11

Application of the Nikiforov-Uvarov Method in Quantum Mechanics

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1. Introduction

This book chapter is addressed to readers who want to learn how to solve the time-independent Schrödinger equation (Schrödinger, 1926) in an alternative method that was introduced by A. F. Nikiforov and V. B. Uvarov (Nikiforov & Uvarov, 1988). The requirement for understanding the chapter is a knowledge of quantum mechanics in an introductory level and partial differential equations. The primary of the chapter is intended for undergraduate students in physics and chemistry however, it may be used as a reference guide for graduate students and researchers as well.

The solution of the Schrödinger equation for a physical system in quantum mechanics is of great importance, because the knowledge of wavefunction $\Psi(\mathbf{r},t)$ and energy E contains all possible information about the physical properties of a system. This knowledge is ranging from the energy, momentum and coordinate of the particle to the wave characteristics of the particle, frequency and wavelength if we describe the quantum mechanical system by the probability amplitude $|\Psi(\mathbf{r},t)|^2$ and its phase (Tang, 2005). $\Psi(\mathbf{r},t)$ is supposed to describe the "state" of a particle subject to the potential energy function $V(\mathbf{r})$, where $\mathbf{r}$ represents the spatial position of the particle. For a one-particle, one-dimensional system in cartesian coordinates, we have $\Psi(\mathbf{r},t) = \Psi(x,t)$ and $V(\mathbf{r}) = V(x)$ or for a one-particle, three-dimensional system in spherical coordinates, we have $\Psi(\mathbf{r},t) = \Psi(r,\theta,\phi,t)$ and $V(\mathbf{r}) = V(r,\theta,\phi)$. If we want to know how the state of the particle changes with time, we need to specify the future state, $\Psi(\mathbf{r},t)$, of a quantum mechanical system from the knowledge of its initial state, $\Psi(\mathbf{r},t=0)$. To do that an equation postulated by the Austrian physicist Erwin Schrödinger (1887-1961) can help us

$$-\frac{\hbar}{i}\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t), \tag{1}$$

where the constant $\hbar$ is defined as $\hbar \equiv h/2\pi$, μ is the mass of particle and ∇^2 is an operator that can be described in any coordinate system. Eq.(1) is known as the time-dependent Schrödinger equation and it can be reduced to the time-independent one using an appropriate wavefunction $\Psi(\mathbf{r},t) = e^{-iEt/\hbar}\Psi(\mathbf{r})$ that corresponds to states of constant E. For the states of the form $\Psi(\mathbf{r},t) = e^{-iEt/\hbar}\Psi(\mathbf{r})$, the probability density $|\Psi(\mathbf{r},t)|^2$ is given by $|\Psi(\mathbf{r})|^2$ and it does

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not change with time. So, we can now call the states by the "stationary state" that would be concerned mostly with states of constant energy (Levine, 2008). If we insert this wavefunction into Eq.(1), we have an equation called the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{2}$$

For simplicity, we will refer to Eq.(2) as the Schrödinger equation (SE). The solution of the SE not only depends on the potential energy function $V(\mathbf{r})$ but also depends on the coordinate system. Although many quantum mechanical system can be solved by writing the one-particle, one-dimensional SE in cartesian coordinates, we will pay our attention to the one-particle, three-dimensional SE in spherical coordinates. Therefore, in this book chapter, we will deal with any one-particle problem with a spherically symmetric potential energy function $V(r)$, where we suppose that $V(r)$ just depends on the radial variable, r, of spherical coordinates, i.e., $V(\mathbf{r}) = V(r,\theta,\phi) \equiv V(r)$. Moreover, the stationary-state wavefunction $\Psi(\mathbf{r})$ would be of the form $\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$, in which $R(r)$ is the unknown radial wavefunction and $Y(\theta,\phi)$ are referred to as the spherical harmonics.

The solution of the SE is an interesting issue in many fields of physics and chemistry. To obtain an accurate solution of the SE is only possible for a few potentials such as harmonic oscillator potential, Coulomb potential, Kratzer potential, etc. For these potentials, one can try to solve the SE for the unknown radial wavefunction $R(r)$ and hence implicitly provide all relevant information about the behavior of a particle. The standard analytical method for solving such an equation with a variable coefficient is to expand the solution in a power series of the independent variable r and then find the recursion relationships for all the expansion coefficients (Flügge, 1971). However, the power series method has more details to reach the solution. The algebraic methods based on Lie algebra (Adams, 1994; Iachello & Levine, 1995; Iachello & Oss, 1996; Iachello & Ibrahim, 1998) are another tool to solve the SE in the framework of quantum mechanics. To constitute a suitable Lie algebra, the quantum system we are trying to find an exact solution has to be displayed a dynamical symmetry. If it is so, the ladder operators of the quantum system for some potentials are constructed by the factorization method or the supersymmetric quantum mechanics approach. The advantage of the factorization method is that the energy spectrum and the wavefunction of a quantum system are obtained algebraically if the SE is factorizable (Frank & Isacker, 1994; Infeld & Hull, 1951).

The solution of the SE is fundamental to understand the energy spectrum of a particle since the early days of quantum mechanics (Flügge, 1971). It often happens in some quantum mechanical problems that the solution of the SE with the potential $V(r)$ is not known accurately (for example, when considering the motion of a particle subject to the Morse potential together with the centrifugal term $\ell(\ell+1)/r$ coming from the radial part of the SE in spherical coordinate). Therefore, in such cases, there is no need for an exact solution of the SE, and we must look for efficient approximate methods for its solution. From this point of view, if the SE is exactly solvable for a given potential, the wavefunction will be able to describe such a system completely, otherwise an approximated solution will be nearly describe the system. Numerical and analytical methods are complementary to find an exact or approximate solution of the SE with/without the centrifugal term $\ell(\ell+1)/r$ for a particle in the potential $V(r)$, and each would be much poorer without the other. However, simple "hand-power methods" namely analytical methods are often more revealing because we will see the solution stages of the problem and so it would be more meaningful than the numerical solution.

An alternative method to solve the SE by the "hand-power" is to use the Nikiforov-Uvarov (NU) method which can be described in terms of the hypergeometric-type second-order differential equations. The method based on the solutions of the general second order linear differential equation with special orthogonal functions (Szego, 1934) provides an exact solution of the SE for certain kind of potentials. The NU method is able to apply the solution of the SE in a more direct, easy and elegant way as well as the methods given in the standard textbooks.

By using the main equation given by Eq.(2), the SE can be solved by separating it in spherical coordinates for a single particle of mass μ. After separating the SE, the eigenvalue equations are solved by using the NU method and the energy levels of the discrete spectrum are obtained for a single particle. In spherical coordinates, the SE is written as follows:

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\}\Psi(r,\theta,\phi)$$
$$+V(\mathbf{r})\Psi(r,\theta,\phi)=E\Psi(r,\theta,\phi). \tag{3}$$

The energy E in Eq.(3) is real and it is either discrete for bound states ($E < 0$) or continuous for scattering states ($E > 0$). Consequently, this equation is separable for several potential such as Harmonic oscillator, Coulomb potential, Kratzer potential, Morse potential, Hulthen potential and so on. It is expected that an interesting extension of this book chapter would be to study the solution of the SE for a given potential.

This book chapter is organized as follows: in Section 2, we reviewed the NU method in detail and at the end of this section we introduced a "guide" like a "cooking list" that will show us a faster way, how to apply the NU to the solution of the SE. Section 3 is devoted to the separable variables of the SE in spherical coordinates. Application of the NU method in quantum mechanics is presented in Section 4 and so the solution of the SE for the selected potentials, i.e., Harmonic oscillator potential, Coulomb potential, Kratzer potential, Morse potential and Hulthen potential, is obtained in the same section. Finally, a few concluding remarks are given in Section 5.

2. The Nikiforov-Uvarov method

The Nikiforov-Uvarov (NU) method is based on solving the hypergeometric-type second-order differential equations by means of the special orthogonal functions (Szego, 1934). For a given potential, the Schrödinger or the Schrödinger-like equations in spherical coordinates are reduced to a generalized equation of hypergeometric-type with an appropriate coordinate transformation $r \to s$ and then they can be solved systematically to find the exact or particular solutions. The main equation which is closely associated with the method is given in the following form (Nikiforov & Uvarov, 1988)

$$\psi''(s)+\frac{\widetilde{\tau}(s)}{\sigma(s)}\psi'(s)+\frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi(s)=0, \tag{4}$$

where $\sigma(s)$ and $\widetilde{\sigma}(s)$ are polynomials at most second-degree, $\widetilde{\tau}(s)$ is a first-degree polynomial and $\psi(s)$ is a function of the hypergeometric-type.

