STUDY OF ONE DIMENSIONAL POSITION DEPENDENT EFFECTIVE MASS PROBLEM IN SOME QUANTUM MECHANICAL SYSTEMS

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ABSTRACT

STUDY OF ONE DIMENSIONAL POSITION DEPENDENT EFFECTIVE MASS PROBLEM IN SOME QUANTUM MECHANICAL SYSTEMS

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The one dimensional position dependent effective mass problem is studied by solving the Schrödinger equation for some well known potentials, such as the deformed Hulthen, the Mie, the Kratzer, the pseudoharmonic, and the Morse potentials. Nikiforov-Uvarov method is used in the calculations to get energy eigenvalues and the corresponding wave functions exactly. By introducing a free parameter in the transformation of the wave function, the position dependent effective mass problem is reduced to the solution of the Schrödinger equation for the constant mass case. At the same time, the deformed Hulthen potential is solved for the position dependent effective mass case by applying the method directly. The Morse potential is also solved for a mass distribution function, such that the solution can be reduced to the constant mass case.

Keywords: Schrödinger Equation, Nikiforov-Uvarov Method, Position Dependent Mass, Morse Potential, Hulthen Potential, Mie Potential, Kratzer Potential, Pseudoharmonic Potential

ÖZ

BAZI KUVANTUM MEKANİK SİSTEMLERDE TEK BOYUTLU KONUMA BAĞLI EFEKTİF KÜTLE PROBLEMİ ÇALIŞMASI

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Tek boyutlu konuma bağlı efektif kütle problemi deforme Hulthen, Mie, Kratzer, psüdoharmonik ve Morse gibi bilinen bazı potansiyeller için Schrödinger denklemi çözülerek çalışıldı. Enerji öz değerleri ve ilgili dalga fonksiyonlarının hesaplamalarında Nikiforov-Uvarov metodu kullanıldı. Dalga fonksiyonu transformasyonunda yeni bir serbest parametre tanımlanarak konuma bağlı efektif kütle problemi sabit kütleli Schrödinger denkleminin çözüm durumuna indirgendi. Aynı zamanda doğrudan bu metot uygulanarak deforme Hulthen potansiyeli konuma bağlı efektif kütle durumu için çözüldü. Morse potansiyeli de sonucun sabit kütle durumuna indirgenmesini sağlayacak bir kütle dağılım fonksiyonu için çözüldü.

Anahtar Kelimeler: Schrödinger Denklemi, Nikiforov-Uvarov Metodu, Konuma Bağlı Kütle, Morse Potansiyeli, Hulthen Potansiyeli, Mie Potansiyeli, Kratzer Potansiyeli, Psüdoharmonik Potansiyel

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CHAPTER 1

INTRODUCTION

The concept of position dependent effective mass (PDEM) is known to play an important role in different branch of nonrelativistic and relativistic physics. This formalism has been extensively used in nuclei, quantum liquids, quantum wells, graded alloys, semiconductor heterostructures, ^3He and metal clusters. Special applications of these subjects are carried out in the investigation of electronic properties of semiconductors such as quantum wells and quantum dots [1-5], lasers [6], ^3He clusters [7], quantum liquids [8], graded alloys and semiconductor heterostructures [9-18].

The PDEM applications stimulated a lot of work in the literature on the development of methods for studying systems with mass that depends on position. These methods are applied in the application of various physical, shape invariant and PT-symmetric potentials. Besides these, many authors attempted to approach PDEM problem with point canonical transformation [19-23], supersymmetry [24-36], series solution [37-39], transfer matrix [40, 41], Green's Function [42, 43] and Lie algebra [44-46] methods. Furthermore, several classes of solvable PT-symmetric potentials are also studied [47-56] in a PDEM background. The equivalence of a PDEM Hamiltonian to a non-Hermitian PT-symmetric one was shown in [57] and PDEM systems with Dirac equations for PT-symmetric potentials are are found in [58-61].

The nonrelativistic Hamiltonian of PDEM systems is always under the constraint of ordering ambiguity in the kinetic energy term. On the other hand, its relativistic counterpart, the relativistic Dirac equation, does not suffer from such ambiguity [62] and the ordering ambiguity problem of the kinetic energy operator with PDEM is resolved in [57]. The Dirac equation with PDEM is solved by using the basic concepts of the supersymmetric quantum mechanics formalism and the functional analysis method for the relativistic problem of neutral fermions subject to PT-symmetric trigonometric potential in [58]. On the other hand, it is approximately solved for the generalized Hulthén potential in the case of the smooth step mass distribution [63] and also for a charged particle with a spherically symmetric singular mass distribution in the Coulomb field in [64-66] and for PT-symmetric and non-PT-symmetric potentials [59, 60]. The Kepler problem for a particle whose potential energy and mass are inversely proportional to the distance from the force center [67] is also studied within the framework of the Dirac PDEM equation. Klein-Gordon equation with PDEM is studied with vector and scalar Hulthen type potential [68], with Coulomb like scalar plus vector potentials [69], with vector and scalar exponential type potentials [70], with scalar and vector Rosen-Morse-type potential [71], with linear scalar potential [72], the generalized Hulthen potential [73] and for the Woods-Saxon potential in the case of an exponentially mass distribution in [74]. Duffin-Kemmer-Petiau equation is also studied with a PDEM for a system with an external smooth potential [75].

The exact solution of the one dimensional Schrödinger equation (SE) with PDEM is studied for some physical potentials in this thesis. The deformed Hulthen potential is solved with a coordinate transformation involving mass term with a power of η. As a second type of solution, by choosing an appropriate value of η in the coordinate transformation, all the PDEM wave equations are transformed into the solution of the constant mass form of SE for the Mie, the Kratzer, the pseudoharmonic and the Morse potentials and the energy eigenvalues and the corresponding wave functions are obtained analytically. The Nikiforov-Uvarov method (NUM) is used generally in the both computations.

The contents of the thesis are as follows, the PDEM Schrodinger equation is introduced in chapter 2. In chapter 3, brief introduction of the one dimensional molecular potentials are given. In chapter 4, the solutions of the Schrodinger equation for some potentials are given for constant and PDEM. In the last chapter, the results are discussed.

CHAPTER 2

METHOD

In dealing with quantum mechanical systems one aims at determining the wave function of a single electron or of the whole system. The wave function in quantum mechanics is sufficient to describe a particle or even a system of particles. In other words, if the wave function of an electron system in a solid is known, all of the macroscopic parameters that define the electronic performance of an electronic device element, i.e. diode, can be calculated. Thus, one of the main tasks of the quantum mechanics is to find exact solutions to the SE for certain potentials.

The wave function $\Psi(x,t)$ of an electron or an electron system satisfies the time dependent SE,

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} - H\Psi(x,t) = 0 \tag{2.1}$$

where H is the Hamiltonian operator of the system,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{2.2}$$

where $\hbar$ is the Plank's constant divided by 2π, m is mass and $V(x)$ is the potential energy. The form of Eq. (2.1) is that of a wave function and its solutions are expected to be wavelike in nature. If $V(x)$ is time independent, one may separate the dependencies on the time and spatial coordinates:

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x) \tag{2.3}$$

where ψ is a function of only spatial coordinates. Substituting Eq. (2.3) into Eq. (2.1), the time independent SE is obtained:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x) \tag{2.4}$$

where E is the energy of a particle or a system of particles.

2.1 One dimensional Schrödinger Equation with Position Dependent Effective Mass

The motivation for obtaining exact solutions of the wave equation with PDEM comes from the wide range of applications of these solutions in various areas of material science and condensed matter in the framework of the effective mass theory which is proposed to describe impurities in crystals [76]. The study of quantum mechanical systems with PDEM raises some important conceptual problems, such as the ordering ambiguity of the momentum and mass operators in the kinetic energy term, the boundary conditions at abrupt interfaces characterized by discontinuities in the mass function, and the Galilean invariance of the theory [77,78].

The growing interest in semiconductor physics parallel to the modern development in fabricating nanostructure technology creates a renewed attention to study the behaviour of one dimensional eigenvalue equation

$$H(x)\psi(x)\equiv\left[T(x)+V(x)\right]\psi(x)=E\psi(x) \tag{2.5}$$

from a theoretical standpoint [78]. In this equation $T(x)$ is the kinetic energy operator and $\psi(x)$ is the wave function (also known as envelope wave function in the literature [80, 81]). In order to have the special properties of the eigenvalue equation Eq. (2.5), the first step is certainly to choose a suitable form of the Hermitian kinetic energy operator arising from non-commutativity of momentum operator

$$p\equiv -i\hbar\frac{d}{dx} \tag{2.6}$$

and the coordinate operator. Different forms had been proposed in the literature, most of which may be written as a special class of the general two-parameter family proposed in [15]:

$$T(x) = \frac{1}{4}\left(m^{\alpha}pm^{\beta}pm^{\gamma} + m^{\gamma}pm^{\beta}pm^{\alpha}\right) \tag{2.7}$$

with the constraint $\alpha + \beta + \gamma = -1$ over the ordering parameters.

Considerable efforts were made to remove the non-uniqueness of the kinetic energy operator Eq. (2.7) or, in other words, to fix the values of the ordering parameters α, β, γ:

1. In [82] a step potential and a step mass were considered, and it was shown that $\alpha = \gamma$ is the only physical choice for an abrupt heterojunction.

2. Later in an attempt to fix β, two different conclusions were drawn, namely $\beta = 0$ for a one-dimensional model and $\beta = -1$ for a three-dimensional model [83].

3. On the other hand, in a series of works [84-86], the authors concluded that $\alpha = \gamma = 0$, $\beta = -1$ for an abrupt heterojunction. Among these works, [86] deserves to be mentioned separately because it presented the first example of a continuous function $m(x)$ across the heterojunction.

4. A new kind of kinetic energy operator was proposed [10] for strained heterostructure, which is not included in Eq. (2.7), in general, for position dependent lattice constant. It should be mentioned that the choice $\alpha = \gamma = 0$, $\beta = -1$ gives rise to the kinetic energy operator $T = p(\frac{1}{2m})p$ which was first proposed in [87].

5. Choosing the same operator some interesting pedagogical models were considered [86] to show the qualitative differences in quantum mechanical observables (e.g. reflection and transmission coefficient, band-structure, etc) between PDEM and constant mass case.

6. Many other forms of kinetic energy operator have also been proposed; e.g., $\alpha = -1$, $\beta = 0$ and $\gamma = 0$ which gives from Eq. (2.7), $T = \frac{1}{4m}p^2 + p^2\frac{1}{4m}$ [12], $\alpha = \gamma = -1/2$, $\beta = 0$ which $T = (1/2\sqrt{m})p^2(1/2\sqrt{m})$ [88], etc.

7. A different variation was derived, via path-integral formalism [89], which comes from Eq. (2.7) for the following values: $\alpha = \frac{(-\sqrt{2}+i)}{3\sqrt{2}}$, $\beta = -\frac{1}{3}$, $\gamma = \alpha$.

