are mainly interested in the discrete eigenvalues of the problem. The first main result of this conclusion gives necessary and sufficient conditions for the termination of the Taylor series expansion of the wave function.

The process presented here is iterative and number of iteration is given by m. The results are obtained as follows: in our Mathematica program, we use an iteration number, say $m = 30$, then we obtain another result for $m = 40$, so on, then we compare values of the parameter (eigenvalue) in each case till 10 digits. If values of the parameter reach its asymptotic value then we use these values and omit the others. For instance, if one can obtain values of the parameters for $m = 40$, first few of them will be reached its asymptotic values, say first 8 values. The following comment for the function is considerable: for such a solution it is suitable to take sum of first 8 term in the (4.6).

It will be shown that ATEM gives accurate results for PDM Schrödinger equations. In the following sections, it is shown that this approach opens the way to the treatment of PDM Schrödinger equation including large class of potentials of practical interest.

4.2 Solution of the PDM Schrödinger equation by using ATEM

In the PDM Schrödinger equation the mass and momentum operator no longer commute, so there are several ways to define kinetic energy operator. The general expression for the Hamiltonian with the kinetic energy operator introduced by von Roos [1] and potential energy (x) , can be written as (2.18):

$$H = \frac{1}{4}(m^{\eta}pm^{\varepsilon}pm^{\rho} + m^{\rho}pm^{\varepsilon}pm^{\eta} + V(x)$$

where $\eta + \varepsilon + \rho = -1$ is a constraint and is position dependent mass. There are many debates for the choice of the parameters η , ε and ρ, in our approach, we will obtain the solution of the PDM Schrödinger equation for the Hamiltonians of

(2.18a), (2.18b), (2.18c) and (2.18d) [1,46,97].

Here we take a new look at the solution of the PDM Schrödinger equation by using the method of ATEM developed in the previous section.

Before going further we share one of our significant observation during our calculations. If the mass distribution is not appropriate for a given potential, the eigenvalues do not reach their asymptotic values and resultant eigenfunction cannot be terminated when $x \to \pm\infty$. In order to illustrate semi analytical solution of the eigenvalue equations (2.19):

$$H_i\psi(x) = E\psi(x), (i = 1,2,3,4)$$

including harmonic oscillator potential:

$$V(x) = \frac{1}{2}m_0w^2x^2,$$

we use the mass distributions

$$m(x) = m_0(1 + \gamma x^2)$$

where γ is arbitrary positive constant. By the way, we emphasize that the wave function of harmonic oscillator potential is well defined in the region of $\pm\infty$ and satisfy that $\lim_{x\to\pm\infty} \frac{|\psi(x)|^2}{\sqrt{m}} \to 0$. In this limit the mass distributions to be continuous.

It is well known that asymptotic behavior of constant mass Schrödinger equation including harmonic oscillator potential is given by

$$\psi = e^{-\left(\frac{x^2}{2}\right)}f(x),$$

for simplicity we set $\hbar = m_0 = \omega = 1$. Thus, this change of wave function guaranties $\lim_{x\to\pm\infty} \frac{|\psi(x)|^2}{\sqrt{m}} \to 0$. After this transformation, we present an iteration algorithm to calculate both eigenvalues and eigenfunctions of the eigenvalue equation (2.19). Using this algorithm, we develop a Mathematica program in appendix part, which demonstrates that it is easier to be implemented into a computer program, and produces a highly accurate solution with analytical expression efficiently.

4.2.1 Asymptotic Analysis

The term asymptotic means the function approaching to a given value as the iteration number tends to infinity. By the aid of a Mathematica program we calculate eigenvalues and eigenfunction of H_1 for $\gamma = 0.1$ using number of iterations $k = \{20,30,40,50,60\}$. The function $f(x)$ for $n = 2$ state is given in (4.9) and

eigenvalues are presented in Table 4.1.

$$k = 20;\ f(x) = 1 - 1.857x^2 - 1.619 \times 10^{-1}x^4 + 2.060 \times 10^{-2}x^6 + 1.515 \times 10^{-3}x^8 - 1.261 \times 10^{-4}x^{10} - 6.495 \times 10^{-6}x^{12}$$

$$k = 40;\ f(x) = 1 - 1.856x^2 - 1.622 \times 10^{-1}x^4 + 2.051 \times 10^{-2}x^6 + 1.505 \times 10^{-3}x^8 - 1.271 \times 10^{-4}x^{10} - 6.662 \times 10^{-6}x^{12}$$

$$k = 60;\ f(x) = 1 - 1.856x^2 - 1.622 \times 10^{-1}x^4 + 2.051 \times 10^{-2}x^6 + 1.504 \times 10^{-3}x^8 - 1.271 \times 10^{-4}x^{10} - 6.663 \times 10^{-6}x^{12} \quad (4.9)$$