By taking $\psi(s) = \phi(s)y(s)$ and choosing an appropriate function $\phi(s)$, Eq.(4) is reduced to a comprehensible form;

$$y''(s) + \left(2\frac{\phi'(s)}{\phi(s)} + \frac{\widetilde{\tau}(s)}{\sigma(s)}\right)y'(s) + \left(\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)}\frac{\widetilde{\tau}(s)}{\sigma(s)} + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\right)y(s) = 0. \tag{5}$$

The coefficient of $y'(s)$ is taken in the form $\tau(s)/\sigma(s)$, where $\tau(s)$ is a polynomial of degree at most one, i.e.,

$$2\frac{\phi'(s)}{\phi(s)} + \frac{\widetilde{\tau}(s)}{\sigma(s)} = \frac{\tau(s)}{\sigma(s)}, \tag{6}$$

and hence the most regular form is obtained as follows,

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \tag{7}$$

where

$$\pi(s) = \frac{1}{2}[\tau(s) - \widetilde{\tau}(s)]. \tag{8}$$

The most useful demonstration of Eq.(8) is

$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s). \tag{9}$$

The new parameter $\pi(s)$ is a polynomial of degree at most one. In addition, the term $\phi''(s)/\phi(s)$ which appears in the coefficient of $y(s)$ in Eq.(5) is arranged as follows

$$\frac{\phi''(s)}{\phi(s)} = \left(\frac{\phi'(s)}{\phi(s)}\right)' + \left(\frac{\phi'(s)}{\phi(s)}\right)^2 = \left(\frac{\pi(s)}{\sigma(s)}\right)' + \left(\frac{\pi(s)}{\sigma(s)}\right)^2. \tag{10}$$

In this case, the coefficient of $y(s)$ is transformed into a more suitable form by taking the equality given in Eq.(7);

$$\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)}\frac{\widetilde{\tau}(s)}{\sigma(s)} + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)} = \frac{\bar{\sigma}(s)}{\sigma^2(s)} \tag{11}$$

where

$$\bar{\sigma}(s) = \widetilde{\sigma}(s) + \pi^2(s) + \pi(s)[\widetilde{\tau}(s) - \sigma'(s)] + \pi'(s)\sigma(s). \tag{12}$$

Substituting the right-hand sides of Eq.(6) and Eq.(11) into Eq.(5), an equation of hypergeometric-type is obtained as follows

$$y''(s) + \frac{\tau(s)}{\sigma(s)}y'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}y(s) = 0. \tag{13}$$

As a consequence of the algebraic transformations mentioned above, the functional form of Eq.(4) is protected in a systematic way. If the polynomial $\bar{\sigma}(s)$ in Eq.(13) is divisible by $\sigma(s)$, i.e.,

$$\bar{\sigma}(s) = \lambda\sigma(s), \tag{14}$$

where λ is a constant, Eq.(13) is reduced to an equation of hypergeometric-type

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \tag{15}$$

and so its solution is given as a function of hypergeometric-type. To determine the polynomial $\pi(s)$, Eq.(12) is compared with Eq.(14) and then a quadratic equation for $\pi(s)$ is obtained as follows,

$$\pi^2(s) + \pi(s)[\widetilde{\tau}(s) - \sigma'(s)] + \widetilde{\sigma}(s) - k\sigma(s) = 0, \tag{16}$$

where

$$k = \lambda - \pi'(s). \tag{17}$$

The solution of this quadratic equation for $\pi(s)$ yields the following equality

$$\pi(s) = \frac{\sigma'(s) - \widetilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \widetilde{\tau}(s)}{2}\right)^2 - \widetilde{\sigma}(s) + k\sigma(s)}. \tag{18}$$

In order to obtain the possible solutions according to the plus and minus signs of Eq.(18), the parameter k within the square root sign must be known explicitly. To provide this requirement, the expression under the square root sign has to be the square of a polynomial, since $\pi(s)$ is a polynomial of degree at most one. In this case, an equation of the quadratic form is available for the constant k. Setting the discriminant of this quadratic equal to zero, the constant k is determined clearly. After determining k, the polynomial $\pi(s)$ is obtained from Eq.(18), and then $\tau(s)$ and λ are also obtained by using Eq.(8) and Eq.(17), respectively.

A common trend that has been followed to generalize the solutions of Eq.(15) is to show that all the derivatives of hypergeometric-type functions are also of the hypergeometric-type. For this purpose, Eq.(15) is differentiated by using the representation $v_1(s) = y'(s)$

$$\sigma(s)v_1''(s) + \tau_1(s)v_1'(s) + \mu_1 v_1(s) = 0, \tag{19}$$

where $\tau_1(s) = \tau(s) + \sigma'(s)$ and $\mu_1 = \lambda + \tau'(s)$. $\tau_1(s)$ is a polynomial of degree at most one and μ_1 is a parameter that is independent of the variable s. It is clear that Eq.(19) is an equation of hypergeometric-type. By taking $v_2(s) = y''(s)$ as a new representation, the second derivative of Eq.(15) becomes

$$\sigma(s)v_2''(s) + \tau_2(s)v_2'(s) + \mu_2 v_2(s) = 0, \tag{20}$$

where

$$\tau_2(s) = \tau_1(s) + \sigma'(s) = \tau(s) + 2\sigma'(s), \tag{21}$$

$$\mu_2 = \mu_1 + \tau_1'(s) = \lambda + 2\tau'(s) + \sigma''(s). \tag{22}$$

In a similar way, an equation of hypergeometric-type can be constructed as a family of particular solutions of Eq.(15) by taking $v_n(s) = y^{(n)}(s)$;

$$\sigma(s)v_n''(s) + \tau_n(s)v_n'(s) + \mu_n v_n(s) = 0, \tag{23}$$

and here the general recurrence relations for $\tau_n(s)$ and μ_n are found as follows, respectively,

$$\tau_n(s) = \tau(s) + n\sigma'(s), \tag{24}$$

$$\mu_n = \lambda + n\tau'(s) + \frac{n(n-1)}{2}\sigma''(s). \tag{25}$$

When $\mu_n = 0$, Eq.(25) becomes as follows

$$\lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad (n = 0, 1, 2, \ldots) \tag{26}$$

and then Eq.(23) has a particular solution of the form $y(s) = y_n(s)$ which is a polynomial of degree n. To obtain an eigenvalue solution through the NU method, the relationship between λ and λ_n must be set up by means of Eq.(17) and Eq.(26). $y_n(s)$ is the hypergeometric-type function whose polynomial solutions are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[\sigma^n(s)\rho(s)\right], \tag{27}$$

where B_n is a normalization constant and the weight function ρ(s) must satisfy the condition below

$$(\sigma(s)\rho(s))' = \tau(s)\rho(s). \tag{28}$$

It could be facilitative to introduce a "guide" to figure out the solution of SE in a faster way. To obtain the unknown radial wavefunction $R(r)$ and the energy eigenvalue E of the SE by means of the NU method, let us look at the following guide in the ten-steps;
1) reduce the differential equation that satisfies the SE into the differential equation given in Eq.(4),
2) compare each equations and determine the values of polynomials $\widetilde{\tau}(s)$, $\sigma(s)$ and $\widetilde{\sigma}(s)$. In this stage, don't forget to make some abbreviations in the original differential equation,
3) arrange the polynomial $\pi(s)$ given in Eq.(18) by inserting the polynomials $\widetilde{\tau}(s)$, $\sigma(s)$ and $\widetilde{\sigma}(s)$ we have found in the second stage and compose an equation of quadratic form under the square root sign of the $\pi(s)$,
4) set up the discriminant of this quadratic equal to zero, using the expression $\triangle = b^2 - 4ac = 0$ and find two roots regarding with the k, i.e., $k_\pm$,
5) substitute these values of k into the $\pi(s)$ and obtain the four possible forms of $\pi(s)$. Now we have two forms of the $\pi(s)$ for k_+ and two forms for k_-. At this stage one can ask a question which of the four forms is physically valid.
6) try to find a negative derivative of the $\tau(s)$ given in Eq.(9) using the four forms of the $\pi(s)$ and keep this form to use it in the further stages because that would be physically valid.
7) recall Eq.(17) for λ and Eq.(26) for λ_n, and compare them with each other, i.e., $\lambda = \lambda_n$, and so it would be energy spectrum.
8) insert the values of $\sigma(s)$ and $\pi(s)$ into Eq.(7), so the result would be the functional form of $\phi(s)$,
9) satisfy Eq.(28) with the weight function $\rho(s)$ and obtain the hypergeometric-type function $y_n(s)$ which can be given by the Rodrigues relation in Eq.(27),
10) combine the $\phi(s)$ and the $y_n(s)$ to form the $\psi(s)$, and so it would be the radial wavefunction $R(r)$.