In previous studies [2, 19, 26-29, 30, 31, 37, 40, 42, 45, 90-95] authors either started from a preferred ad hoc choice for α, β, γ or they kept them arbitrary. In both cases attention had been paid to solvability for various smooth functional forms of $V(x)$ and $m(x)$ by employing the existing tools like supersymmetry [10, 24, 25, 29, 30, 40, 81, 84, 96], Lie-algebraic approach [44, 45, 91, 92], shape-invariance [93, 94], etc. The connection between solvability and the ordering parameters in equations Eq. (2.5) and Eq. (2.7) was discussed in [97]. Smooth functions (in the sense that m' and m'' are also continuous) were chosen for the first time in [90], where the authors however concluded again that $\alpha = \gamma = 0$, $\beta = -1$ by comparing their results with a limiting case where the potential and mass become abrupt. It may be mentioned that in several works [26, 45, 91] mass function was kept arbitrary and thus the solutions provided there were only formal. In contrast, in most cases where smooth functional forms were chosen for $m(x)$, we note that $m(x) \to 0$ as $|x| \to \infty$. One possible way of eliminating this nonphysical situation is to consider the variation of the mass in a finite region (being constant outside), which is also natural on realistic grounds. Of course, this correction will force one to obtain correct matching conditions for the model.

The study of semiconductor heterostructures, or more generally of inhomogeneous crystals, has given rise to an extended discussion concerning the use of simple PDEM model descriptions, which are related to the envelope function approximations, for the dynamics of electrons in such systems. The PDEM problem arises from the boundary conditions at abrupt interfaces, where the discontinuities in the solid cause the spatial dependence of the mass function $m(x)$.

Generally, the mass is taken as a constant and so that the form of the kinetic energy Hamiltonian is defined as

$$H(x) = \frac{\hat{p}^2}{2m(x)} + V(x) \tag{2.8}$$

Here, $m(x)$ is the PDEM and $\hat{p}$ is the momentum operator. As momentum operator and PDEM function do not commute, the PDEM Hamiltonian written in this form becomes non-Hermitian. The kinetic energy Hamiltonian can be written in the form

$$H = \frac{1}{4}\left(m^{\alpha} p m^{\beta} p m^{\gamma} + m^{\gamma} p m^{\beta} p m^{\alpha}\right) \tag{2.9}$$

with the constraint $\alpha + \beta + \gamma = -1$ as introduced by Von Roos [15]. As a result, one of the correct forms of the kinetic energy Hamiltonian can be written as

$$H(x) = \hat{p}\frac{1}{2m(x)}\hat{p} + V(x) \tag{2.10}$$

Now, the SE with PDEM is defined in one dimension as

$$\left[\frac{d}{dx}\left(\frac{1}{m(x)}\right)\frac{d}{dx}\right]\psi(x) + \frac{2}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{2.11}$$

The first term can be rewritten by acting the derivative operator:

$$\begin{aligned}\left[\frac{d}{dx}\left(\frac{1}{m(x)}\right)\frac{d}{dx}\right] &= \left[\frac{d}{dx}\left(\frac{1}{m(x)}\right)\right]\frac{d}{dx} + \frac{1}{m(x)}\frac{d^2}{dx^2} \\ &= -\frac{m'(x)}{m^2(x)}\frac{d}{dx} + \frac{1}{m(x)}\frac{d^2}{dx^2}\end{aligned} \tag{2.12}$$

where $m'(x)$ denotes the derivative with respect to x. When the result of Eq. (2.12) is substituted into Eq. (2.11), the SE with a variable mass becomes:

$$\frac{1}{m(x)}\frac{d^2\psi(x)}{dx^2} - \frac{m'(x)}{m^2(x)}\frac{d\psi(x)}{dx} + \frac{2}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{2.13}$$

or by multiplying each term with $m(x)$, the final form of the equation becomes:

$$\frac{d^2\psi(x)}{dx^2} - \frac{m'(x)}{m(x)}\frac{d\psi(x)}{dx} + \frac{2m(x)}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{2.14}$$

2.2 The Nikiforov-Uvarov Method

The Nikiforov-Uvarov method (NUM) [98] provides an exact solution for the SE. This method is developed for constructing solutions of the general second-order linear differential equation which are special orthogonal polynomials. It is well known that any given one-dimensional or radial SE can be written as a second-order linear differential equation and then the equation is reduced to the hypergeometric type one with an appropriate coordinate transformation $x = x(s)$.

$$\frac{d^2\Psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)}\frac{d\Psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0 \tag{2.15}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials with at most second degree, and $\tilde{\tau}(s)$ is a polynomial with at most first degree. $\Psi(s)$ can be written as

$$\Psi(s) = \phi(s)\ y(s), \tag{2.16}$$

Then, the Eq. (2.15) becomes,

$$\sigma(s)\frac{d^2y(s)}{ds^2} + \tau(s)\frac{dy(s)}{ds} + \lambda y(s) = 0, \tag{2.17}$$

where λ is a constant and $\sigma(s)$ is defined as

$$\sigma(s) = \pi(s)\frac{d}{ds}[\ln\phi(s)], \tag{2.18}$$

and $\tau(s)$ is

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{2.19}$$

λ is given as

$$\lambda = \lambda_n = -n\tau' - \frac{[n(n-1)\sigma'']}{2}, \quad n = 0, 1, 2, \ldots \tag{2.20}$$

and it is also defined as

$$\lambda = k + \pi'(s) \tag{2.21}$$

where the energy eigenvalues can be calculated by equating Eq. (2.20) with Eq. (2.21). The $\pi(s)$ function is defined as

$$\pi(s) = \frac{(\sigma' - \tilde{\tau})}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}. \tag{2.22}$$

Here, $\pi(s)$ is a polynomial with the parameter s and prime factors denote the differentials at first degree. The determination of k is the essential point in the calculation of $\pi(s)$. It is simply defined as by setting the discriminant of the square root to zero. As a result of this, a general quadratic equation for k is obtained.

In order to write the wave function, the Rodriguez relation can be defined by considering Eq. (2.18) as

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[\sigma^n(s)\ \rho(s)\right], \tag{2.23}$$

where B_n is normalizable constant and the weight function $\rho(s)$ satisfy the following relation

$$\frac{d}{ds} \left[\sigma(s)\ \rho(s)\right] = \tau(s)\ \rho(s). \tag{2.24}$$

where

$$\frac{\phi'}{\phi} = \frac{\pi}{\sigma}. \tag{2.25}$$

Eq. (2.23) refers to the classical orthogonal polynomials. It has many important properties such as orthogonality relation which can be defined as

$$\int_a^b y_n(s) y_m(s) \rho(s)\ ds = 0, \quad m \neq n. \tag{2.26}$$

CHAPTER 3

MOLECULAR POTENTIALS IN ONE DIMENSION

3.1 The Basic Structure of Diatomic Molecules

A simple molecule consists of two atoms bonded together by forces. The empirical results of molecular spectroscopy show that the energy of the molecule (aside from translational energy) consist of three parts [99]. They are called the electronic energy, vibrational energy and the rotational energy. The energy levels fall into widely separated groups. They correspond to the different electronic states of the molecule [100]. 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. This is 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 suggests 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. Just for an atomic system, the Hamiltonian for a diatomic or polyatomic molecule is the sum of the kinetic energy and the potential energy. For a molecule, the kinetic energy consists of two parts. The contributions to the energy come from the motions of the electrons and nuclei. 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 [101]. The energy changes involved in a transition from one electronic state of a molecule to another are very large. They also correspond to the 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 specialized to study of electronic spectra of polyatomic molecules like benzene or ions.

3.2 Molecular Potentials

Intermolecular forces are important as they are required to solve a wide class of problems in physics, chemistry and biology. In physics, they are used to determine the properties of crystals, the binding energy, phonon spectra, etc. In biology, they are accounted for the stability of important compounds such as DNA and RNA and they also play an essential role in muscle contraction. In chemistry, intermolecular interactions are involved in the formation of complicated chemical complexes, such as charge-transfer and hydrogen-bond complexes [102].

Intermolecular forces are not measured directly in any experiment. They are determined indirectly by measuring some other characteristics which are related with the intermolecular forces. The experimental procedures used to determine these forces are:

- scattering experiments in atomic-molecular beams
- spectroscopic measurements (vibrational-rotational spectra, etc.)
- data on thermophysical properties of gases and liquids (virial coefficients, viscosity and transport coefficients, etc.)
- data on crystal properties (elastic constants, phonon spectra, etc.)
- experiments on the formation of radioactive defects in solids
- nuclear magnetic resonance experiments in solids and liquids (the time of spin and spin-lattice relaxations)

After getting data from the experiments, some semiemprical model potentials are used to fit these data. The choose of the model potential depends on the studied problem.

The potential describing the interaction between two molecules is represented by a potential curve depending only on one variable, if the interaction is averaged over all molecular orientations in space. This potential, $V(R)$, where R is the distance between the centers of masses of the molecules, is named the potential of intermolecular interaction, or briefly, the intermolecular potential. The types of intermolecular interactions are shown in Figure 3.1. They are classified according to the three ranges of interatomic separation for a typical interatomic potential.

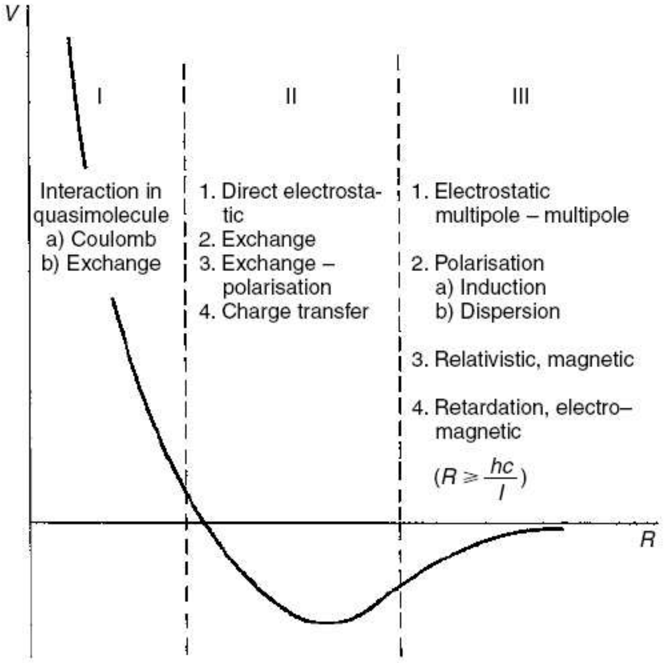


Figure 3.1: The classification of intermolecular interactions

These three ranges are:

I At short distances the potential has a repulsive nature and the electronic exchange, due to the overlap of the molecular electronic shells, dominates.

II At intermediate distances the repulsive and attractive forces are in balance.

III At large distances, the electronic exchange is negligible and the intermolecular forces are attractive.