Table 4.1 Eigenvalues of the PDM H_1 for different iteration numbers k and $\gamma = 0.1$.

k	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
20	0.468 89047	1.433 41211	2.357 65542	3.283 97486	4.213 60362	4.353 99596
30	0.468 89665	1.433 48058	2.356 42259	3.246 60834	4.120 86916	4.983 21327
40	0.468 89650	1.433 48582	2.356 55507	3.245 85555	4.105 43833	4.957 55341
50	0.468 89651	1.433 48553	2.356 54885	3.245 99291	4.107 03835	4.941 14551
60	0.468 89651	1.433 48555	2.356 54908	3.245 98255	4.106 94346	4.943 37909

Our calculation [26] gives an accurate result for first 8 eigenvalues and eigenfunctions after 40 iterations. Here we have used 60 iterations. Figure 4.1, 4.2, 4.3, 4.4, 4.5, 4.6 shows the plot of normalized wave functions for first 6 state.

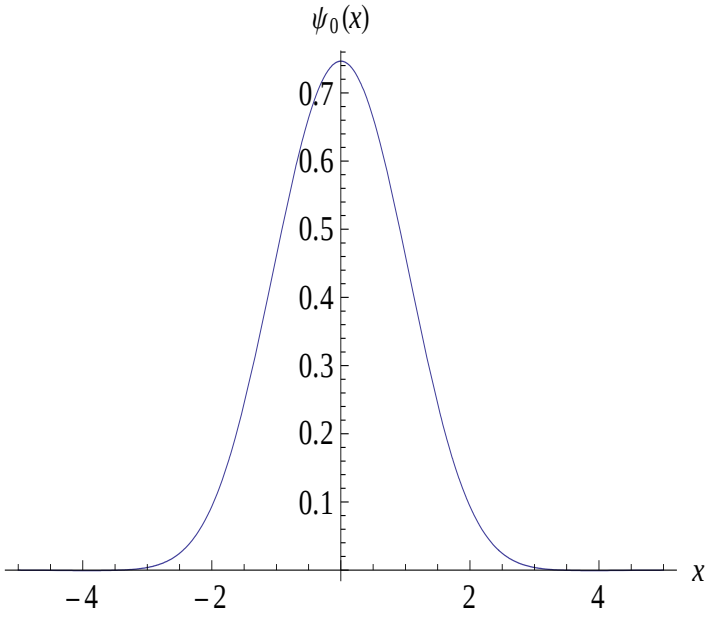

Figure 4.1 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 0$.

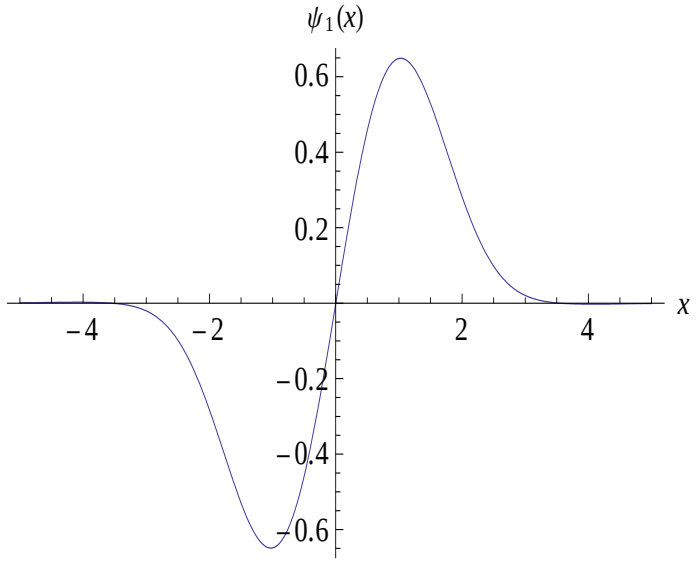

Figure 4.2 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 1$.