3. The Schrödinger equation in spherical coordinates

Many of the potentials that are used together with the SE are the central potentials and they are just the function of a distance between a particle and some point of origin. In spherical coordinates, a point in space is defined in terms of its distance r from the origin of the coordinate system and in terms of two angles, zenith angle θ and azimuthal angle ϕ. Therefore, we can specify a single point of three-dimensional space using these triplets (r, θ, ϕ). In order to define a unique set of spherical coordinates for each point, we have to restrict their ranges. A common choice is $r \geq 0$, $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. At this section, one could ask a question about why we need to take into account the spherical coordinate to solve the SE for a particle subject to a potential function. For the realistic potentials in physics, as an answer, the SE in spherical coordinates can be solved by using the separation of the wavefunction in terms of independent wavefunctions, i.e., $\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. The motion of a rotating molecule or of an electron moving around an atomic nucleus could be better described in spherical coordinates by using only a single coordinate. For example, the Coulomb potential that represents the electromagnetic interaction between an electron and a proton can be written $V(x,y,z) = -e'^2/\sqrt{x^2+y^2+z^2}$ in cartesian coordinate, where $e' = e/\sqrt{4\pi\varepsilon_0}$, e is the elementary electric charge and ε_0 is the electric permittivity of free space. It might not straightforward to solve the SE with the potential $V(x,y,z)$ because the potential has there variables which are not separable in cartesian coordinate even if the wavefunction became separable. Transformation to spherical coordinates from cartesian one would be easier to solve the SE because in this case the potential $V(x,y,z)$ would be turned to $V(r) = -e'^2/r$ which depends only on r. For this transformation, we used the conversion $r = \sqrt{x^2+y^2+z^2}$. Further, the variables (x,y,z) in cartesian coordinate could be related to the variables (r,θ,ϕ) in spherical coordinates as follows;

$$x = rsin\theta cos\phi, \quad y = rsin\theta sin\phi, \quad z = rcos\theta, \quad \theta = cos^{-1}\left(\frac{z}{r}\right). \quad \phi = tan^{-1}\left(\frac{y}{x}\right). \tag{29}$$

Now let us look at the separable variables in spherical coordinates. Keeping in mind the SE given in Eq.(2), we will use the relation of ∇^2 in spherical coordinates as we develop the SE in the same coordinate. So, the SE may be written as

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)+V(r)\right]\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi), \tag{30}$$

where the ∇^2 is given in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{31}$$

The potential we are interesting is central because it only depends on the distance r from the origin and we look for separable solution of the SE;

$$\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi). \tag{32}$$

Using the assumed form of $\Psi(r,\theta,\phi)$, we may write the SE as

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\frac{2\mu}{\hbar^2}r^2(E-V(r)) = -\frac{1}{Y(\theta,\phi)}\left[\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial Y(\theta,\phi)}{\partial\theta}\right)+\frac{1}{sin^2\theta}\frac{\partial^2 Y(\theta,\phi)}{\partial\phi^2}\right]. \tag{33}$$

The two sides of this equation depend on different variables and so they can equal each other only if they are equal to a constant L. Therefore, the following two equations have to be true simultaneously

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\left[\frac{2\mu}{\hbar^2}(E-V(r))-\frac{L}{r^2}\right]R(r) = 0, \tag{34}$$

$$\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial Y(\theta,\phi)}{\partial\theta}\right)+\frac{1}{sin^2\theta}\frac{\partial^2 Y(\theta,\phi)}{\partial\phi^2}+LY(\theta,\phi) = 0. \tag{35}$$

Now, we have two different equations and we can deal with each separately because only radial variables come into Eq.(34) and only angular variables come into Eq.(35). The solution of the angular part given in Eq.(35) is straightforward because this part hasn‘t a potential or an energy term and so we can again attempt the method of separation of variables by assuming that the angular function $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$. It should be noted that Eq.(35) is separable by inserting $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$. $\Theta(\theta)$ and $\Phi(\phi)$ satisfy the differential equations as follows

$$\frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta(\theta)}{d\theta}\right)+\left(L-\frac{m^2}{sin^2\theta}\right)\Theta(\theta)=0, \tag{36}$$

$$\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2}=-m^2. \tag{37}$$

We definitely know that someone can solve these equations easily. There is no need for us to "reinvent the wheel" here. Therefore we will not give general solutions of these equations but we will just mention about their results that are related with the L and m, and discuss their physical significance. Based on the physically acceptable solution of the equation that depends on the variable ϕ, we can say that the separable constant m must be a positive or negative integer, i.e., $m = 0, \pm 1, \pm 2, ...$ The constant m is also known the magnetic quantum number. If we return to the more difficult equation that depends on the variable θ, we can rewrite Eq.(36) by a change of variables $\omega = cos\theta$. The equation with the function $\Theta(\theta)$ becomes

$$\frac{d}{d\omega}\left[(1-\omega^2)\frac{dP(\omega)}{d\omega}\right]+\left(L-\frac{m^2}{1-\omega^2}\right)P(\omega)=0, \tag{38}$$

where $P(\omega)$ is the Legendre polynomial. Generally Eq.(38) has two independent solutions that became infinite for $\omega = \pm 1$. However, the wavefunctions that satisfy the boundary conditions in Eq.(38) are finite and single-valued everywhere spatially because we are studying the bound-state solutions of the SE. Nevertheless, if the constant L is of the form

$$L=\ell(\ell+1), \tag{39}$$

where the ℓ is introduced as the orbital quantum number and the values of ℓ are equal to;

$$\ell=0,1,2,3,.... \tag{40}$$

For these values of ℓ, one of the solutions can be finite for all values of ω. In the definition of the associate Legendre function, the magnitude of the magnetic quantum number m must be limited to values less than or equal to ℓ because the Legendre polynomials are polynomials of order ℓ;

$$\mid m \mid = 0,1,2,3,... \leq \ell. \tag{41}$$

On the other hand, there are $(2\ell+1)$ allowed values for m, i.e., $-\ell \leqslant m \leqslant \ell$. Substituting $L = \ell(\ell+1)$ into Eq.(34) shows that the radial wavefunction $R(r)$ and the eigenvalue E of the SE depend on the quantum number ℓ and satisfy the equation;

$$\frac{d^2R(r)}{dr^2}+\frac{2}{r}\frac{dR(r)}{dr}+\frac{2\mu}{\hbar^2}\left[E-V(r)-\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]R(r)=0, \tag{42}$$

This equation can be figured an ordinary differential equation with variable coefficient and can be solved by the standard methods which have been already given in quantum mechanics text books (Flügge, 1971). However, the analytical solution of Eq.(42) would be definitely depended on the potential function $V(r)$.

4. Application of the Nikiforov-Uvarov method

4.1 Harmonic oscillator potential

The harmonic motion of a physical system means that it oscillates around a mean value at one or more characteristic frequencies. Such a system describes the motion of a bound particle in a potential well that increases quadratically with the distance from the minimum of the potential well. For example, pulling a particle subject to the end of a spring from its equilibrium position results in a contrary force pushing back toward the equilibrium position. Letting the particle go back from a position of tension results in a harmonic motion of the particle, so the particle is now a harmonic oscillator. As such, the harmonic oscillator is a model for many physical systems whose natural motions are described by the harmonic oscillator equation, such as the vibrational motion of molecules, acoustic vibration of solid, electromagnetic waves, etc.

The conventional way to deal with the harmonic oscillator problem is to obtain the energy eigenvalues and eigenfunctions of the Hamiltonian by solving the SE given in the form of Eq.(42). Now we will consider the solution of the SE for the three dimensional harmonic oscillator in spherical coordinates. Thus, in three dimensions and spherical coordinates, the SE is written as follows,

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 r^2 - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]R(r) = 0. \tag{43}$$

where $V(r) = \frac{1}{2}\mu\omega^2 r^2$ is the harmonic oscillator potential and ω is the angular frequency of the oscillator. The method used for solving such a differential equation with a variable coefficient is to expend the solution in a power series of the independent variable r and then find the recursion relationship for all the expansion coefficient. However, this method has been already applied to the solution of Eq.(43) in the past and the solution are well known after so many solution step. "Please don‘t panic"; because we don‘t need to barge into the power series solution of this equation. We will follow a pretty well organized method that is termed the NU method.

Let us apply the NU method to solve Eq.(43). To begin the solution we have to get an equivalent equation with the equation given in Eq.(4) that is a key introduction to the NU method (see (Büyükkilic et al., 1997), for a more detailed solution and explanations). It could be written an unknown radial function $R(r) = U(r)/r$ to reduce Eq.(43) into Eq.(4). The radial equation becomes

$$\frac{d^2U(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 r^2 - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]U(r) = 0, \tag{44}$$

where we used the derivatives

$$\frac{dR(r)}{dr} = \frac{1}{r}\frac{dU(r)}{dr} - \frac{U(r)}{r^2}, \quad r^2\frac{dR(r)}{dr} = r\frac{dU(r)}{dr} - U(r), \quad \frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) = r\frac{d^2U(r)}{dr^2}. \tag{45}$$

To make this more manageable mathematically, it would be convenient to introduce dimensionless variables

$$r = \alpha\zeta, \quad \alpha = \sqrt{\frac{hbar}{\mu\omega}}, \quad \epsilon = \frac{E}{\hbar\omega}, \tag{46}$$

and to use the following derivatives

$$\frac{d}{dr} = \frac{d\zeta}{dr}\frac{d}{d\zeta}, \qquad \frac{d^2}{dr^2} = \frac{1}{\alpha^2}\frac{d^2}{d\zeta^2}. \tag{47}$$

Putting these into Eq.(44), we have

$$\frac{d^2U(\zeta)}{d\zeta^2} + \left(2\epsilon - \frac{\ell(\ell+1)}{\zeta^2} - \zeta^2\right)U(\zeta) = 0. \tag{48}$$

By performing transformations $\zeta^2 = s$ and $U(\zeta) \to \psi(s)$ in Eq.(48), we can rewrite it in terms of s and so we can get an equation that would be comparable with Eq.(4);

$$\frac{d^2\psi(s)}{ds^2} + \frac{1}{2s}\frac{d\psi(s)}{ds} + \frac{(-s^2 + \beta^2 s - \ell(\ell+1))}{4s^2}\psi(s) = 0, \tag{49}$$

where the variable s is in the range of $0 \leq s \leq \infty$. Furthermore we used the derivative and definition, respectively;

$$\frac{d^2U(\zeta)}{d\zeta^2} = 4s\frac{d^2\psi(s)}{ds^2} + 2\frac{d\psi(s)}{ds}, \tag{50}$$

$$\beta^2 = 2\epsilon. \tag{51}$$

A comparison of Eq.(49) with Eq.(4) identifies the relevant polynomials as follows

$$\widetilde{\tau} = 1, \quad \sigma(s) = 2s, \quad \widetilde{\sigma} = -s^2 + \beta^2 s - \ell(\ell+1)). \tag{52}$$