A consistent theory of intermolecular forces can only be developed on the basis of quantum mechanical principles. Because of the quantum nature of the electronic and nuclear motions, the solution of the intermolecular interaction problem reduces to solving the SE. The problem under study can be solved analytically by the SE for a physical potential. There are various model potentials used in the molecular dynamics and Monte Carlo simulation studies of condensed matter physics, i.e., for determining the properties of crystal structures [102]. Some of the most interested ones are the Morse, Kratzer's, Pöschl-Teller and Mie potentials.

3.3 The Morse Potential

The Morse potential was proposed by Morse [103] for defining the vibrational energy levels of diatomic molecules. It is much used in spectroscopic applications as it is possible to solve SE for this system. The functional form of the potential has two exponential terms:

$$V(R) = D\left[e^{-2\alpha(R-R_m)} - 2e^{-\alpha(R-R_m)}\right] \tag{3.1}$$

where D is the electronic energy and R_m defines the minimum as shown in the Figure 3.2. At $R = 0$ the potential becomes finite, that is,

$$V(0) = De^{\alpha R_m}\left[e^{\alpha R_m} - 2\right] \tag{3.2}$$

The energy levels observed experimentally and described by the formula

$$E_\nu = -D + \hbar\omega_0\left[\left(\nu + \frac{1}{2}\right) - a\left(\nu + \frac{1}{2}\right)^2\right] \tag{3.3}$$

where ω_0 is the vibrational frequency and n indicates the vibrational levels and a is a constant. Morse fitted the three parameters a, D and R_m on the basis of spectroscopic data. The Morse potential does not work at large distances. At $R = 0$ the potential has a finite value which is not correct. However, it describes the vibrational levels quite satisfactorily.

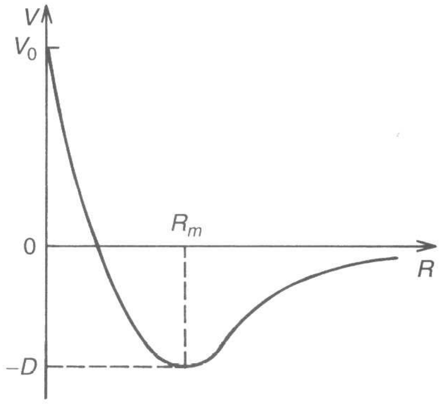


Figure 3.2: The Morse Potential

3.4 The Pseudoharmonic Potential

The pseudoharmonic potential [104] is a type of exactly solvable potential like Mie-type potentials other than the Coulombic and anharmonic oscillator. The potential has the form

$$V(x) = V_0 \left(\frac{x}{x_0} - \frac{x_0}{x} \right)^2 \tag{3.4}$$

It may be used for the energy spectrum of linear and nonlinear systems. It is generally used for discussion of molecular vibrations. One of the advantages of the pseudoharmonic potential over the harmonic oscillator is that it can be treated exactly in three as well as in one dimension. The Morse potential is commonly used for an anharmonic oscillator. However, its wave function does not vanish at the origin, but the Mie type and the pseudoharmonic potentials do. The Mie type potential has the general features of the true interaction energy, interatomic and intermolecular and dynamical properties of solids. This potential may be considered as an intermediate potential between the harmonic oscillator potential and anharmonic potentials, as the Morse oscillator potential, which is a more realistic potential, in good agreement with the experimental spectroscopical data.

3.5 The Kratzer Potential

Kratzer proposed his potential in 1920 [105] to describe the vibrational-rotational energy levels in diatomic molecules. The potential has the form:

$$V(x) = -\frac{a}{x + x_0} + \frac{b}{(x + x_0)^2} \tag{3.5}$$

where x_0 is not a free parameter, it is expressed via a and b, $x_0 = 2b/a$. The Kratzer potential is a two parameter potential with a minimum at $x = 0$, $V(0) = -a^2/4b = -D$. It tends to infinity as $x \to -x_0$ and converges to zero as $x \to \infty$ as shown in Figure 3.3. When Kratzer potential is compared with the others, the curve seen in figure has to be shifted by x_0 along the x-axis. So that, $R = x + x_0$ is introduced and when $V(R = 0) \equiv V(x = -x_0) = \infty$ and $V(R = x_0) \equiv V(x = 0) = -D$. The point $R = x_0$ corresponds to a minimum, denoted as R_m. The SE can also be solved analytically for the Kratzer potential as Morse and Pöschl-Teller potentials.

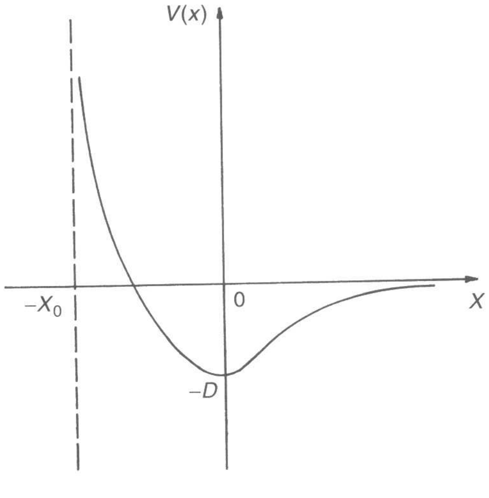


Figure 3.3: The Kratzer's Potential

3.6 The Mie Potential

The Mie potential was introduced by Mie [106] which is used to study the dynamical properties of solids. It is a special kind of exactly solvable power-law and inverse power-law potentials other than the Coulombic and harmonic oscillator. The wave functions of the potential vanish at the origin and it is given by

$$V(x) = \varepsilon \left[\frac{k}{l-k} \left(\frac{a}{x} \right)^l - \frac{l}{l-k} \left(\frac{a}{x} \right)^k \right] \tag{3.6}$$

where ε is the interaction energy between two atoms in a solid at $x = a$, and $l > k$ is always satisfied. When $l = 2k$ and by choosing the special case $k = 1$, corresponding to a Coulombic-type potential with an additional centrifugal potential barrier, the form of the potential shown in Figure 3.4 can be simplified. The maximum depth of the potential is ε.

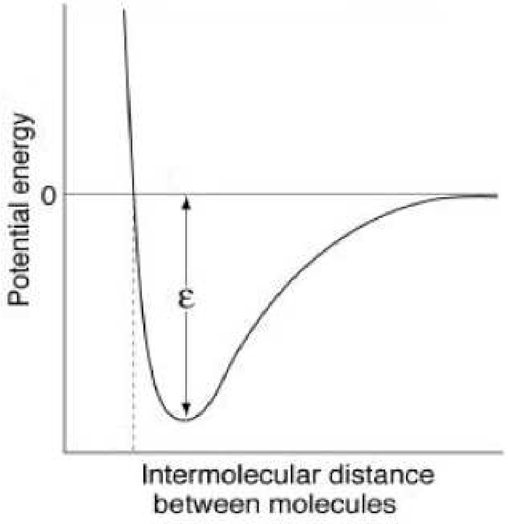


Figure 3.4: The Mie Potential

The Mie potential plays an important role in many fields, such as condensed matter physics, because it is of central importance for the general understanding of the behaviour and the application of a condensed matter. The Mie potential of crystalline solids have been deeply investigated [107-108]. There are some applications of Mie type potentials such as bulk metallic glass[109], and other applications in solid state physics [110, 111], molecular spectroscopy [112], fluid mechanics [113], the interatomic interaction potential in molecular physics [114-117], $1/r_n$ potential in three dimensions [118].

CHAPTER 4

APPLICATIONS AND CALCULATIONS

4.1 Solution of the Schrödinger Equation with Constant Mass

There are several applications involving the SE with constant mass in nonrelativistic form with some well known potentials like ring-shaped [119, 120], non-central [121] and central [122], Woods-Saxon [123-126], Morse [127, 128], Hulthen [129], symmetrical [130] and deformed hyperbolic [131, 132] potentials. In relativistic form [133, 134] there are applications of the Klein-Gordon [135], the Duffin-Kemmer-Petiau [136] and the Dirac equation for the Hulthen [137] and the Woods-Saxon [138, 139] potentials with various methods. In this section some selected physical potentials are solved by using NUM. These solutions are used in the solution of the SE with PDEM.

4.1.1 The Mie Potential

As a first application, Mie potential is studied [140]. The Mie-type potentials are given by

$$V(r) = \epsilon \left[\frac{k}{\ell - k} \left(\frac{a}{r} \right)^{\ell} - \frac{\ell}{\ell - k} \left(\frac{a}{r} \right)^{k} \right] \tag{4.1}$$

where ϵ is the interaction energy between two atoms in a solid at $r = a$, and $\ell > k$ is always satisfied. One-dimensional Mie potential [106] is solved with $\ell = 2k$ combination. By choosing the special case $k = 1$, corresponding to a Coulombic-type potential with an additional centrifugal potential barrier, we get the following form:

$$V(r)=V_0\left[\frac{1}{2}\left(\frac{a}{r}\right)^2-\left(\frac{a}{r}\right)\right];\ V_0=2\epsilon k \tag{4.2}$$

where V_0 is the dissociation energy and a is the positive constant which is strongly repulsive at shorter distances. The radial part of the SE for a diatomic molecule potential is

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}+V(r)\right]R_{n\ell}(r)=E_{n\ell}R_{n\ell}(r) \tag{4.3}$$

where μ is the reduced mass of the diatomic molecules. n denotes the radial quantum number (n and ℓ are named as the vibration-rotation quantum numbers in molecular chemistry). r is the internuclear separation. Substituting the explicit form of $V(r)$,

$$\begin{aligned}\frac{d^2R_{n\ell}(r)}{dr^2} &+ \frac{2}{r}\frac{dR_{n\ell}(r)}{dr}+\frac{2\mu}{\hbar^2}\left[E_{n\ell}-V_0\left(\frac{1}{2}\left(\frac{a}{r}\right)^2-\frac{a}{r}\right)\right]R_{n\ell}(r)\\ &- \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}R_{n\ell}(r)=0 \qquad (4.4)\end{aligned}$$

is obtained. By defining the following variables:

$$\varepsilon^2=E \tag{4.5}$$

$$\beta=-\frac{2\mu}{\hbar^2}V_0a \tag{4.6}$$

$$\gamma=\frac{2\mu}{\hbar^2}\left(\frac{1}{2}V_0a^2+\frac{\ell(\ell+1)\hbar^2}{2\mu}\right) \tag{4.7}$$

The SE takes the simple form:

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+\frac{1}{r^2}\left(\varepsilon^2r^2-\beta r-\gamma\right)\right]R_{n\ell}(r)=0 \tag{4.8}$$

From Eq. (4.8), it is clear that

$$\sigma(r)=r \tag{4.9}$$

$$\tilde{\tau} = 2 \tag{4.10}$$

$$\tilde{\sigma} = \varepsilon^2 r^2 - \beta r - \gamma \tag{4.11}$$

$\pi(r)$ becomes

$$\pi(r) = -\frac{1}{2} \pm \begin{cases} i\varepsilon r + \frac{1}{2}\sqrt{4\gamma+1}, & k_1 = -\beta + \varepsilon\sqrt{-1-4\gamma} \\ i\varepsilon r - \frac{1}{2}\sqrt{4\gamma+1}, & k_2 = -\beta - \varepsilon\sqrt{-1-4\gamma} \end{cases} \tag{4.12}$$

and $\tau(r)$ can be written as

$$\tau(r) = \begin{cases} 1 + 2i\varepsilon r + \sqrt{4\gamma+1}, & k_1 = -\beta + \varepsilon\sqrt{-1-4\gamma} \\ 1 - 2i\varepsilon r + \sqrt{4\gamma+1}, & k_2 = -\beta - \varepsilon\sqrt{-1-4\gamma} \end{cases} \tag{4.13}$$