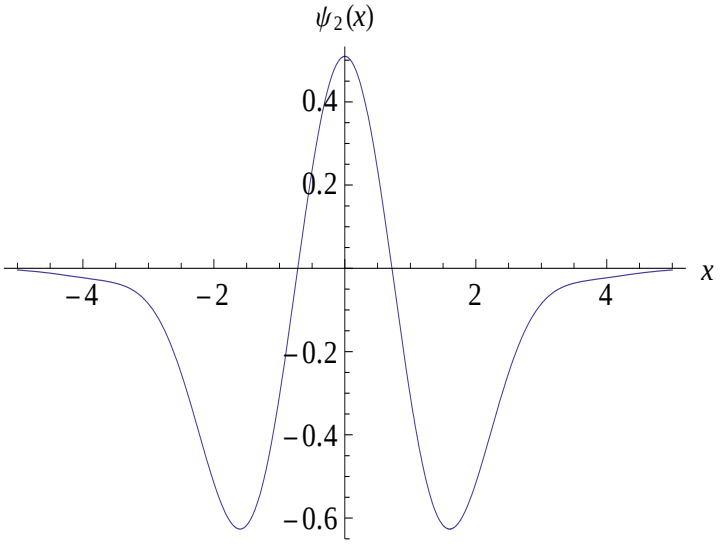

Figure 4.3 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 2$.

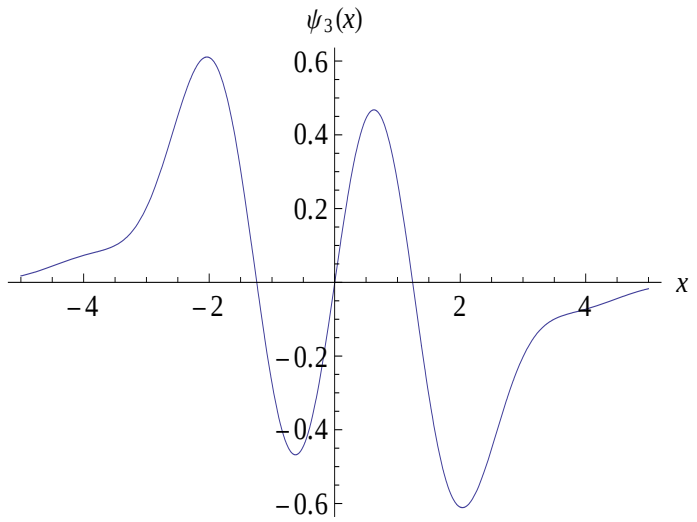

Figure 4.4 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 3$.

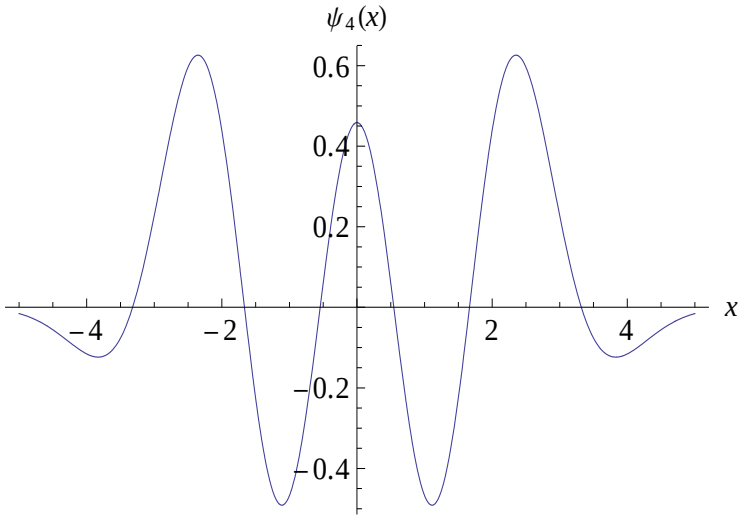

Figure 4.5 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 4$.

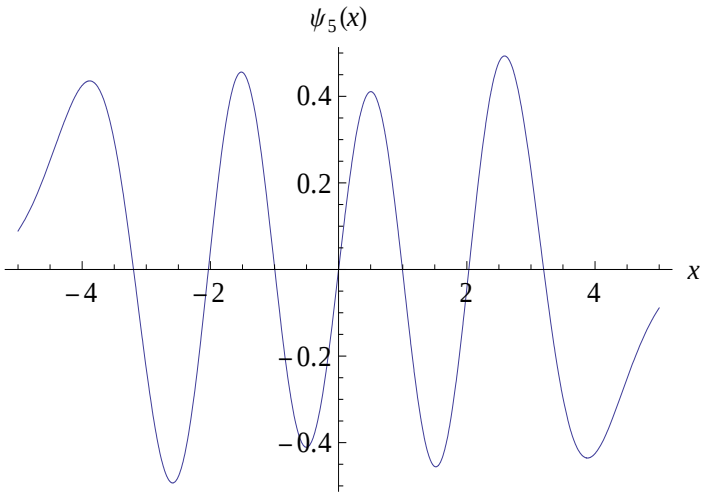

Figure 4.6 Plot of the normalized wavefunction of the PDM Hamiltonian (2.18a) for $n = 5$.