Inserting the polynomials given by Eq.(52) into Eq.(18) gives the polynomial $\pi(s)$:

$$\pi(s) = \frac{1}{2} \pm \sqrt{s^2 + (2k - \beta^2)s + \ell(\ell+1) + 1/4}. \tag{53}$$

The equation of quadratic form under the square root sign of Eq.(53) must be solved by setting the discriminant of this quadratic equal to zero, i.e., $\triangle = b^2 - 4ac = 0$. This discriminant gives a new quadratic equation which can be solved for the constant k to obtain the two roots;

$$\triangle = (2k - \beta^2)^2 - 4\left(\ell(\ell+1) + \frac{1}{4}\right) = 0, \tag{54}$$

$$k^2 - k\beta^2 + \frac{\beta^4}{4} - \left(\ell(\ell+1) + \frac{1}{4}\right) = 0, \tag{55}$$

$$k_{\pm} = \frac{\beta^2 \pm \sqrt{1 + 4\ell(\ell+1)}}{2}. \tag{56}$$

When the two values of k given in Eq.(56) are substituted into Eq.(53), the four possible forms of $\pi(s)$ are obtained as

$$\pi(s) = \frac{1}{2} \pm \begin{cases} s + \frac{\sqrt{1+4\ell(\ell+1)}}{2}, & \text{for} \quad k_{+} = \frac{\beta^2 + \sqrt{1+4\ell(\ell+1)}}{2} \\ s - \frac{\sqrt{1+4\ell(\ell+1)}}{2}, & \text{for} \quad k_{-} = \frac{\beta^2 - \sqrt{1+4\ell(\ell+1)}}{2}. \end{cases} \tag{57}$$

One of the four values of the polynomial $\pi(s)$ is just proper to obtain the bound-state solution because $\tau(s)$ given by Eq.(9) has a zero and a negative derivative for this value of $\pi(s)$ in the interval $(0, \infty)$ (Büyükkilic et al., 1997). Therefore, the most suitable expression of $\pi(s)$ is chosen as

$$\pi(s) = \frac{1}{2} - s + \frac{\sqrt{1+4\ell(\ell+1)}}{2}, \tag{58}$$

for $k_- = \left(\beta^2 - \sqrt{1+4\ell(\ell+1)}\right)/2$. By using $\pi(s)$ given in Eq.(53) and remembering $\widetilde{\tau} = 1$, we can obtain the expression $\tau(s) = \widetilde{\tau} + 2\pi(s)$ that is introduced in Eq.(9),

$$\tau(s) = 2 + \sqrt{1+4\ell(\ell+1)} - 2s, \tag{59}$$

and the derivative of this expression would be negative, i.e., $\tau'(s) = -2 < 0$, where $\tau'(s)$ represents the derivative of $\tau(s)$. The expressions $\lambda = k_- + \pi'(s)$ in Eq.(17) and $\lambda_n = -n\tau'(s) - n(n-1)\sigma''(s)/2$ in Eq.(26) are obtained as follows

$$\lambda = \frac{\beta^2 - \sqrt{1+4\ell(\ell+1)}}{2} - 1, \tag{60}$$

$$\lambda_n = 2n. \tag{61}$$

When we compare these expressions, $\lambda = \lambda_n$, we can obtain the energy of the harmonic oscillator,

$$\frac{\beta^2 - \sqrt{1+4\ell(\ell+1)}}{2} - 1 = 2n, \tag{62}$$

$$\frac{E}{\hbar\omega} = 2n + \ell + \frac{3}{2}, \tag{63}$$

$$E = \left(2n + \ell + \frac{3}{2}\right)\hbar\omega, \tag{64}$$

recalling $\beta^2 = 2\epsilon = 2E/\hbar\omega$. Here n is the number of nodes of the radial wave functions and if we define $n_p = 2n + \ell$ as the principal quantum number, Eq.(25) is written as

$$E_{n_p} = \left(n_p + \frac{3}{2}\right)\hbar\omega, \tag{65}$$

where $n_p = 0, 1, 2, 3, ...$ We inserted the quantum number n_p into Eq.(26) because the harmonic oscillator's energy is usually described by the single quantum number, i.e., $n_p \equiv 2n + \ell$. n is a non-negative integer, for every even n we have $\ell = 0, 2, ..., n-2, n$ and for every odd n we have $\ell = 1, 3, ..., n-2, n$. So for every n and ℓ there are $2\ell + 1$ different quantum states, labeled by m that is an integer satisfying $-\ell \leq m \leq \ell$. Thus, the degeneracy at level n is $\sum_{\ell=...,n-2,n}(2\ell+1) = \frac{(n+1)(n+2)}{2}$, where the sum starts from 0 or 1, according to whether n is even or odd.

Let us turn to the calculation of the wavefunction $\psi(s)$. If we remember the definition of the $\psi(s)$ that is given in Section 2, i.e., $\psi(s) = \phi(s)y_n(s)$, we can see that we have to calculate the polynomials $\phi(s)$ and $y_n(s)$. By inserting the values of $\sigma(s)$ and $\pi(s)$ given in Eq.(52) and Eq.(53) into Eq.(7), one can find the first part of the $\psi(s)$ as

$$\frac{\phi'(s)}{\phi(s)} = \frac{d\phi(s)}{d(s)}\frac{1}{\phi(s)} = \frac{\left(1 + \sqrt{1+4\ell(\ell+1)}\right)/2 - s}{2s}, \tag{66}$$

$$\frac{d\phi(s)}{d(s)}\frac{1}{\phi(s)} = \frac{\delta_1}{s} - \frac{1}{2}, \tag{67}$$

$$\int \frac{d\phi(s)}{\phi(s)} = \int \left(\frac{\delta_1}{s} - \frac{1}{2}\right) ds, \tag{68}$$

$$log\phi(s) = \delta_1 logs - s/2, \tag{69}$$

$$\phi(s) = s^{\delta_1} e^{-s/2}, \tag{70}$$

where $\delta_1 = \left(1 + \sqrt{1 + 4\ell(\ell+1)}\right)/4 = (\ell+1)/2$. On the other hand, to find a solution for $y_n(s)$ we should first obtain the weight function $\rho(s)$ which is already inserted into Eq.(28). The weight function $\rho(s)$ given in Eq.(28) can be written in a simple form and obtained as

$$\frac{d\rho(s)}{d(s)}\frac{1}{\rho(s)} = \frac{\tau(s) - \sigma'(s)}{\sigma(s)} = \frac{2 + \sqrt{1 + 4\ell(\ell+1)} - 2s - 2}{2s}, \tag{71}$$

$$\frac{d\rho(s)}{d(s)}\frac{1}{\rho(s)} = \frac{\sqrt{1 + 4\ell(\ell+1)}/2}{s} - 1, \tag{72}$$

$$\int \frac{d\rho(s)}{\rho(s)} = \int \left(\frac{\delta_2}{s} - 1\right) ds, \tag{73}$$

$$log\rho(s) = \delta_2 logs - s, \tag{74}$$

$$\rho(s) = s^{\delta_2} e^{-s}, \tag{75}$$

where $\delta_2 = \sqrt{1 + 4\ell(\ell+1)}/2 = \ell + 1/2$. Substituting $\rho(s)$ into Eq.(27) allows us to obtain the polynomial $y_n(s)$ as follows

$$y_n(s) = B_n 2^n e^s s^{\delta_2} \frac{d^n}{ds^n}\left(e^{-s} s^{n+\delta_2}\right). \tag{76}$$

If we recall the Rodrigues' formula of the associated Laguerre polynomials

$$L_n^{\delta_2}(s) = \frac{1}{n!} e^s s^{\delta_2} \frac{d^n}{ds^n}\left(e^{-s} s^{n+\delta_2}\right), \tag{77}$$

Eq.(76) and Eq.(77) will yield $y_n(s) \equiv L_n^{\delta_2}(s)$, where $1/n! = B_n 2^n$. By using $\psi(s) = \phi(s) y_n(s)$, we have

$$\psi(s) = N_{n\ell} s^{\delta_1} e^{-s/2} L_n^{\delta_2}(s). \tag{78}$$

where $N_{n\ell}$ is a normalization constant. It would be useful to keep in mind that the relationship between the $\psi(s)$ and the $R(r)$ is $\psi(s) \equiv rR(r)$ with the transformations $r = \alpha\zeta$ and $\zeta^2 = s$.