For appropriate solutions $\tau^{'}(r) < 0$ [98]. Therefore,

$$k_2 = -\beta - \varepsilon\sqrt{-1-4\gamma} \tag{4.14}$$

$$\pi_2 = -\frac{1}{2} - i\varepsilon r - \frac{1}{2}\sqrt{1+4\gamma} \tag{4.15}$$

are used, and

$$\tau(r) = 1 - 2i\varepsilon r + \sqrt{1+4\gamma} \tag{4.16}$$

for obtaining eigenvalues and eigenfunctions. Using Eqs. (2.20-2.21) we find energy spectrum as

$$E_n = -\left(\frac{2\mu V_0 a}{\hbar^2}\right)^2 \left[2n + 1 + \sqrt{1 + \frac{8\mu}{\hbar^2}\left(\frac{V_0 a^2}{2} + \frac{\ell(\ell+1)\hbar^2}{2\mu}\right)}\right]^{-2} \tag{4.17}$$

The wave function is calculated from Eqs. (2.23-2.25).

$$\phi(r) = r^{\frac{1}{2}(-1+\sqrt{1+4\gamma})} e^{-i\varepsilon r} \tag{4.18}$$

and

$$\rho(r) = r^{\sqrt{1+4\gamma}} e^{-2i\varepsilon r} \tag{4.19}$$

and the radial part of the wave function becomes

$$R_{n,\ell} = C_n r^{\frac{1}{2}(-1+\sqrt{1+4\gamma})} e^{-i\varepsilon r} L_n^{\sqrt{1+4\beta}}(2i\varepsilon r) \tag{4.20}$$

If Eq. (4.17) is rewritten in atomic units,

$$E_n = -V_0^2 a^2 \left(2n + 1 + \sqrt{(2\ell+1)^2 + 2V_0 a^2}\right)^{-2} \tag{4.21}$$

is obtained. The calculated energy eigenvalues of the Mie potential for N_2, CO, NO and CH diatomic molecules with different values of n and ℓ in eV are given in Figure 4.1. The data for the potential parameters are taken from [141] and the values shown in Figure 4.1 are similar to the calculations given in [142] with the same parameters [141] for the given quantum numbers $n = 0, 1, 2, 3, 4, 5$.

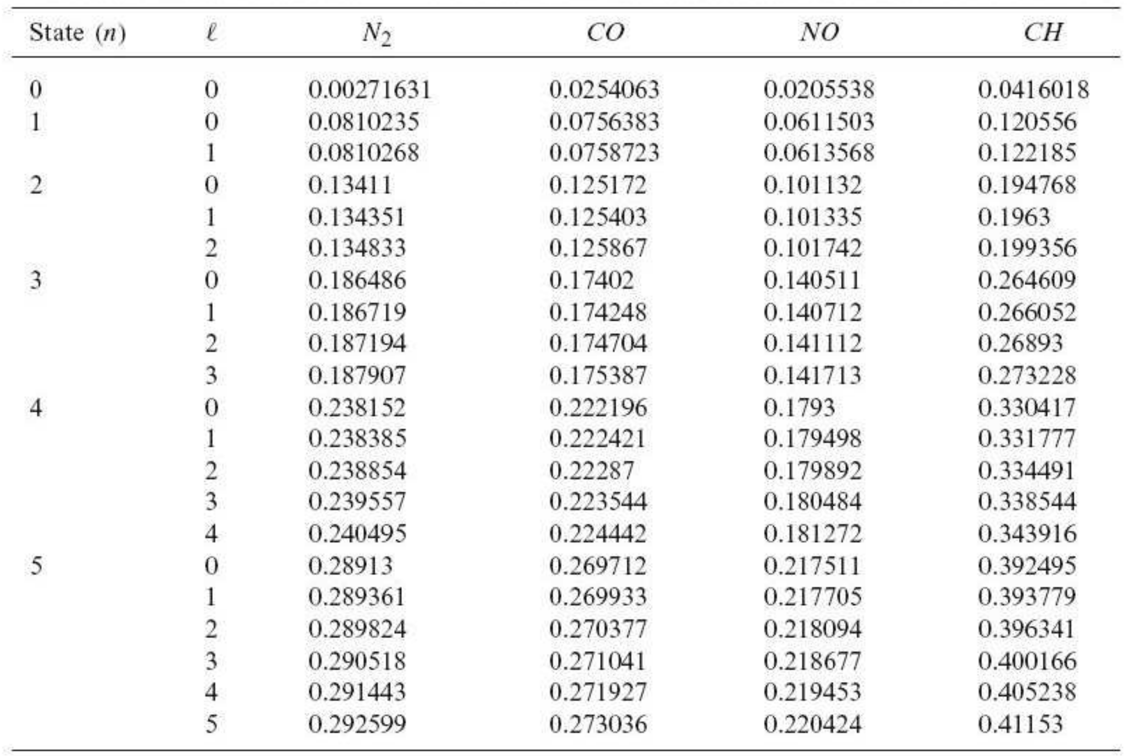
4.1.2 The Pseudoharmonic Potential

In this section, one-dimensional SE with pseudoharmonic potential is solved with NUM. The radial part of the SE for a diatomic molecular potential is given as

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r)\right] R_{n,\ell}(r) = E_{n,\ell} R_{n,\ell}(r) \tag{4.22}$$

where μ is reduced mass of the diatomic molecules, r is the intermolecular separation, n, ℓ are the vibration-rotation quantum numbers in molecular chemistry. For the pseudoharmonic potential [143]

$$V(r) = V_0 \left(\frac{r}{r_0} - \frac{r_0}{r}\right)^2 \tag{4.23}$$



State (n)	ℓ	N_2	CO	NO	CH
0	0	0.00271631	0.0254063	0.0205538	0.0416018
1	0	0.0810235	0.0756383	0.0611503	0.120556
	1	0.0810268	0.0758723	0.0613568	0.122185
2	0	0.13411	0.125172	0.101132	0.194768
	1	0.134351	0.125403	0.101335	0.1963
	2	0.134833	0.125867	0.101742	0.199356
3	0	0.186486	0.17402	0.140511	0.264609
	1	0.186719	0.174248	0.140712	0.266052
	2	0.187194	0.174704	0.141112	0.26893
	3	0.187907	0.175387	0.141713	0.273228
4	0	0.238152	0.222196	0.1793	0.330417
	1	0.238385	0.222421	0.179498	0.331777
	2	0.238854	0.22287	0.179892	0.334491
	3	0.239557	0.223544	0.180484	0.338544
	4	0.240495	0.224442	0.181272	0.343916
5	0	0.28913	0.269712	0.217511	0.392495
	1	0.289361	0.269933	0.217705	0.393779
	2	0.289824	0.270377	0.218094	0.396341
	3	0.290518	0.271041	0.218677	0.400166
	4	0.291443	0.271927	0.219453	0.405238
	5	0.292599	0.273036	0.220424	0.41153

Figure 4.1: The energy eigenvalues of the Mie potential.

Eq. (4.22) turns to be

$$\frac{d^2R_{n,\ell}(r)}{dr^2}+\frac{2}{r}\frac{dR_{n,\ell}}{dr}+\frac{2\mu}{\hbar^2}\left[E_{n,\ell}-V_0\left(\frac{r}{r_0}-\frac{r_0}{r}\right)^2-\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R_{n,\ell}=0 \qquad (4.24)$$

By defining the coordinate transformation

$$r^2=s \qquad (4.25)$$

and using the following dimensionless parameters

$$\alpha^2=\frac{V_0}{r_0^2}\frac{\mu}{2\hbar^2} \qquad (4.26)$$

$$\epsilon=\frac{\mu}{2\hbar^2}(E_{n,\ell}+2V_0) \qquad (4.27)$$

and

$$\beta = \frac{\mu}{2\hbar^2}\left[V_0 r_0^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu}\right] \tag{4.28}$$

$$\frac{d^2R}{ds^2} + \frac{3/2}{s}\frac{dR}{ds} + \frac{1}{s^2}(-\alpha^2 s^2 + \epsilon s - \beta)R(s) = 0 \tag{4.29}$$

is obtained. The energy eigenvalue solution is given as [143]

$$\epsilon = \left(2n + 1 + 2\sqrt{\beta + \frac{1}{16}}\right)\alpha \tag{4.30}$$

which can also be written in the form

$$E_{n\ell} = -2V_0 + \frac{\hbar}{r_0}\sqrt{\frac{2V_0}{\mu}}\left[2n + 1 + 2\sqrt{\frac{\mu}{2\hbar^2}\left(V_0 r_0^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu}\right) + \frac{1}{16}}\right] \tag{4.31}$$

and the wave function is obtained as

$$R_{n,\ell} = B_n s^{-\frac{1}{4}+\sqrt{\beta+1/16}} e^{-\alpha s} L_n^{2\sqrt{\beta-1/16}}(2\alpha s) \tag{4.32}$$

The energy eigenvalues of pseudoharmonic potential for N_2, CO, NO and CH diatomic molecules with different values of n and ℓ in eV are given in Figure 4.2. The data for potential parameters are taken from [141] and the values shown in Figure 4.2 are similar to the calculations given in [142] with the same parameters [141].