4.2.2 Solution of the Hamiltonians H_2, H_3 and H_4

In the previous section we have illustrated applicability of our method by solving Hamiltonian H_1. In this section we apply the same procedure to solve the Hamiltonians H_2, H_3 and H_4. Again we have used 60 iterations for each Hamiltonians and checked stability of the eigenvalues. Here we calculated eigenvalues for 30 iterations and they are listed in Table 4.2. We have also checked that for the given eigenvalues, the wave functions are normalizable and it tends to zero when $x \to \infty$.

Table 4.2 The eigenvalue Hamiltonians H_2, H_3 and H_4, for $\gamma = 0.1$. The result is obtained after 30 iterations.

n	E_{H_2}	E_{H_3}	E_{H_4}
0	0.507 732 26	0.488 333 47	0.509 493 36
1	1.455 513 69	1.444 518 56	1.459 729 23
2	2.369 412 82	2.362 868 81	2.374 618 96
3	3.255 441 87	3.251 372 13	3.261 064 59
4	4.132 353 79	4.128 826 19	4.138 052 87
5	4.959 975 06	4.963 053 56	4.964 789 01

The results given in Table 4.2 shows that eigenvalues and eigenfunctions are also depends on the choices of the parameters, ε , ρ and η of Hamiltonian (2.18).

CHAPTER 5

CONCLUSION

In this thesis, we have reviewed the articles about (1) construction of the PDM Hamiltonians, (2) methods of solutions of the PDM Hamiltonians including physical potentials and various mass functions. We have also suggested a method for solving PDM Schrödinger equation.

The history of Schrödinger equation has been studied and solved for spherical coordinate to obtain quantum numbers. Approximations of kinetic energy operators which are used in calculations for PDM Hamiltonian, have been discussed. We have seen better kinetic energy operator approximations like the one used by von Roos.

We have introduced some of methods to solve PDM Schrödinger, Klein-Gordon and Dirac equations. We benefit from some of the articles [48, 64, 70, 78, 91,98] which use different methods, potentials and masses for solving PDM equations. For example, Series Expansion Method gives information about the solution of N-dimensional Schrödinger equation which is a method without mapping potential into mass space or vice versa. If we discuss the methods about transformations, we can say NU method, Lie algebraic technique and SUSYQM method have transformations. Certainly, these methods which include transformations have lots of good results (wavefunctions, energy eigenvalues).

We have suggested a new method to solve PDM Hamiltonian, it is called Asymptotic Taylor Expansion Method. The importance of this method is that it does not transform potential into mass space. We have solved PDM Schrödinger equation for four different kinetic energy operators including harmonic oscillator potential with the variable mass function of the form $m(x) = m_0(1 + \gamma x^2)$. It is shown that energy levels of the PDM Schrödinger equation depends on the mass distributions. It is important to remark that the results presented here, shows that eigenvalues also depends on the ordering parameters of the PDM Schrödinger equation [99]. Normalized wave functions for first six state and eigenvalues of PDM Hamiltonians

(H_1, H_2, H_3, H_4) have been shown in Figure 4.1, Table 4.1 and 4.2. The results are highly accurate. ATEM is useful for obtaining both eigenvalues and eigenfunctions of the Schrödinger type equations. Therefore, the results have been obtained here, allowing further comparisons between the models.

As a further work the method presented here can be used to built more realistic models for the PDM physical systems. Before ending this work a remark is in order. When the potential mapped to the mass space, the both constant and PDM Hamiltonian has the same eigenvalues. It will be worthwhile to discuss physical acceptability of such an isospectrality in the position dependent mass background. Therefore we have to develop methods for solving PDM Schrödinger equation without connecting mass to potential or vice versa [26].