4.2 Coulomb potential

As another illustration of the application of the NU method, we will take up the Coulomb potential which concerns an electron of charge $-e$ moving in the Coulomb electrostatic field of the nucleus. If nucleus is proton of positive charge e, the problem studied is that of the hydrogen atom that is a real physical system in three dimensions. So, the hydrogen atom consists of an electron moving in a spherical potential well due to the Coulomb attraction of the proton. This two-particle system (electron and proton) can be converted into a one-particle system by considering the motion of the electron relative to that of the proton in the center-of-mass frame of the two particles according to the principles of classical mechanics. In this frame, we can replace the electron of mass by a particle of reduced mass μ moving relatively to a proton. If we have a system which consist of one electron and a nucleus of charge Ze, Z being the atomic number, we can consider a slightly more general problem, known as a hydrogen-like atom. For $Z = 1$, we have hydrogen atom; for $Z = 2$, the He$^+$ ion; for $Z = 3$, the Li$^+$ ion and so on. This means that the hydrogen-like atom would be an ionized atom. The potential energy $V(r)$ of the electron due to the Coulomb attraction of the nucleus is

$$V(r) = -\frac{Ze'^2}{r} \tag{79}$$

where $e' = e/\sqrt{4\pi\varepsilon_0}$. The corresponding SE for the Coulomb potential given in Eq.(79) satisfy

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E + \frac{Ze'^2}{r} - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]R(r) = 0. \tag{80}$$

To save time in writing, we define the constants as follows

$$a = \hbar^2/\mu e'^2 = 4\pi\varepsilon_0\hbar^2/\mu e^2 \tag{81}$$

and so Eq.(80) becomes

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left[\frac{2E}{ae'^2} + \frac{2Z}{ar} - \frac{\ell(\ell+1)}{r^2}\right]R(r) = 0. \tag{82}$$

Now let us explicitly solve for the problem of the hydrogen-like atom using the NU method. To make our mathematics comparable with Eq.(4), we choice a function in the form of $R(r) \equiv \psi(s)$, where the transformation $r \to s$ is valid. With this choice we obtain the convenient simplification of the radial equation given in Eq.(82);

$$\frac{d^2\psi(s)}{ds^2} + \frac{2}{s}\frac{d\psi(s)}{ds} + \frac{1}{s^2}\left[-\alpha s^2 + \beta s - \gamma\right]\psi(s) = 0. \tag{83}$$

where the reduced quantities are given as

$$\alpha = -2E/ae'^2, \quad \beta = 2Z/a, \quad \gamma = \ell(\ell+1). \tag{84}$$

We restrict ourselves to bound states of negative energy E. This means that the parameter α is positive. Eq.(83) is now comparable with Eq.(4) and then the following expressions are obtained;

$$\widetilde{\tau} = 2, \quad \sigma(s) = s, \quad \widetilde{\sigma} = -\alpha s^2 + \beta s - \gamma. \tag{85}$$

We are able to find four possible solutions of the polynomial $\pi(s)$ as follows. To do that we insert the polynomials given by Eq.(85) into Eq.(18) and hence the polynomial $\pi(s)$ is obtained in terms of k;

$$\pi(s) = -\frac{1}{2} \pm \frac{1}{2}\sqrt{4\alpha s^2 + (k-\beta)s + 1 + 4\gamma}. \tag{86}$$

The equation of quadratic form under the square root sign of Eq.(86) must be solved by setting the discriminant of this quadratic equal to zero, i.e., $\triangle = b^2 - 4ac = 0$. This discriminant gives a new quadratic equation which can be solved for the constant k to obtain the two roots;

$$\triangle = 16(k-\beta)^2 - 16\alpha\,(1+4\gamma) = 0, \tag{87}$$

$$k^2 - 2k\beta + \beta^2 - \alpha\,(1+4\gamma) = 0, \tag{88}$$

$$k_\pm = \beta \pm \sqrt{\alpha(1+4\gamma)}. \tag{89}$$

When the two values of k given in Eq.(89) are substituted into Eq.(86), the four possible forms of $\pi(s)$ are obtained as

$$\pi(s) = -\frac{1}{2} \pm \frac{1}{2} \begin{cases} \left(2\sqrt{\alpha}s + \sqrt{1+4\gamma}\right), & \text{for} \quad k_+ = \beta + \sqrt{\alpha(1+4\gamma)} \\ \left(2\sqrt{\alpha}s - \sqrt{1+4\gamma}\right), & \text{for} \quad k_- = \beta - \sqrt{\alpha(1+4\gamma)}. \end{cases} \tag{90}$$

In order to make the derivative of the polynomial $\tau(s)$ to be negative, we must select the most suitable form of the polynomial $\pi(s)$. Therefore, the most suitable expression of $\pi(s)$ is chosen as

$$\pi(s) = -\frac{1}{2} - \frac{1}{2}\left(2\sqrt{\alpha}s - \sqrt{1+4\gamma}\right) \tag{91}$$

for $k_- = \beta - \sqrt{\alpha(1+4\gamma)}$. By using $\pi(s)$ given in Eq.(91) and remembering $\widetilde{\tau} = 2$, we can obtain the expression $\tau(s)$,

$$\tau(s) = 1 + \sqrt{1+4\gamma} - 2\sqrt{\alpha}s, \tag{92}$$

and the derivative of this expression would be negative, i.e., $\tau'(s) = -2\sqrt{\alpha} < 0$. The expressions $\lambda = k_- + \pi'(s)$ in Eq.(17) and $\lambda_n = -n\tau'(s) - n(n-1)\sigma''(s)/2$ in Eq.(26) are obtained as follows

$$\lambda = \beta - \sqrt{\alpha(1+4\gamma)} - \sqrt{\alpha}, \tag{93}$$

$$\lambda_n = 2n\sqrt{\alpha}, \tag{94}$$

When we compare these expressions, $\lambda = \lambda_n$, we can obtain the energy of the hydrogen-like atom,

$$\beta - \sqrt{\alpha(1+4\gamma)} - \sqrt{\alpha} = 2n\sqrt{\alpha}, \tag{95}$$

$$\sqrt{\alpha}\left(1 + 2n + \sqrt{1+4\gamma}\right) = \beta, \tag{96}$$

$$\alpha = \frac{\beta^2}{\left(1+2n+\sqrt{1+4\gamma}\right)^2}, \tag{97}$$

$$-\frac{2E}{ae'^2} = \frac{(2Z/a)^2}{\left(1+2n+\sqrt{1+4\ell(\ell+1)}\right)^2}, \tag{98}$$

$$E = -\frac{Z^2\mu e'^4}{2\hbar^2(1+n+\ell)^2}, \tag{99}$$

recalling the quantities given in Eq.(84). Here n $(n = 0, 1, 2, 3, ...)$ and ℓ are integers and we now define a new integer n_p, called the principle quantum number, by

$$n_p \equiv n + \ell + 1, \quad n_p = 1, 2, 3, ... \tag{100}$$

The quantum number ℓ must satisfy $\ell \leq n_p - 1$ and hence it ranges from 0 to $n_p - 1$. So Eq.(99) becomes

$$E_{n_p} = -\frac{Z^2\mu e'^4}{2n_p^2\hbar^2}, \tag{101}$$

This expression represents the bound-state energy levels of the hydrogen-like atom, and the levels are discrete.

Let us now find the corresponding eigenfunctions for the radial equation. The polynomial solution of the hypergeometric-type function $y_n(s)$ depends on the determination of the weight function $\rho(s)$. Thus, using equation Eq.(7), we obtain

$$\frac{\phi'(s)}{\phi(s)} = \frac{d\phi(s)}{d(s)}\frac{1}{\phi(s)} = \frac{-\frac{1}{2} - \frac{1}{2}(2\sqrt{\alpha}s - \sqrt{1+4\gamma})}{s}, \tag{102}$$

$$\frac{d\phi(s)}{d(s)}\frac{1}{\phi(s)} = \frac{-1+\sqrt{1+4\gamma}}{2s} - \sqrt{\alpha}, \tag{103}$$

$$\int \frac{d\phi(s)}{\phi(s)} = \int \left(\frac{-1+\sqrt{1+4\gamma}}{2s} - \sqrt{\alpha}\right) ds, \tag{104}$$

$$log\phi(s) = \frac{-1+\sqrt{1+4\gamma}}{2} logs - \sqrt{\alpha}s, \tag{105}$$

$$\phi(s) = s^{\frac{-1+\sqrt{1+4\gamma}}{2}} e^{-\sqrt{\alpha}s}, \tag{106}$$

$$\phi(s) = s^{\ell} e^{-\sqrt{\alpha}s}. \tag{107}$$

where $\sqrt{1+4\gamma} = \sqrt{1+4\ell(\ell+1)} = 2(\ell+1/2)$ and $\sqrt{\alpha} = Z\mu e'^2/\hbar^2 n_p$. On the other hand, to find a solution for $y_n(s)$ we should first obtain the weight function $\rho(s)$ which is already inserted into Eq.(28). The weight function $\rho(s)$ given in Eq.(28) can be written in a simple form and obtained as

$$\frac{d\rho(s)}{d(s)}\frac{1}{\rho(s)} = \frac{\tau(s) - \sigma'(s)}{\sigma(s)} = \frac{1+\sqrt{1+4\gamma} - 2\sqrt{\alpha}s - 1}{s}, \tag{108}$$

$$\frac{d\rho(s)}{d(s)}\frac{1}{\rho(s)} = \frac{\sqrt{1+4\gamma}}{s} - 2\sqrt{\alpha}, \tag{109}$$

$$\int \frac{d\rho(s)}{\rho(s)} = \int \left(\frac{\sqrt{1+4\gamma}}{s} - 2\sqrt{\alpha}\right) ds, \tag{110}$$

$$log\rho(s) = \sqrt{1+4\gamma} logs - 2\sqrt{\alpha}s, \tag{111}$$

$$\rho(s) = s^{\sqrt{1+4\gamma}} e^{-2\sqrt{\alpha}s}. \tag{112}$$

Substituting $\rho(s)$ into Eq.(27) allows us to obtain the polynomial $y_n(s)$ as follows

$$y_n(s) = B_n e^{2\sqrt{\alpha}s} s^{-\sqrt{1+4\gamma}} \frac{d^n}{ds^n}\left(e^{-2\sqrt{\alpha}s} s^{n+\sqrt{1+4\gamma}}\right). \tag{113}$$