4.1.3 The Morse Potential

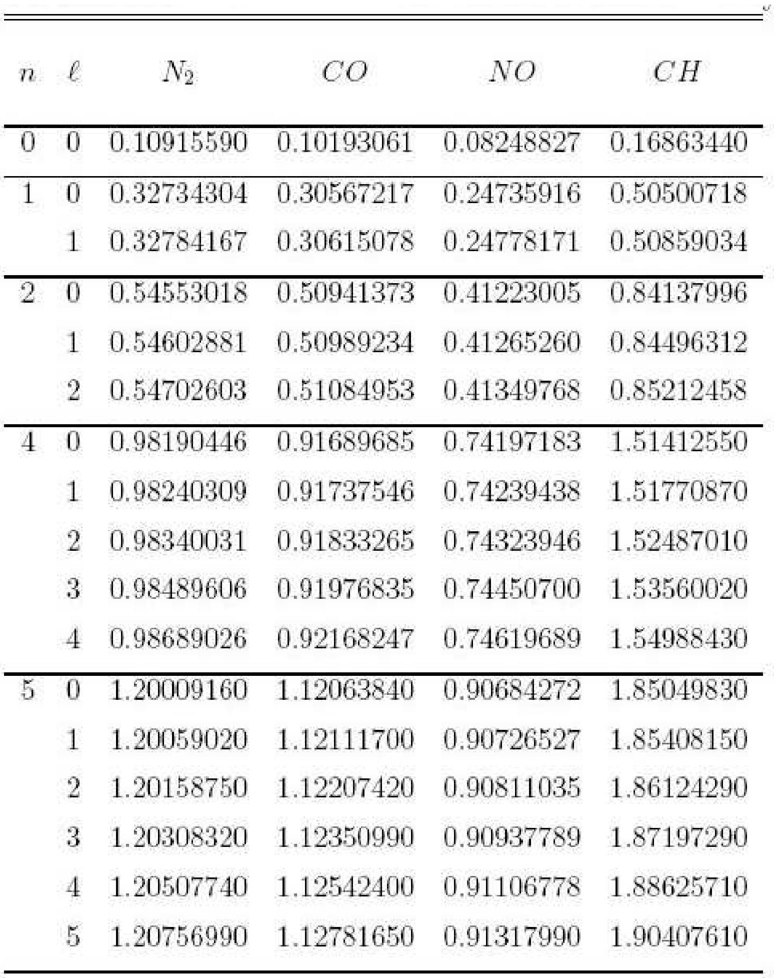
The SE is given as

$$\psi''(x) + \frac{2\mu}{\hbar^2}(E - V)\psi(x) = 0 \tag{4.33}$$

When the Morse potential

$$V(x) = V_1 e^{-2\lambda x} - V_2 e^{-\lambda x} \tag{4.34}$$

is substituted to the SE and by using the following variable



n	ℓ	N_2	CO	NO	CH
0	0	0.10915590	0.10193061	0.08248827	0.16863440
1	0	0.32734304	0.30567217	0.24735916	0.50500718
	1	0.32784167	0.30615078	0.24778171	0.50859034
2	0	0.54553018	0.50941373	0.41223005	0.84137996
	1	0.54602881	0.50989234	0.41265260	0.84496312
	2	0.54702603	0.51084953	0.41349768	0.85212458
4	0	0.98190446	0.91689685	0.74197183	1.51412550
	1	0.98240309	0.91737546	0.74239438	1.51770870
	2	0.98340031	0.91833265	0.74323946	1.52487010
	3	0.98489606	0.91976835	0.74450700	1.53560020
	4	0.98689026	0.92168247	0.74619689	1.54988430
5	0	1.20009160	1.12063840	0.90684272	1.85049830
	1	1.20059020	1.12111700	0.90726527	1.85408150
	2	1.20158750	1.12207420	0.90811035	1.86124290
	3	1.20308320	1.12350990	0.90937789	1.87197290
	4	1.20507740	1.12542400	0.91106778	1.88625710
	5	1.20756990	1.12781650	0.91317990	1.90407610

Figure 4.2: The energy eigenvalues of pseudoharmonic potential.

$$s = \sqrt{V_1} e^{-\lambda x} \tag{4.35}$$

reduces to [144]

$$\frac{d^2\psi}{ds^2} + \frac{1}{s}\frac{d\psi}{ds} - \frac{1}{s^2}\left(\frac{2\mu s^2}{\hbar^2\lambda^2} - \frac{2\mu V_2 s}{\hbar^2\lambda^2\sqrt{V_1}} - \frac{4\mu E}{2\hbar^2\lambda^2}\right)\psi = 0. \tag{4.36}$$

Defining

$$\epsilon^2 = -\frac{\mu E}{2\hbar^2\lambda^2} \tag{4.37}$$

and

$$\gamma^2 = \frac{2\mu}{\hbar^2\lambda^2} \tag{4.38}$$

Eq. (4.36) becomes

$$\frac{d^2\psi}{ds^2} + \frac{1}{s}\frac{d\psi}{ds} - \frac{1}{s^2}(\gamma^2 s^2 - \gamma^2 a s + 4\epsilon^2)\psi = 0 \tag{4.39}$$

where $a = \frac{V_2}{\sqrt{V_1}}$. From Eq. (4.39), it is clear that

$$\sigma(s) = s \tag{4.40}$$

$$\tilde{\tau}(s) = 1 \tag{4.41}$$

$$\tilde{\sigma}(s) = -\gamma^2 s^2 + \gamma^2 a s - 4\epsilon^2 \tag{4.42}$$

By using the same procedure followed from Eq. (4.12) to Eq. (4.21) the energy eigenvalue and the wave function solutions [144] are are given as

$$E_n = -\frac{\lambda^2}{4}\left(2n + 1 - \frac{V_2}{\lambda\sqrt{V_1}}\right)^2 \tag{4.43}$$

and

$$\psi_n(s) = C_n s^{2\epsilon} e^{-\gamma s} L_n^{4\epsilon}(2\gamma s) \tag{4.44}$$

Here, both the energy eigenvalue and the wave function depend on the potential parameters λ, V_1 and V_2. $L_n^{4\epsilon}(2\gamma s)$ stands for associated Laguerre polynomials. The ground state wave function behaves as $\psi_0(s \to 0) \to 0$.

4.1.4 The Kratzer Potential

The modified Kratzer potential is given as [141]

$$V(r) = D_e\left(\frac{r - r_e}{r}\right)^2 \tag{4.45}$$

where D_e is the dissociation energy and r_e is the equilibrium internuclear separation. The radial part of the SE for a diatomic molecular potential is given as

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right)+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}+V(r)\right]R_{n,\ell}(r)=E_{n,\ell}R_{n,\ell}(r) \tag{4.46}$$

When Eq. (4.45) is substituted into Eq. (4.46) and by using the coordinate transformation

$$r=s \tag{4.47}$$

$$\frac{d^2R_{n,\ell}}{ds^2}+\frac{2}{s}\frac{dR_{n,\ell}(s)}{ds}+\frac{1}{s^2}(\epsilon^2 s^2-\beta s-\gamma)R_{n,\ell}(s)=0. \tag{4.48}$$

is obtained where

$$\epsilon^2=\frac{2\mu(E_{n,\ell}-D_e)}{\hbar^2} \tag{4.49}$$

$$\beta=-\frac{4\mu D_e r_e}{\hbar^2} \tag{4.50}$$

and

$$\gamma=\frac{2\mu}{\hbar^2}\left(D_e r_e^2+\frac{\ell(\ell+1)\hbar^2}{2\mu}\right) \tag{4.51}$$

When Eq. (4.48) is solved the energy eigenvalue becomes [141]

$$\epsilon^2=-\beta^2(2n+1+\sqrt{1+4\gamma})^{-2} \tag{4.52}$$

or

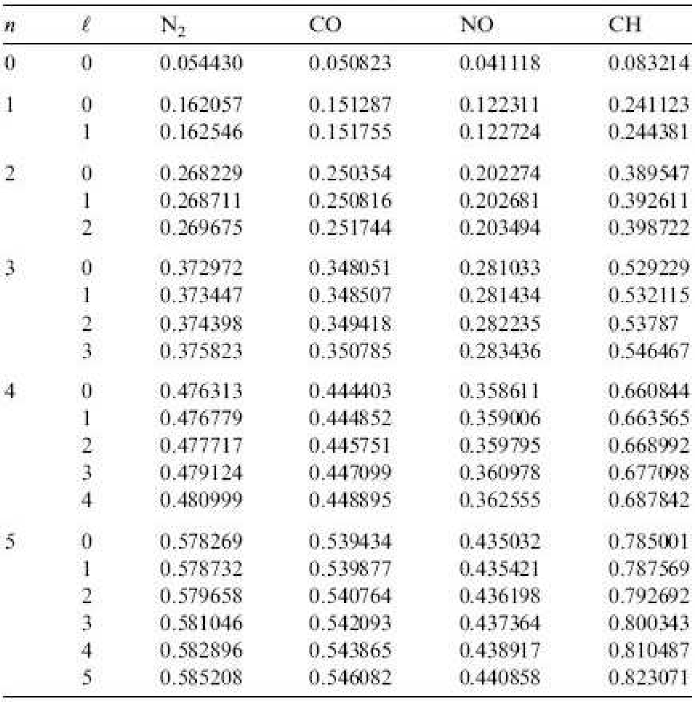
$$E_{n\ell}=D_e-\frac{\hbar^2}{2\mu}\left[\left(\frac{4\mu D_e r_e}{\hbar^2}\right)^2\left(2n+1+\sqrt{1+4\left(\frac{2\mu D_e r_e^2}{\hbar^2}+\ell(\ell+1)\right)}\right)^{-2}\right] \tag{4.53}$$

and the wave function is

$$R_{n,\ell}(r) = A_{n,\ell}\upsilon^{-\frac{1}{2}(1-\sqrt{1-4\gamma})}e^{-\frac{1}{2}(1-\sqrt{1-4\gamma})}L_n^{1+4\gamma}(\upsilon) \tag{4.54}$$

where

$$\upsilon(s) = 2i\epsilon s \tag{4.55}$$



n	ℓ	N_2	CO	NO	CH
0	0	0.054430	0.050823	0.041118	0.083214
1	0	0.162057	0.151287	0.122311	0.241123
	1	0.162546	0.151755	0.122724	0.244381
2	0	0.268229	0.250354	0.202274	0.389547
	1	0.268711	0.250816	0.202681	0.392611
	2	0.269675	0.251744	0.203494	0.398722
3	0	0.372972	0.348051	0.281033	0.529229
	1	0.373447	0.348507	0.281434	0.532115
	2	0.374398	0.349418	0.282235	0.53787
	3	0.375823	0.350785	0.283436	0.546467
4	0	0.476313	0.444403	0.358611	0.660844
	1	0.476779	0.444852	0.359006	0.663565
	2	0.477717	0.445751	0.359795	0.668992
	3	0.479124	0.447099	0.360978	0.677098
	4	0.480999	0.448895	0.362555	0.687842
5	0	0.578269	0.539434	0.435032	0.785001
	1	0.578732	0.539877	0.435421	0.787569
	2	0.579658	0.540764	0.436198	0.792692
	3	0.581046	0.542093	0.437364	0.800343
	4	0.582896	0.543865	0.438917	0.810487
	5	0.585208	0.546082	0.440858	0.823071

Figure 4.3: The energy eigenvalues of the Kratzer potential.

The computed energy eigenvalues for N_2, CO, NO and CH molecules with different values of n and ℓ in eV are given in Figure 4.3 [141] and the numerical calculations in Figure 4.3 are similar to the calculations given in [141].