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APPENDIX

A Mathematica Program for Solving PDM Schrödinger Equation within the framework of ATEM

```
Remove[f, g, h] (*Command of Remove: removes symbols of f,g,
h completely, so that their names no longer recognized by
 Mathematica*)
```

▪ Construction of Hamiltonian

General form of the PDM eigenvalue equation $H\psi(x) - En\psi(x) = 0$:
General *Mathematica* form of PDM Hamiltonian:

```
HE = 1/4 (m[x]^η (-i ħ D[m[x]^ϵ (-i ħ D[m[x]^ρ ψ[x], x]), x]) +
        m[x]^ρ (-i ħ D[m[x]^ϵ (-i ħ D[m[x]^η ψ[x], x]), x])) +
     (V[x] - En) ψ[x];
```

For 4 different PDM Hamiltonians, selected values of the parameters are ϵ, ρ, η

```
sp[1] = {ϵ → -1, ρ → 0, η → 0};
sp[2] = {ϵ → 0, ρ → 0, η → -1};
sp[3] = {ϵ → -1/2, ρ → 0, η → -1/2};
sp[4] = {ϵ → 0, ρ → -1/2, η → -1/2};
```

Potential, mass and values of the other parameters can be writen as:

```
st = {V[x] -> 1/2 m0 ω0^2 x^2, m[x] → m0 (1 + γ x^2), m^(j_)[x] → D[m0 (1 + γ x^2),
      {x, j}], m0 → 1, ħ → 1, ω0 → 1};
```

For given potential, mass and parameters the Hamiltonians can be expressed as:

```
Do[
 H[i] =
  Collect[Simplify[e^(x^2/2) HE /. sp[i] //. st /. ψ → Function[x, f[x] e^(-x^2/2)]],
   {f[x], f'[x], f''[x], FullSimplify}], {i, 1, 4}]
```

▪ Iteration of the Hamiltonians

Here in is iteration number, i is ith Hamiltonian defined in previous *Mathematica* section

```
k = 60; γ = 1 / 10; i = 1;
Do[g[n] = Simplify[D[H[i], {x, n}] /. x → 0], {n, 0, k}]
Do[f^(n)[0] = Solve[g[n - 2] == 0, f^(n)[0]][[1, 1, 2]], {n, 2, k}]
```

Solution of H[i] is given by

$$h[x] = \text{Sum}\left[\frac{x^n}{n!} f^{(n)}[0], \{n, 0, k\}\right];$$

Coefficient of even power of x in h[x] gives eigenvalues of the even functions and vice versa

```
enr =
 Sort[Solve[Coefficient[h[x], x^k] * Coefficient[h[x], x^(k-1)] == 0, En] // N]
```

```
{{En → 0.468897}, {En → 1.43349}, {En → 2.35655},
 {En → 3.24598}, {En → 4.10694}, {En → 4.94338}, {En → 5.75817},
 {En → 6.52942}, {En → 7.26923}, {En → 7.87023 - 0.748681 i},
 {En → 7.87023 + 0.748681 i}, {En → 8.343 - 0.904071 i},
 {En → 8.343 + 0.904071 i}, {En → 9.00544 - 2.32083 i},
 {En → 9.00544 + 2.32083 i}, {En → 9.38394 - 2.47609 i},
 {En → 9.38394 + 2.47609 i}, {En → 10.2559 - 4.08237 i},
 {En → 10.2559 + 4.08237 i}, {En → 10.5458 - 4.25468 i},
 {En → 10.5458 + 4.25468 i}, {En → 11.6534 - 6.09392 i},
 {En → 11.6534 + 6.09392 i}, {En → 11.8844 - 6.29248 i},
 {En → 11.8844 + 6.29248 i}, {En → 13.2671 - 8.46745 i},
 {En → 13.2671 + 8.46745 i}, {En → 13.4738 - 8.68153 i},
 {En → 13.4738 + 8.68153 i}, {En → 15.2835 - 11.4632 i},
 {En → 15.2835 + 11.4632 i}, {En → 15.4865 - 11.6842 i},
 {En → 15.4865 + 11.6842 i}, {En → 17.4868}, {En → 20.1232},
 {En → 27.8564}, {En → 30.5342}, {En → 39.1497}, {En → 42.2922},
 {En → 52.8735}, {En → 56.6667}, {En → 70.0167}, {En → 74.6128},
 {En → 91.6103}, {En → 97.1661}, {En → 118.907}, {En → 125.598},
 {En → 153.536}, {En → 161.564}, {En → 197.725}, {En → 207.334},
 {En → 254.729}, {En → 266.219}, {En → 329.738}, {En → 343.508},
 {En → 432.344}, {En → 448.969}, {En → 586.204}, {En → 606.717}}
```