It is shown from the Rodrigues' formula of the associated Laguerre polynomials

$$L_n^{2\ell+1}(2\sqrt{\alpha}s) = \frac{1}{n!} e^{2\sqrt{\alpha}s} s^{-(2\ell+1)} \frac{d^n}{ds^n}\left(e^{-2\sqrt{\alpha}s} s^{n+2\ell+1}\right) \tag{114}$$

where $1/n! = B_n$. Eq.(76) and Eq.(77) yield $y_n(s) \equiv L_n^{2\ell+1}(2\sqrt{\alpha}s)$. By using $\psi(s) = \phi(s)y_n(s)$, we have

$$\psi(s) = N_{n\ell} s^{\ell} e^{-\sqrt{\alpha}s} L_n^{2\ell+1}(2\sqrt{\alpha}s). \tag{115}$$

where $N_{n\ell}$ is a normalization constant and the $\psi(s)$ represents the radial wavefunction $R(r)$ through the transformation $s \to r$.

4.3 Kratzer potential

The Kratzer potential (Kratzer, 1920), which was named in B. Adolf Kratzer's honor, is one of the widely used potential models in molecular physics and chemistry. The model potential means that we can describe molecular structures and interactions by using analytical and computational methods. These methods which are used in the fields of computational and materials science have been developing for studying molecular systems ranging from small molecules (or a set of interacting molecules like clusters) to large material assemblies. However, the advancing of studies not only depends on the super-computers in modern-day science but also needs computational methods such as *ab initio* and semi-empirical methods which present complementary advantages (Herzberg, 1950).

The simplest calculations can be performed by hand, but inevitably computers are required to perform molecular modelling of any reasonably sized system. The common feature of molecular modeling techniques is the atomistic level description of the molecular systems; the lowest level of information is individual atoms (or a small group of atoms). This is in contrast to quantum chemistry (also known as electronic structure calculations) where electrons are considered explicitly. The benefit of molecular modeling is that it reduces the complexity of the system, allowing many more particles (atoms) to be considered during simulations.

Supposed that we have a model potential that is known in the form of the Kratzer potential as follows

$$V(r) = A - \frac{B}{r} + \frac{C}{r^2}, \tag{116}$$

where the parameters A, B and C are constants which are related with the Kratzer potential. If we set up the constants A and C to zero, i.e., $A = 0$ and $C = 0$, Eq.(116) can be presented in the form of Coulomb potential $V(r) = -Ze'^2/r^2$, where $B = Ze'^2$ and $e' = e/\sqrt{4\pi\varepsilon_0}$. The solution of the Coulomb potential in the framework of the SE is already given in the previous subsection. So it could be said that the Coulomb potential is a special form of the so-called Kratzer potential. If we re-arrange the potential's parameters $A = D_e$, $B = 2D_e r_e$ and $C = D_e r_e^2$, Eq.(116) turns to the modified Kratzer potential, i.e., $V(r) = D_e\left((r-r_e)/r\right)^2$ Berkdemir et al (2006). The dissociation energy, D_e, is the vertical distance between the dissociation limit and the minimum point of the potential curve, which is found at the equilibrium inter-atomic separation $r = r_e$. If the potential curve flattens out at the large inter-atomic distance, i.e, $r \to \infty$, it is named the dissociation limit. At this limit the potential curve converges to zero, i.e., $V(\infty) = 0$. So the dissociation energy is defined $V(r_e) - V(\infty) = -D_e$. It would be meaningful to explain the word "modified". It is not "amazing" to include the "modified" into the Kratzer potential because the modified Kratzer potential represents the Kratzer-Fues potential setting up $A = 0$, i.e., $V(r) = D_e\left[((r-r_e)/r)^2 - 1\right]$, which is shifted in amount of D_e (Fues, 1926; Pliva, 1999).

Let us try to solve the SE with the potential given by Eq.(116). Substitution of the potential $V(r) = A - B/r + C/r^2$ into Eq.(42) allows us to write down the SE;

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left(E - \left[A - \frac{B}{r} + \frac{C}{r^2}\right] - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)R(r) = 0. \tag{117}$$

In order to make further arrangements, we can rewrite the above equation as follows;

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{1}{r^2}\left[\frac{2\mu(E-A)}{\hbar^2}r^2 + \frac{2\mu B}{\hbar^2}r - \left(\frac{2\mu C}{\hbar^2} + \ell(\ell+1)\right)\right]R(r) = 0. \tag{118}$$

For the sake of simplicity, it is convenient to introduce arbitrary parameters;

$$\begin{aligned} \alpha &= -\frac{2\mu(E-A)}{\hbar^2}, \\ \beta &= \frac{2\mu B}{\hbar^2}, \\ \gamma &= \frac{2\mu C}{\hbar^2} + \ell(\ell+1), \end{aligned} \tag{119}$$

with $\alpha > 0$ means that we are dealing with the bound state energy solutions, assuming $|E| < A$, $\beta > 0$ and $\gamma > 0$. In particular, from Eqs. (118) and (119) it follows:

$$\frac{d^2\psi(s)}{ds^2} + \frac{2}{s}\frac{d\psi(s)}{ds} + \frac{1}{s^2}\left(-\alpha s^2 + \beta s - \gamma\right)\psi(s) = 0, \tag{120}$$

which is expressed in terms of the functional $R(r) \equiv \psi(s)$ and the variable $r \to s$. In order to apply the NU method, it is necessary to compare Eq.(120) with the differential equation given in Eq.(4). A simple comparison reveals that the relevant polynomials $\widetilde{\tau}(s)$, $\sigma(s)$ and $\widetilde{\sigma}(s)$ are the same with Eq.(85), i.e.;

$$\begin{aligned} \widetilde{\tau} &= 2, \\ \sigma(s) &= s, \\ \widetilde{\sigma} &= -\alpha s^2 + \beta s - \gamma. \end{aligned} \tag{121}$$

This means that we don't need further calculations up to Eq.(97). Let us recall Eq.(97) for the bound state energy solution,

$$\alpha = \frac{\beta^2}{\left(1 + 2n + \sqrt{1+4\gamma}\right)^2}, \tag{122}$$

and keeping the values of arbitrary parameters α, β and γ given by Eq.(119) in our mind,

$$-\frac{2\mu(E-A)}{\hbar^2} = \frac{\left(\frac{2\mu B}{\hbar^2}\right)^2}{\left(1 + 2n + \sqrt{1 + 4\left(\frac{2\mu C}{\hbar^2} + \ell(\ell+1)\right)}\right)^2}, \tag{123}$$

$$E = A - \frac{\hbar^2}{2\mu}\left[\left(\frac{2\mu B}{\hbar^2}\right)^2 \left(1 + 2n + \sqrt{1 + 4\left(\frac{2\mu C}{\hbar^2} + \ell(\ell+1)\right)}\right)^{-2}\right], \tag{124}$$

$$E = A - \frac{\frac{\mu B^2}{2\hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{2\mu C}{\hbar^2} + \left(\ell + \frac{1}{2}\right)^2}\right)^2}. \tag{125}$$

This expression indicates that we have a solution of the bound state energy spectrum for a family of the Kratzer potential. Of course, it is clear that by imposing appropriate values of the parameters A, B and C, the bound state energy spectrum for a particle in the modified Kratzer potential can be calculated immediately.

As an analogy, if we set up the parameters $A = 0$, $B = Ze'^2$ and $C = 0$, it is easy to demonstrate that Eq.(125) reduces to the bound state energy spectrum of a particle in the

Coulomb potential, i.e., $E_{n_p} = -Z^2\mu e'^4/2n_p^2\hbar^2$, where $n_p \equiv n + \ell + 1$. The principal quantum number n_p ranges from 1 to infinite. Thus the particle that is in the Coulomb potential will have the quantize energy levels due to the n_p. If we assume that the particle is an electron that is bound to the nucleus in a hydrogen-like atom, the electron energy would be negative relative to that of a free electron. Moreover, the electron would be confined within the Coulomb potential well owing to the presence of the positively charged nucleus. Numerically, the ground-state ($n_p = 1$) energy E_1 of the hydrogen atom ($Z = 1$) is -13.6 eV below the ionization limit $E_\infty = 0$ for the state $n_p = \infty$. In other words, the minimum amount of energy required to release the electron from a hydrogen atom is -13.6 eV that is the ground state energy of electron in the Coulomb potential. The electron can remain in this stationary ground state forever because it is stable and the electron never collapses into the nucleus. If we apply our knowledge of classical mechanics, we can see that this information is not correct. But quantum mechanically it is. Why these results are not compatible with each other? Readers are strongly encouraged to discuss the reason.