4.2 Solution of the Schrödinger Equation with PDEM

In this next section, first the PDEM hamiltonian is introduced and then, the effective potential is defined with the sum of the physical potential and the sum of the ambiguity parameters. The Hamiltonian introduced at Eq. (2.9) is used and then the one-dimensional PDEM Hamiltonian becomes [139]

$$H_{eff} = -\frac{d}{dx}\left[\frac{1}{M(x)}\frac{d}{dx}\right] + V_{eff}(x) \tag{4.56}$$

where V_{eff}(x) is defined as

$$V_{eff}(x) = V(x) + \frac{1}{2}(\beta+1)\frac{M''}{M^2} - [\alpha(\alpha+\beta+1)+\beta+1]\frac{M'^2}{M^3} \tag{4.57}$$

where α and β are ambiguity parameters and $\gamma = 0$, $\hbar = 1$. The SE for the PDEM Hamiltonian given in Eq. (4.56) becomes:

$$\left(-\frac{1}{M}\frac{d^2}{dx^2} + \frac{M'}{M^2}\frac{d}{dx} + V_{eff} - E\right)\varphi(x) = 0. \tag{4.58}$$

4.2.1 The Deformed Hulthen Potential

The Hulthen potential is a short range potential which behaves like a Coulomb potential for small values of r and decreases exponentially for large values of r. The Hulthen potential is a special case of the Eckart potential which has been used in many different areas like nuclear, atomic, solid state and chemical physics and its bound-state and scattering properties have been investigated by a variety of techniques and the SE for this potential can be solved exactly for constant mass for $l \neq 0$ by applying a number of methods.

In this section, the general form of PDEM SE is obtained by using a more general transformation of the wave function as $\varphi = M^{\eta}(x)\psi(x)$. NUM is adapted to this general equation. Then, using an appropriate mass function, it is solved for the deformed Hulthen potential within this generalization. Energy eigenvalues and the corresponding wave functions are obtained. The one-dimensional PDEM Hamiltonian of the SE is written as Eq. (4.56) with effective potential V_{eff} in Eq. (4.57). Then the SE is obtained as Eq. (4.58). After making the transformation

$$\varphi(x) = M^{\eta}(x)\ \psi(x) \tag{4.59}$$

the SE takes the form

$$
\begin{aligned}
-\frac{d^2\psi}{dx^2} &- (2\eta-1)\frac{M^{'}}{M}\frac{d\psi}{dx} - [\eta(\eta-2)+\alpha(\alpha+\beta+1)+\beta+1]\left(\frac{M^{'}}{M}\right)^2\psi \\
&+ \left[\frac{1}{2}(\beta+1)-\eta\right]\frac{M^{''}}{M}\psi + M(V-E)\psi = 0 \qquad (4.60)
\end{aligned}
$$

The deformed Hulthen potential is given by [137]

$$
V(x) = -V_0\frac{e^{-\lambda x}}{1-qe^{-\lambda x}} \qquad (4.61)
$$

Here, V_0 is the compact form of the three parameters which are atomic number, screening parameter and the deformation parameter q which determine the range for the potential. The deformed Hulthen potential reduces to the general deformed Hulthen form for $q = 1$, to the standard Wood-Saxon potential for $q = -1$ and to the exponential potential for $q = 0$. The following parameters are introduced for Eq. (4.60):

$$
A = \alpha(\alpha+\beta+1)+\beta+1 \qquad (4.62)
$$

$M(x) = m_0 m(x)$, where m_0 has a mass unit and taken as $m_0 = 1$ where

$$
m(x) = (1-qe^{-\lambda x})^{-1} \qquad (4.63)
$$

$$
\frac{m^{'}}{m} = -q\lambda\frac{e^{-\lambda x}}{1-qe^{-\lambda x}} \qquad (4.64)
$$

$$
\frac{m^{''}}{m} = q\lambda^2 e^{-\lambda x}\frac{1+qe^{-\lambda x}}{(1-qe^{-\lambda x})^2} \qquad (4.65)
$$

and then the transformation

$$
s = \frac{1}{1-qe^{-\lambda x}} \qquad (4.66)
$$

is applied to Eq. (4.60) and if Eqs. (4.61)-(4.66) are substituted into Eq. (4.60), then it becomes

$$\left[\frac{d^2}{ds^2}+\frac{2\eta-(2\eta+1)s}{s(1-s)}\frac{d}{ds}+\frac{1}{s^2(1-s)^2}(-\xi_1 s^2+\xi_2 s-\xi_3)\right]\psi=0 \tag{4.67}$$

where

$$\begin{aligned} -\xi_1 &= [\eta(\eta-2)+A]-2\left[\frac{1}{2}(\beta+1)-\eta\right]+\frac{V_0}{q\lambda^2} && (4.68)\\ \xi_2 &= -2\left[\eta(\eta-2)+A\right]+3\left[\frac{1}{2}(\beta+1)-\eta\right]-\frac{V_0}{q\lambda^2}+\frac{E}{\lambda^2} && (4.69)\\ -\xi_3 &= \eta(\eta-2)+A-\left[\frac{1}{2}(\beta+1)-\eta\right] && (4.70)\end{aligned}$$

and $V(s)=\frac{V_0}{q}(1-s)$. Now, NUM is applied starting from its standard form as it is introduced in Eq. (2.15). When Eqs.(4.67) and (2.15) are compared

$$\begin{gathered}\sigma=s(1-s),\\ \tilde{\tau}(s)=2\eta-(2\eta+1)s,\\ \tilde{\sigma}(s)=-\xi_1 s^2+\xi_2 s-\xi_3\end{gathered} \tag{4.71}$$

are obtained. After applying the procedure explained from Eq.(2.16) and to Eq.(2.26) and using $z=\frac{1}{2}(1-2\eta)$, one obtains

$$\pi=z(1-s)\pm\left\{\begin{array}{ll}(\sqrt{\xi_1-\xi_2+\xi_3}-\sqrt{\xi_3+z^2})s+\sqrt{\xi_3+z^2} & k_1=\xi_2-2\xi_3+2\zeta;\\ (\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})s-\sqrt{\xi_3+z^2} & k_2=\xi_2-2\xi_3-2\zeta.\end{array}\right. \tag{4.72}$$

where $\zeta=\sqrt{\xi_3(\xi_1-\xi_2+\xi_3+z^2)-z^2(\xi_2-\xi_1)}$. Now, $\tau(s)$ can be introduced as,

$$\tau(s)=\left\{\begin{array}{l}1-2s+2((\sqrt{\xi_1-\xi_2+\xi_3}-\sqrt{\xi_3+z^2})s+\sqrt{\xi_3+z^2})\\ 1-2s-2((\sqrt{\xi_1-\xi_2+\xi_3}-\sqrt{\xi_3+z^2})s+\sqrt{\xi_3+z^2})\\ 1-2s+2((\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})s-\sqrt{\xi_3+z^2})\\ 1-2s-2((\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})s-\sqrt{\xi_3+z^2})\end{array}\right. \tag{4.73}$$

Derivative of $\tau(s)$ is obtained as

$$\tau^{'} = \begin{cases} -2+2(\sqrt{\xi_1-\xi_2+\xi_3}-\sqrt{\xi_3+z^2}) \\ -2-2(\sqrt{\xi_1-\xi_2+\xi_3}-\sqrt{\xi_3+z^2}) \\ -2+2(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2}) \\ -2-2(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2}) \end{cases} \tag{4.74}$$

Here, first derivative of τ should be $\tau^{'} < 0$ in order to obtain physical solutions. Thus, k and related functions are chosen which help to derive the energy eigenvalues and eigenfunctions:

$$\begin{aligned} k &= \xi_2-2\xi_3-2\sqrt{\xi_3(\xi_1-\xi_2+\xi_3+z^2)-z^2(\xi_2-\xi_1)} && (4.75) \\ \tau &= 1-2s-2[(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})s-\sqrt{\xi_3+z^2}] && (4.76) \\ \pi &= z(1-s)-[(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})s-\sqrt{\xi_3+z^2}] && (4.77) \\ \tau^{'} &= -2-2(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2}). && (4.78) \end{aligned}$$

Using Eq. (2.21), the relation given below

$$\lambda = z^2-z+\xi_1-(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})^2-(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2}) \tag{4.79}$$

is obtained. With the aid of Eq. (2.20), this equality can be written:

$$\lambda = \lambda_n = -n[-2-2(\sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2})]+n(n-1) \tag{4.80}$$

Substituting $\Lambda = \sqrt{\xi_1-\xi_2+\xi_3}+\sqrt{\xi_3+z^2}$, Λ can be written

$$\Lambda = \frac{1}{2}\left[-(2n+1)\pm\sqrt{1+4\gamma}\right] \tag{4.81}$$

where $\gamma = \xi_1+z(z-1)$. Now two cases can be considered with respect to the sign of Λ.

Case 1:

$$\sqrt{\xi_1 - \xi_2 + \xi_3} + \sqrt{\xi_3 + z^2} = \frac{1}{2}\left[-(2n+1) + \sqrt{1+4\gamma}\right] \tag{4.82}$$

then, ξ_3 is obtained as

$$\xi_3 = \left[\frac{\xi_2 - \xi_1 + z^2}{2n+1-\sqrt{1+4\gamma}} + \frac{1}{4}\left(2n+1-\sqrt{1+4\gamma}\right)\right]^2 \tag{4.83}$$

Using the definitions of ξ_1, ξ_2 and ξ_3, E_n is given by

$$E_n = -\frac{\lambda^2}{4}\left(2n+1-\sqrt{1+4\gamma} - 2\sqrt{-\eta(\eta-1) - A^* + \frac{\beta+1}{2}}\right)^2 - \lambda^2(\eta - \frac{1}{2})^2 \tag{4.84}$$

Case 2:

$$\sqrt{\xi_1 - \xi_2 + \xi_3} + \sqrt{\xi_3 + z^2} = \frac{1}{2}\left[-(2n+1) - \sqrt{1+4\gamma}\right] \tag{4.85}$$

then, ξ_3 becomes

$$\xi_3 = \left[\frac{\xi_2 - \xi_1 + z^2}{2n+1+\sqrt{1+4\gamma}} - \frac{1}{4}\left(2n+1+\sqrt{1+4\gamma}\right)\right]^2 \tag{4.86}$$

Energy eigenvalues can be written:

$$E_n = \frac{\lambda^2}{4}\left(2n+1+\sqrt{1+4\gamma} + 2\sqrt{-\eta(\eta-1) - A^* + \frac{\beta+1}{2}}\right)^2 - \lambda^2(\eta - \frac{1}{2})^2 \tag{4.87}$$

Using Eqs.(2.24) and (2.25), ϕ and ρ are obtained as

$$\phi = s^{z+\sqrt{\xi_3+z^2}}(1-s)^{\sqrt{\xi_1-\xi_2+\xi_3}} \tag{4.88}$$

and

$$\rho(s) = s^{2\sqrt{\xi_3+z^2}}(1-s)^{2\sqrt{\xi_1-\xi_2+\xi_3}} \tag{4.89}$$

Solution of y can be obtained from Eq. (2.23):

$$y_n(s) = P_n^{(2\sqrt{\xi_3+z^2},2\sqrt{\xi_1-\xi_2+\xi_3})}(1-2s) \tag{4.90}$$

Hence, the wave function has the following form:

$$\psi_n = s^{z+\sqrt{\xi_3+z^2}}(1-s)^{\sqrt{\xi_1-\xi_2+\xi_3}}P_n^{(2\sqrt{\xi_3+z^2},2\sqrt{\xi_1-\xi_2+\xi_3})}(1-2s) \tag{4.91}$$

If $z+\sqrt{\xi_3+z^2} < 0$ and $\sqrt{\xi_1-\xi_2+\xi_3} > 0$, it is required that $|z+\sqrt{\xi_3+z^2}| \geq \sqrt{\xi_1-\xi_2+\xi_3}$ and if $\sqrt{\xi_1-\xi_2+\xi_3} < 0$, $z+\sqrt{\xi_3+z^2} > 0$, $|\sqrt{\xi_1-\xi_2+\xi_3}| \geq z+\sqrt{\xi_3+z^2}$ for physical solutions.