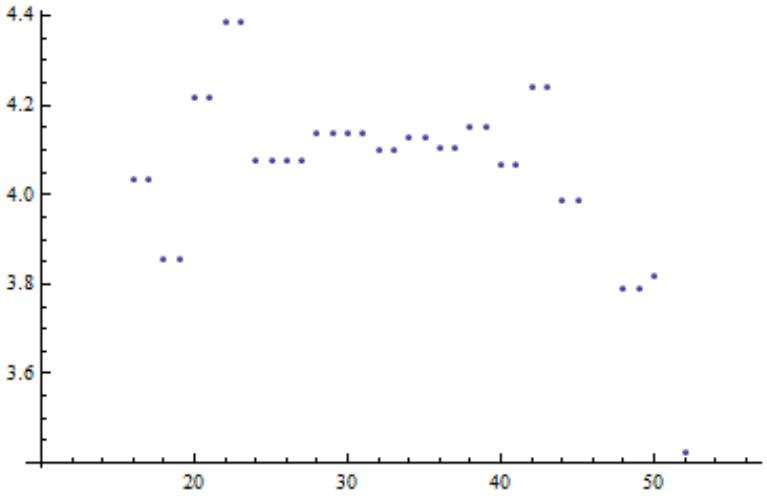
```
Clear[enr]
(*Command of Clear: clears value and definition for the enr*)

Do[
 enr[i] =
  Sort[Solve[Coefficient[h[x], x^(k-i)] * Coefficient[h[x], x^(k-1-i)] == 0,
     En] // N], {i, 4, 56}]

Chop[Table[{60 - i, enr[i][[5, 1, 2]]}, {i, 4, 50}]]
```

```
{{56, 2.85455}, {55, 3.59289 - 1.0536 i}, {54, 3.34621 + 0.54855 i},
 {53, 3.34621 + 0.54855 i}, {52, 3.42528}, {51, 4.01227 - 0.783501 i},
 {50, 3.81849}, {49, 3.79087}, {48, 3.79087}, {47, 4.35046 - 0.454178 i},
 {46, 4.35046 - 0.454178 i}, {45, 3.98576}, {44, 3.98576}, {43, 4.24191},
 {42, 4.24191}, {41, 4.06744}, {40, 4.06744}, {39, 4.15143},
 {38, 4.15143}, {37, 4.10255}, {36, 4.10255}, {35, 4.12568},
 {34, 4.12568}, {33, 4.10021}, {32, 4.10021}, {31, 4.13805},
 {30, 4.13805}, {29, 4.1352}, {28, 4.1352}, {27, 4.07547},
 {26, 4.07547}, {25, 4.07807}, {24, 4.07807}, {23, 4.38776},
 {22, 4.38776}, {21, 4.21558}, {20, 4.21558}, {19, 3.8563},
 {18, 3.8563}, {17, 4.03627}, {16, 4.03627}, {15, 4.17888 - 0.936684 i},
 {14, 3.73576 + 0.347326 i}, {13, 3.73576 + 0.347326 i},
 {12, 3.50462 + 0.404398 i}, {11, 3.50462 - 0.404398 i}, {10, 3.14806}}
```

```
ListPlot[%]
```



Graph of the eigen function for given energy values.nr is normalization constant.

```
Do[pe[i] = h[x] /. f'[0] → 0 /. f[0] → 1 /. En → enr[[i, 1, 2]];
  pfe[i] = Take[pe[i], 7]; nr = 1/Sqrt[∫_-∞^∞ e^-x^2 pfe[i]^2 dx];
  plem[i] = Plot[nr e^-x^2/2 pfe[i], {x, -5, 5}, AxesLabel → {x, ψ_i-1[x]},
    LabelStyle → Directive[FontSize → 14]], {i, 1, 6, 2}]
Do[po[i] = h[x] /. f'[0] → 1 /. f[0] → 0 /. En → enr[[i, 1, 2]];
  pfo[i] = Take[po[i], 7]; nr = 1/Sqrt[∫_-∞^∞ e^-x^2 pfo[i]^2 dx];
  plom[i] = Plot[nr e^-x^2/2 pfo[i], {x, -5, 5}, AxesLabel → {x, ψ_i-1[x]},
    LabelStyle → Directive[FontSize → 14]], {i, 2, 6, 2}]
```