Another analogy is to be on the Kratzer potential. When we take $A = 0$, $B = 2D_er_e$ and $C = D_er_e^2$, Eq.(125) turns to the bound state energy spectrum of a vibrating-rotating diatomic molecule subject to the Kratzer potential as follows

$$E = -\frac{\frac{2\mu D_e^2 r_e^2}{\hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{2\mu D_e r_e^2}{\hbar^2} + \left(\ell + \frac{1}{2}\right)^2}\right)^2}. \tag{126}$$

Although this result came from an exact solution of the SE for the energy levels, it has not been properly used by spectroscopists because the Kratzer potential supports an infinite number of vibrational and rotational levels which is not related with the actual diatomic molecules. To see this number we can get the derivative of Eq.(126) according to n that gives the maximum vibrational quantum number n_{max} in the case of Kratzer potential (Berkdemir et al, 2006; Berkdemir & Sever, 2009);

$$\frac{dE}{dn} = \frac{\frac{4\mu D_e^2 r_e^2}{\hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{2\mu D_e r_e^2}{\hbar^2} + \left(\ell + \frac{1}{2}\right)^2}\right)^3} = 0, \tag{127}$$

$$n \to n_{max} = \infty. \tag{128}$$

If we take the derivative of Eq.(126) with respect to ℓ, we can reach the maximum rotational quantum number, i.e., $\ell_{max} = \infty$. As a main conclusion of these results, the Kratzer potential (or the modified Kratzer potential with $A = D_e$) does not describe the spectrum of a vibrating-rotating diatomic molecule correctly. To make sure about this knowledge the readers should be applied the selection rules to diatomic molecules by means of Eq.(126) (Fues, 1926). They will probably recognize that the spectrum that is obtained from Eq.(126) would be far away the spectroscopic results (Fernandez, 2011).

Let us now find the corresponding eigenfunctions for the Kratzer potential. According to the NU method, the wavefunction $\psi(s)$ is defined in terms of the separable functions $\phi(s)$ and $y_n(s)$. For the $\phi(s)$, we have

$$\phi(s) = s^{\frac{-1+\sqrt{1+4\gamma}}{2}} e^{-\sqrt{\alpha}s}, \tag{129}$$

where $\gamma = \frac{2\mu C}{\hbar^2} + \ell(\ell+1)$ and $\alpha = -\frac{2\mu(E-A)}{\hbar^2}$. The polynomial solution of the hypergeometric-type function $y_n(s)$ depends on the determination of the weight function $\rho(s)$ which must satisfy the condition $(\sigma(s)\rho(s))' = \tau(s)\rho(s)$. Thus, $\rho(s)$ can be calculated by falling back on Eq.(121) and Eq.(92);

$$\rho(s) = s^{\sqrt{1+4\gamma}} e^{-2\sqrt{\alpha}s}. \tag{130}$$

Substituting Eq.(130) into the Rodrigues' formula given by Eq.(27), the hypergeometric-type function $y_n(s)$ is obtained in the following form

$$y_n(s) = B_n e^{2\sqrt{\alpha}s} s^{-\sqrt{1+4\gamma}} \frac{d^n}{ds^n}\left(e^{-2\sqrt{\alpha}s} s^{n+\sqrt{1+4\gamma}}\right). \tag{131}$$

It is shown from the Rodrigues‘ formula of the associated Laguerre polynomials

$$L_n^{\sqrt{1+4\gamma}}(2\sqrt{\alpha}s) = \frac{1}{n!} e^{2\sqrt{\alpha}s} s^{-\sqrt{1+4\gamma}} \frac{d^n}{ds^n}\left(e^{-2\sqrt{\alpha}s} s^{n+\sqrt{1+4\gamma}}\right) \tag{132}$$

where $1/n! = B_n$. Eq.(131) and Eq.(132) yield $y_n(s) \equiv L_n^{\sqrt{1+4\gamma}}(2\sqrt{\alpha}s)$. By using $\psi(s) = \phi(s)y_n(s)$, we have

$$\psi(s) = N_{n\ell} s^{\frac{-1+\sqrt{1+4\gamma}}{2}} e^{-\sqrt{\alpha}s} L_n^{\sqrt{1+4\gamma}}(2\sqrt{\alpha}s). \tag{133}$$

where $N_{n\ell}$ is the normalization constant.

4.4 Morse potential

The Morse potential (Morse, 1920), named after physicist Philip M. Morse, is one of the convenient models for the potential energy of a diatomic molecule. It is a better approximation for the vibrational structure of a molecule than the harmonic oscillator model because it explicitly includes the effects of bond breaking, such as the existence of unbound states. For a diatomic molecular system with reduced mass μ, the Morse potential (Morse, 1920) can be written as

$$V(r) = D_e[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}] \qquad (D_e > 0, a > 0, r_e > 0), \tag{134}$$

where D_e is the dissociation energy, r_e is the equilibrium internuclear distance and a is a parameter controlling the width of the potential well. If anyone wants to modify this potential, shifting through the positive axis, it would be quite enough to insert an additional D_e into the potential. So the potential would be called the "modified" Morse potential. In an obvious manner, the word "modified" is not an "amazing" greatly. The vibrations and rotations of a two-atomic molecule can be exactly described by this potential in the case of $\ell = 0$ (Flügge, 1971). If we want to obtain the solution for $\ell \neq 0$, the centrifugal term has to be approximated to the Morse potential. In order to calculate the bound state energy spectrum and the corresponding radial wavefunction, the potential function given by Eq.(134) is inserted into the radial SE

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E - D_e[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}] - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]R(r) = 0, \tag{135}$$

where n and ℓ can be defined the vibrational and rotational quantum numbers, respectively, and E is the appropriate energy (Berkdemir & Han, 2005; Zuniga et al., 2008). With a transformation from $R(r)$ to $U(r)/r$, Eq.(135) turns into the following one;

$$\frac{d^2U(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - D_e[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}] - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]U(r) = 0. \tag{136}$$

An analytical solution of this differential equation can not be obtained without an approximation because Eq.(136) includes both exponential and radial terms. For this reason, we outline a procedure given by Pekeris (Flügge, 1971; Pekeris, 1934) to suggest an approximation to the solution of SE given in Eq.(136).

The approximation is based on the expansion of the centrifugal term in a series of exponential depending on the internuclear distance, keeping terms up to second order. In this way, the centrifugal term can be rearranged by keeping the parameters in the Morse potential. However, by construction, this approximation is valid only for the low vibrational energy states. Therefore, we can take into account the rotational term in the following way, using the Pekeris approximation. We first simplify the centrifugal part of Eq.(136) by changing the coordinates $x = (r - r_e)/r_e$ around $x = 0$. Hence, it may be expanded into a series of powers as

$$V_{rot}(x) = \frac{\eta}{(1+x)^2} = \eta(1 - 2x + 3x^2 - 4x^3 + ...), \tag{137}$$

with

$$\eta = \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r_e^2}, \tag{138}$$

the first few terms should be quite sufficient. Instead, we now replace the rotational term by the potential

$$\tilde{V}_{rot}(x) = \eta\left(D_0 + D_1 e^{-\delta x} + D_2 e^{-2\delta x}\right), \tag{139}$$

where $\delta = a r_e$ and D_i is the coefficients $(i = 0, 1, 2)$. In this point, the expression of Eq.(139) can be expanded up to the terms x^3

$$\tilde{V}_{rot}(x) = \eta\left(D_0 + D_1(1 - \delta x + \frac{\delta^2 x^2}{2!} - \frac{\delta^3 x^3}{3!} + ...) + D_2(1 - 2\delta x + \frac{4\delta^2 x^2}{2!} - \frac{8\delta^3 x^3}{3!} + ...)\right), \tag{140}$$

$$\tilde{V}_{rot}(x) = \eta\left(D_0 + D_1 + D_2 - x(D_1\delta + 2D_2\delta) + x^2(D_1\frac{\delta^2}{2} + 2D_2\delta^2) - x^3(D_1\frac{\delta^3}{6} + D_2\frac{4\delta^3}{3}) + ...\right). \tag{141}$$

Combining equal powers of Eqs.(137) and (141) we obtain the relations between the coefficients and the parameter δ as follows

$$\begin{aligned} D_0 &= 1 - \frac{3}{\delta} + \frac{3}{\delta^2} \\ D_1 &= \frac{4}{\delta} - \frac{6}{\delta^2} \\ D_2 &= -\frac{1}{\delta} + \frac{3}{\delta^2}. \end{aligned} \tag{142}$$

We now can take the potential $\tilde{V}_{rot}$ instead of the true rotational potential V_{rot} and solve the SE for $\ell \neq 0$ in Eq.(136).