4.2.2 The Morse Potential

Case I: $M(x) = \frac{m_0}{(1-\kappa e^{-\lambda x})^2}$

The Morse potential is solved by following two ways by reducing the PDEM solution to constant mass one. In the first way, the solution generally depends on the wave function transformation parameter η and the mass function parameters. The one-dimensional PDEM Hamiltonian of the SE is written as Eq. (4.56) with effective potential V_{eff} in Eq. (4.57). Then, the SE is obtained as Eq. (4.58). After making the transformation

$$\varphi(x) = M^{\eta}(x)\,\psi(x) \tag{4.92}$$

the SE takes the form

$$\begin{aligned}\frac{d^2\psi(x)}{dx^2} &+ (2\eta-1)\left(\frac{M'}{M}\right)\frac{d\psi(x)}{dx} + A_1\left(\frac{M'}{M}\right)^2\psi(x) \\ &- A_2\left(\frac{M''}{M}\right)\psi - M(V-E)\psi(x) = 0\end{aligned} \tag{4.93}$$

where

$$
\begin{aligned}
A_1 &= [\eta(\eta-2)+\alpha(\alpha+\beta+1)+\beta+1] \\
A_2 &= \left[\frac{1}{2}(\beta+1)-\eta\right]
\end{aligned}
\tag{4.94}
$$

with

$$
M(x) = m_0 m(x) \tag{4.95}
$$

and

$$
m(x) = \frac{1}{(1-\kappa e^{-\lambda x})^2} \tag{4.96}
$$

$\hbar$ and m_0 are taken equal to 1 and m_0 has a mass unit, where κ is a dimensionless parameter. The Morse potential is given as

$$
V(x) = V_0 e^{-2\lambda x} - V_1 e^{-\lambda x} \tag{4.97}
$$

When the transformation $s = e^{-\lambda x}$ is used to apply NUM with the necessary derivations of $m(x)$ in Eq. (4.93), it becomes

$$
\begin{aligned}
\psi''(s) &+ \left[\frac{1+(4\eta\kappa-3\kappa)}{s(1-\kappa s)}\right]\psi'(s) \\
&+ \left[\frac{(4A_1\kappa^2-4A_2\kappa^2-\frac{V_0}{\lambda^2})s^2+(\frac{V_1}{\lambda^2}-2A_2\kappa)s+\frac{E}{\lambda^2}}{[s(1-\kappa s)]^2}\right]\psi(s)=0
\end{aligned}
\tag{4.98}
$$

Eq. (4.98) is in the form of

$$
\left[\frac{d^2}{ds^2}+\frac{\alpha_1-\alpha_2 s}{s(1-\alpha_3 s)}\frac{d}{ds}+\frac{-\xi_1 s^2+\xi_2 s-\xi_3}{[s(1-\alpha_3 s)]^2}\right]\psi=0 \tag{4.99}
$$

When Eq. (4.99) is compared with Eq. (2.15)

$$
\tilde{\tau} = \alpha_1 - \alpha_2 s \tag{4.100}
$$

$$\sigma = s(1 - \alpha_3 s) \tag{4.101}$$

$$\tilde{\sigma} = -\xi_1 s^2 + \xi_2 s - \xi_3 \tag{4.102}$$

When Eqs. (4.100)-(4.102) are substituted into Eq. (2.22)

$$\pi(s) = \alpha_4 + \alpha_5 s \pm \sqrt{(\alpha_6 - k\alpha_3)s^2 + (\alpha_7 + k)s + \alpha_8} \tag{4.103}$$

where

$$\alpha_4 = \frac{1}{2}(1 - \alpha_1) \tag{4.104}$$

$$\alpha_5 = \frac{1}{2}(\alpha_2 - 2\alpha_3) \tag{4.105}$$

$$\alpha_6 = \alpha_5^2 + \xi_1 \tag{4.106}$$

$$\alpha_7 = 2\alpha_4\alpha_5 - \xi_2 \tag{4.107}$$

$$\alpha_8 = \alpha_4^2 + \xi_3 \tag{4.108}$$

In Eq. (4.103), the function under square root must be the square of a polynomial according to the NUM, so that

$$k_{1,2} = -(\alpha_7 + 2\alpha_3\alpha_8 \pm 2\sqrt{\alpha_8\alpha_9}). \tag{4.109}$$

Here,

$$\alpha_9 = \alpha_3\alpha_7 + \alpha_3^2\alpha_8 + \alpha_6 \tag{4.110}$$

For each k, the following π's are obtained. When

$$k = -(\alpha_7 + 2\alpha_3\alpha_8) - 2\sqrt{\alpha_8\alpha_9} \tag{4.111}$$

π becomes:

$$\pi = \alpha_4 + \alpha_5 s - [(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}] \tag{4.112}$$

For the same k, from Eq. (2.20), Eq. (4.100) and Eq. (4.112)

$$\tau = \alpha_1 + 2\alpha_4 - (\alpha_2 - 2\alpha_5)s - 2\left[(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}\right] \tag{4.113}$$

and

$$\begin{aligned} \tau' &= -(\alpha_2 - 2\alpha_5) - 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \\ &= -2\alpha_3 - 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \quad < 0 \end{aligned} \tag{4.114}$$

is obtained. When Eq. (2.21) is used with Eq. (4.111) and Eq. (4.112) the following equation is derived:

$$\begin{aligned} \alpha_2 n - (2n+1)\alpha_5 &+ (2n+1)(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) + n(n+1)\alpha_3 \\ &+ \alpha_7 + 2\alpha_3\alpha_8 + 2\sqrt{\alpha_8\alpha_9} = 0 \end{aligned} \tag{4.115}$$

This equation gives the energy spectrum of the problem. The wave function can be derived by using Eq. (2.23) as

$$\rho(s) = s^{\alpha_{10}-1}(1 - \alpha_3 s)^{\frac{\alpha_{11}}{\alpha_3} - \alpha_{10} - 1} \tag{4.116}$$

and when this equation is used in Eq. (2.16)

$$y_n = P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10} - 1)}(1 - 2\alpha_3 s) \tag{4.117}$$

is obtained, where

$$\alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8} \tag{4.118}$$

$$\alpha_{11} = \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \tag{4.119}$$

Using Eq. (2.25)

$$\phi(s) = s^{\alpha_{12}}(1-\alpha_3 s)^{-\alpha_{12}-\frac{\alpha_{13}}{\alpha_3}} \tag{4.120}$$

is obtained and as the general solution equation is

$$\psi = \phi(s)y(s) \tag{4.121}$$

it becomes

$$\psi = s^{\alpha_{12}}(1-\alpha_3 s)^{-\alpha_{12}-\frac{\alpha_{13}}{\alpha_3}} P_n^{(\alpha_{10}-1,\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3 s) \tag{4.122}$$

Here,

$$\alpha_{12} = \alpha_4 + \sqrt{\alpha_8} \tag{4.123}$$

$$\alpha_{13} = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \tag{4.124}$$

By using the definitions from Eq. (4.99) to Eq. (4.124) and the terms in Eq. (4.98), the corresponding ξ and α parameters can be listed as follows:

$$\begin{gathered}
\xi_1 = -\left(4A_1\kappa^2 - 4A_2\kappa^2 - \frac{V_0}{\lambda^2}\right) \\
\xi_2 = \left(\frac{V_1}{\lambda^2} - 2A_2\kappa\right) \\
\xi_3 = -\frac{E}{\lambda^2}
\end{gathered} \tag{4.125}$$

and

$$\alpha_1 = 1 \tag{4.126}$$

$$\alpha_2 = \kappa(3 - 4\eta) \tag{4.127}$$

$$\alpha_3 = \kappa \tag{4.128}$$

$$\begin{aligned}\alpha_4 &= \frac{1}{2}(1 - \alpha_1) \\ &= 0 \qquad (4.129)\end{aligned}$$

$$\begin{aligned}\alpha_5 &= \frac{1}{2}(\alpha_2 - 2\alpha_3) \\ &= \frac{\kappa}{2}(1 - 4\eta) \qquad (4.130)\end{aligned}$$

$$\begin{aligned}\alpha_6 &= \alpha_5^2 + \xi_1 \\ &= [\frac{\kappa}{2}(1 - 4\eta)]^2 + \xi_1 \qquad (4.131)\end{aligned}$$

$$\begin{aligned}\alpha_7 &= 2\alpha_4\alpha_5 - \xi_2 \\ &= -\xi_2 \qquad (4.132)\end{aligned}$$

$$\begin{aligned}\alpha_8 &= \alpha_4^2 + \xi_3 \\ &= -\frac{E}{\lambda^2} \qquad (4.133)\end{aligned}$$

$$\begin{aligned}\alpha_9 &= \alpha_3\alpha_7 + \alpha_3^2\alpha_8 + \alpha_6 \\ &= \xi_1 - \kappa\xi_2 - \frac{E}{\lambda^2}\kappa^2 + \left[\frac{\kappa}{2}(1 - 4\eta)\right]^2 \qquad (4.134)\end{aligned}$$

$$\begin{aligned}\alpha_{10} &= \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8} \\ &= 1 + 2\sqrt{-\frac{E}{\lambda^2}} \qquad (4.135)\end{aligned}$$

$$\begin{aligned}\alpha_{11} &= \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \\ &= 2\kappa \\ &+ 2\left(\sqrt{-\kappa\xi_2 - \frac{E}{\lambda^2}\kappa^2 + \left[-\frac{1}{2}(4\eta\kappa - \kappa)\right]^2 + \xi_1} + \kappa\sqrt{-\frac{E}{\lambda^2}}\right) \qquad (4.136)\end{aligned}$$

$$\begin{aligned}\alpha_{12} &= \alpha_4 + \sqrt{\alpha_8} \\ &= \sqrt{-\frac{E}{\lambda^2}} \\ &= \sqrt{\xi_3} \qquad (4.137)\end{aligned}$$

$$\begin{aligned}\alpha_{13} &= \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \\ &= \left[\frac{1}{2}(-4\eta\kappa + \kappa)\right] \\ &- \left(\sqrt{-\kappa\xi_2 - \frac{E}{\lambda^2}\kappa^2 + \left[-\frac{1}{2}(4\eta\kappa - \kappa)\right]^2 + \xi_1} + \kappa\sqrt{-\frac{E}{\lambda^2}}\right) \qquad (4.138)\end{aligned}$$

The substitution of the related parameters into Eq. (4.115), the energy eigenvalue can be written as

$$E_n = -\lambda^2\left[\frac{\frac{1}{4}(2n+1)^2\kappa + \xi_2 + (-2\eta + \frac{3}{4})\kappa - (2n+1)\sqrt{(2\eta-1)^2\kappa^2 + \xi_1}}{-(2n+1)\kappa + 2\sqrt{(2n-1)^2\kappa^2 + \xi_1}}\right]^2 \qquad (4.139)$$

and the wave function can be written from Eq. (4.122) as

$$\begin{aligned}\psi(s) = {} & s^{\sqrt{\xi_3}}(1-\kappa s)^{-\sqrt{\xi_3}-\frac{1}{\kappa}\left[\frac{1}{2}(-4\eta\kappa+\kappa)-(\sqrt{\xi_1-\kappa\xi_2+\kappa^2\xi_3+\frac{1}{4}(1-4\eta)^2\kappa^2}+\kappa\sqrt{\xi_3})\right]} \\ & P_n^{\left[2\xi_3,\frac{2}{\kappa}-\left[\kappa+\sqrt{\xi_1-\kappa\xi_2+\frac{1}{4}(1-4\eta)^2\kappa^2}+\kappa\sqrt{\xi_3}\right]-2\sqrt{\xi_3}\right]}(1-2\kappa s)\end{aligned} \tag{4.140}$$

Here, both the wave function and the energy eigenvalue depend on the mass and potential function parameters. One can choose a suitable η for the wave function transformation and this changes the solution parameter. These solutions can be reduced to constant mass form by choosing $\kappa \to 0$, i.e. the energy eigenvalue becomes

$$E_n = -\frac{\lambda^2}{4}\left(2n+1-\frac{V_1}{\lambda\sqrt{V_0}}\right)^2 \tag{4.141}$$

The above energy eigenvalue equation is identical with the solution obtained for the constant mass case.

Case II: $M(x) = m_0 e^{-2\lambda x}$

In the second way, the PDEM problem for the Morse potential is again reduced to its constant mass solutions with a different approach. First, the SE in Eq. (4.58) is introduced with the effective potential Eq. (4.57). Then, the transformation in Eq. (4.59) is applied to Eq. (4.58) and this gives Eq. (4.60). The Morse potential is defined as

$$V(x) = V_0 e^{2\lambda x} - V_1 e^{\lambda x} \tag{4.142}$$

and the mass function is defined as $M(x) = m_0 m(x)$ and m_0 has a mass unit and taken as equal to 1 with

$$m(x) = e^{-2\lambda x} \tag{4.143}$$

When Eq. (4.142) and Eq. (4.143) are substituted into Eq. (4.60)

$$\begin{aligned} & - \quad \psi'' - 2\lambda(2\eta-1)\psi' - 4\eta\lambda^2(\eta-1)\psi \\ & + \quad \left[V_0 - V_1 e^{-\lambda x} - E e^{-2\lambda x} + 2(\beta+1)\lambda^2 - 4A^*\lambda^2\right]\psi = 0 \end{aligned} \tag{4.144}$$

is obtained. The transformation $s = e^{-\lambda x}$ in Eq. (4.144) leads to

$$\begin{aligned} & \frac{d^2\psi}{ds^2} + \frac{3-4\eta}{s}\frac{d\psi}{ds} \\ + \quad & \frac{1}{s^2}\left[\frac{E}{\lambda^2}s^2 + \frac{V_1}{\lambda^2}s - \frac{V_0}{\lambda^2} - 2(\beta+1) + 4A^* + 4\eta(\eta-1)\right]\psi = 0 \end{aligned} \tag{4.145}$$

where $A^* = \alpha(\alpha+\beta+1)+\beta+1$. The parameters of the coefficient of ψ in Eq. (4.145) can be defined as

$$\begin{aligned} \xi_1 &= -\frac{E}{\lambda^2} \\ \xi_2 &= -\frac{V_1}{\lambda^2} \\ -\xi_3 &= \frac{V_0}{\lambda^2} + 2(\beta+1) - 4A^* - 4\eta(\eta-1) \end{aligned} \tag{4.146}$$

Then, Eq. (4.145) turns to be

$$\frac{d^2\psi}{ds^2} + \frac{3-4\eta}{s}\frac{d\psi}{ds} - \frac{\xi_1 s^2 + \xi_2 s - \xi_3}{s^2}\psi = 0 \tag{4.147}$$

Eq. (4.147) is the transformed PDEM equation for the Morse potential. Now, if $\eta = 1/2$ and if this equation is compared with the constant mass form of the Morse potential in Eq. (4.39) it is seen that

$$\begin{aligned} \xi_1 &= \gamma^2 \\ \xi_2 &= -\frac{V_2}{\sqrt{V_1}}\gamma^2 \\ \xi_3 &= -4\epsilon^2 \end{aligned} \tag{4.148}$$

Thus, the solution of the PDEM equation Eq. (4.147) is straightforward. The constant mass energy eigenvalue and the wave function solutions are given in Eq. (4.43) and

Eq. (4.44), respectively. The PDEM solutions can be found by substituting the ξ_1 and ξ_3 into Eq. (4.43) and Eq. (4.44) where γ and ϵ are seen. The method is summarized in Figure 4.4.

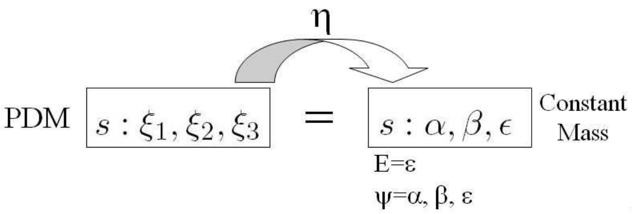


Figure 4.4: The solution of PDEM problem by using constant mass results.

4.2.3 The Pseudoharmonic Potential

The SE with constant mass for pseudoharmonic potential in s transformed form is already given in Eq. (4.29). Now, if $\eta = \frac{3}{8}$ is set and then, when this equation is compared with Eq. (4.147) the equal parameters can be listed as

$$\begin{aligned} \xi_1 &= \alpha^2 \\ \xi_2 &= -\epsilon \\ \xi_3 &= -\beta \end{aligned} \tag{4.149}$$

The solution of Eq. (4.29) for the energy eigenvalue and the wave function is given in Eq. (4.30) and Eq. (4.32), respectively. Thus, the solution of the PDEM problem of pseudoharmonic potential can easily be found by substituting the parameters in Eq. (4.149) to Eq. (4.30) and Eq. (4.32).

4.2.4 The Mie Potential

The SE with constant mass for the Mie potential in s transformed form is already given in Eq. (4.8). Now, if $\eta = \frac{1}{4}$ is set and then, when this equation is compared with Eq. (4.147) the equal parameters can be listed as

$$\begin{aligned}\xi_1 &= -\epsilon^2 \\ \xi_2 &= \beta \\ \xi_3 &= -\gamma\end{aligned} \tag{4.150}$$

where ϵ, β and γ are already defined in Eq. (4.5), Eq. (4.6) and Eq. (4.7), respectively. The constant mass wave function of the Mie potential is given in Eq. (4.20). The PDEM wave function solution of the Mie potential can be obtained by substituting ϵ, β and γ parameters in terms of ξ_1, ξ_2 and ξ_3 where they are introduced in Eq. (4.146).

4.2.5 The Kratzer Potential

The SE with constant mass for the Kratzer potential in s transformed form is already given in Eq. (4.48). Now, if $\eta = \frac{1}{4}$ is set and then, when this equation is compared with Eq. (4.147) the equal parameters can be listed as

$$\begin{aligned}\xi_1 &= -\epsilon^2 \\ \xi_2 &= \beta \\ \xi_3 &= -\gamma\end{aligned} \tag{4.151}$$

where the ϵ, β and γ parameters are defined in Eq. (4.49), Eq. (4.50) and Eq. (4.51), respectively. Then it is clear that the PDEM energy eigenvalue and the wave function solution of the Kratzer potential can easily be determined by substituting to the constant mass solutions defined in Eq. (4.52) and Eq. (4.54).

CHAPTER 5

CONCLUSION

In this thesis, the one dimensional PDEM problem is studied by solving the SE for some well known potentials, such as the deformed Hulthen, the Mie, the Kratzer, the pseudoharmonic, and the Morse potentials. The Nikiforov-Uvarov method is used in the calculations to get energy eigenvalues and the corresponding wave functions exactly. By introducing a free parameter in the transformation of the wave function, the PDEM is reduced to the solution of the SE for the constant mass case. At the same time, the deformed Hulthen potential is solved for the PDEM case by applying the method directly. The Morse potential is also solved for a mass distribution function, such that the solution can be reduced to the constant mass case.

Two different ways are followed for the determination of PDEM problem solutions. In the first way, the SE with PDEM for the deformed Hulthen potential is solved. The Hamiltonian introduced by von Roos [15] is used with the ambiguity parameters α, β, γ. Various numerical combinations for these three parameters are tried in the literature. However, in this study these three constants are used in closed form. A coordinate transformation with a mass term having a power of η is applied to the SE. In the solution of the deformed Hulthen potential, this power factor is also used in closed form. The arbitrary choice of the variable mass function and s transformation for NUM are dependent on the exponential form of the potential to make the calculations easier. The NUM is applied for the first time in the solution of the PDEM SE with the deformed Hulthen potential in this study [145]. In the second way, the solutions of the SE with PDEM are reduced to constant mass solutions for the Mie, the Kratzer, the Morse and the pseudoharmonic potentials with the appropriate choice of η in the coordinate transformation, so that the PDEM equation similar to the constant mass solution in NU form. For the Morse potential η is equal to $1/2$, for the pseudoharmonic potential it is $3/8$ and for the Mie potential it is $1/4$. In the constant mass case, first, the Mie potential is studied in one dimension and the analytical solution of the SE for the Mie potential is obtained. By using a special case of Mie potential $l = 2k$ and $k = 1$ is selected. The energy eigenvalues and the corresponding eigenfunctions are obtained by NUM. This is the first application of NUM for the solution of the Mie potential [140]. Similarly, the pseudoharmonic, the Morse and the Kratzer potentials are solved. The numerical values of the energy eigenvalues for N_2, CO, NO and CH diatomic molecules with different values of principal and angular quantum numbers n and ℓ, respectively are computed in eV and presented for the Mie, the pseudoharmonic and the Kratzer potentials. The Morse potential has exact solution of the SE for angular quantum number $l = 0$. However, one needs to make some approximations to the SE to have analytical solutions for $l \neq 0$ cases. In this study, the SE is solved for $l = 0$ case and by using NUM, the exact solutions of the SE are obtained. The obtained energy eigenvalue not only has a real spectrum as the other potentials mentioned before, but also it is dependent on the potential parameters V_1 and V_2. Moreover, in the special case for $\lambda = 1$, $E_n = -(A - n)^2$ is obtained.

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FOREIGN LANGUAGES

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PUBLICATIONS

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4. R. Sever, C. Tezcan, O. Yesiltas, M. Bucurgat. "Exact Solution of Effective Mass Schrödinger Equation for the Hulthen Potential" (published online: 17 January 2008)