In order to apply the NU method, we rewrite Eq.(136) by using a new variable of the form $s = e^{-\delta x}$ and $U(r) \to \psi(s)$,

$$\frac{d^2\psi(s)}{ds^2} + \frac{1}{s}\frac{d\psi(s)}{ds} + \frac{2\mu r_e^2}{\hbar^2\delta^2 s^2}\left[(E - \eta D_0) + (2D_e - \eta D_1)s - (D_e + \eta D_2)s^2\right]\psi(s) = 0. \tag{143}$$

By introducing the following dimensionless parameters

$$\alpha = -\frac{2\mu r_e^2(E_{nl} - \eta D_0)}{\hbar^2\delta^2},$$
$$\beta = \frac{2\mu r_e^2(2D_e - \eta D_1)}{\hbar^2\delta^2}, \tag{144}$$
$$\gamma = \frac{2\mu r_e^2(D_e + \eta D_2)}{\hbar^2\delta^2},$$

which leads to the main equation defined in Eq.(4), we can rearrange the SE:

$$\frac{d^2\psi}{ds^2} + \frac{1}{s}\frac{d\psi}{ds} + \frac{1}{s^2}\left[-\gamma s^2 + \beta s - \alpha\right]\psi(s) = 0. \tag{145}$$

After the comparison of Eq.(4) with Eq.(145), we obtain the corresponding polynomials as

$$\widetilde{\tau}\,(s) = 1,$$
$$\sigma(s) = s, \tag{146}$$
$$\widetilde{\sigma}\,(s) = -\gamma s^2 + \beta s - \alpha.$$

Substituting these polynomials into Eq.(18), we obtain the polynomial $\pi(s)$;

$$\pi(s) = \pm\sqrt{\gamma s^2 + (k-\beta)s + \alpha} \tag{147}$$

taking $\sigma'(s) = 1$. The discriminant of the upper expression under the square root has to be zero. Hence, the expression becomes the square of a polynomial of first degree;

$$(k-\beta)^2 - 4\alpha\beta = 0. \tag{148}$$

When the required arrangements are prepared with respect to the constant k, its double roots are derived as $k_\pm = \beta \pm 2\sqrt{\alpha\gamma}$. Substituting $k_\pm$ into Eq.(147), the following four possible forms of the $\pi(s)$ are obtained

$$\pi(s) = \pm\begin{cases} \left(\sqrt{\gamma}s + \sqrt{\alpha}\,\right), & \text{for} \quad k_+ = \beta + 2\sqrt{\alpha\gamma} \\ \left(\sqrt{\gamma}s - \sqrt{\alpha}\,\right), & \text{for} \quad k_- = \beta - 2\sqrt{\alpha\gamma}. \end{cases} \tag{149}$$

We just select one of four possible forms of the $\pi(s)$, i.e, $\pi(s) = -\left(\sqrt{\gamma}s - \sqrt{\alpha}\,\right)$ for $k_- = \beta - 2\sqrt{\alpha\gamma}$, because it would be provided a negative derivative of $\tau(s)$ given in Eq.(9). Hence, the $\tau(s)$ satisfies the requirement below

$$\tau(s) = 1 + 2\sqrt{\alpha} - 2\sqrt{\gamma}\,s,$$
$$\tau'(s) = -2\sqrt{\gamma} < 0. \tag{150}$$

From Eq.(17) we obtain

$$\lambda = \beta - 2\sqrt{\alpha\gamma} - \sqrt{\gamma}. \tag{151}$$

and from Eq.(26) we also get

$$\lambda_n = 2n\sqrt{\gamma}. \tag{152}$$

It is seen that the parameter α has the following form

$$\alpha = \left[\frac{\beta}{2\sqrt{\gamma}} - \left(n + \frac{1}{2}\right)\right]^2, \tag{153}$$

remembering the expression $\lambda = \lambda_n$. Substituting the values of α, β and γ into Eq.(153), we can determine the energy spectrum E as

$$E = \frac{\hbar^2 \ell(\ell+1)}{2\mu r_e^2}\left(1 - \frac{3}{ar_e} + \frac{3}{a^2 r_e^2}\right) - \frac{\hbar^2 a^2}{2\mu}\left[\frac{\beta}{2\sqrt{\gamma}} - \left(n + \frac{1}{2}\right)\right]^2, \tag{154}$$

where

$$\frac{\beta}{2\sqrt{\gamma}} = \frac{1}{a^2\sqrt{\gamma}}\left[\frac{2\mu D_e}{\hbar^2} - \frac{\ell(\ell+1)}{r_e^2}\left(\frac{2}{ar_e} - \frac{3}{a^2 r_e^2}\right)\right]. \tag{155}$$

The last equation indicates the energy spectrum of the Morse potential. The derivative of this energy expression according to n gives an idea about the maximum vibrational quantum number so that the result is $n_{max} = \beta/2\sqrt{\gamma} - 1/2$ (Berkdemir & Sever, 2009; Zhang et al., 2011).

Let us now find the corresponding wavefunction of the Morse potential. A simple calculation reveals that $\phi(s)$ can be calculated by recalling Eq.(7) and submitting the $\sigma(s) = s$ and the $\pi(s) = -\left(\sqrt{\gamma}s - \sqrt{\alpha}\right)$;

$$\phi(s) = s^{\sqrt{\alpha}} e^{-\sqrt{\gamma}\, s}, \tag{156}$$

which is one of the separable parts of the wavefunction $\psi(s) = \phi(s) y_n(s)$. The polynomial solution of the hypergeometric-type function $y_n(s)$ depends on the determination of the weight function $\rho(s)$ ($[\sigma(s)\rho(s)]' = \tau(s)\rho(s)$). Thus, $\rho(s)$ is calculated as

$$\rho(s) = s^{2\sqrt{\alpha}} e^{-2\sqrt{\gamma}\, s}. \tag{157}$$

Substituting Eq.(157) into the Rodrigues' formula given in Eq.(27), the other separable part of the wavefunction $\psi(s)$ is given in the following form

$$y_n(s) = B_n s^{-2\sqrt{\alpha}} e^{2\sqrt{\gamma}\, s} \frac{d^n}{ds^n}\left[s^{(n+2\sqrt{\alpha})} e^{-2\sqrt{\gamma}\, s}\right]. \tag{158}$$

The polynomial solution of $y_n(s)$ in Eq.(158) is expressed in terms of the associated Laguerre Polynomials, which is one of the orthogonal polynomials, that is

$$y_n(s) \equiv L_n^{2\sqrt{\alpha}}(2\sqrt{\gamma}\, s). \tag{159}$$

Combining the Laguerre polynomials and $\phi(s)$ in Eq.(155), the radial wavefunction are constructed as

$$\psi(s) = N_{n\ell} s^{\sqrt{\alpha}} e^{-\sqrt{\alpha} s} L_n^{2\sqrt{\alpha}}(2\sqrt{\gamma}\, s), \tag{160}$$

where $N_{n\ell}$ is the normalization constant.

4.5 Hulthen potential

One of the objects of this book chapter is to investigate the solution of the SE with the Hulthen potential (Hulthen, 1942; Rosenfeld, 1948) that is given in the form;

$$V(r) = -\frac{K}{\kappa}\frac{1}{e^{\frac{r}{\kappa}} - 1}, \tag{161}$$

where K and κ are the strength and the range parameter of the potential (on the other word, $1/\kappa$ is known the screening parameter regarding with the potential), respectively. The Hulthen potential has an attractive Coulombic behavior for small values of r with respect to κ, i.e., $r << \kappa$. To see this behavior let us focus the exponential term of the Hulthen potential. If the values of the radial variable r are smaller than those of the κ, the exponential term could be expanded into the Taylor series (Abramowitz & Stegun, 1970), i.e., $e^{\frac{r}{\kappa}} = 1 + r/\kappa + \frac{1}{2!}(r/\kappa)^2 + \frac{1}{3!}(r/\kappa)^3 + ...$ and the higher order terms in the series could be neglected according to the first two terms. So the exponential term is now expressed as $e^{\frac{r}{\kappa}} \approx 1 + r/\kappa$. Inserting this term into Eq.(161), one can reach the attractive Coulomb potential, i.e., $V(r) = -K/r$. Thus, the K can be identified with the atomic number (see Section 4.2 for a comparison). On the other hand, for the large values of r, i.e., $r >> \kappa$, the exponential term would be larger according to the number 1 which is seen in the denominator of the Hulthen potential and hence the number 1 would be neglected. Therefore, the Hulthen potential would be reduced to $V(r) = -\frac{K}{\kappa}e^{-\frac{r}{\kappa}}$.

The Hulthen potential has been used in several branches of physics such as nuclear and particle, atomic, molecular and chemical physics (Durand & Durand, 1981; Xu et al., 2006; Bitensky et al., 1997; Jia et al., 2000; Olson & Micha, 1978). Moreover, its discrete and continuum states have been studied by a variety of techniques such as the supersymmetry and shape invariance property (Varshni, 1990; Filho & Ricotta, 1995; Qian et al., 2002). The solution of the SE for a particle in the Hulthen potential can not be obtained exactly for the case of $\ell \neq 0$ whereas we have an exact solution for the case of $\ell = 0$, namely s-wave solution (Flügge, 1971). To find an approximate solution of the SE with the Hulthen potential, we have to rely on an approximation for the centrifugal term. How can we do that? Let us look at below.

The Hulthen potential given in Eq.(161) can be written in the following form if we recompile it,

$$V(r) = -\frac{K}{\kappa}\frac{e^{-r/\kappa}}{1 - e^{-r/\kappa}}. \tag{162}$$

Inserting Eq.(162) into Eq.(42), we have

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E + \frac{K}{\kappa}\frac{e^{-r/\kappa}}{1 - e^{-r/\kappa}} - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]R(r) = 0. \tag{163}$$

We now want to obtain the solution of Eq.(163) using the NU method. If we define

$$R(r) = \frac{U(r)}{r}, \tag{164}$$

Eq.(163) becomes

$$\frac{d^2U(r)}{dr} + \left[\frac{2\mu}{\hbar^2}\left(E + \frac{K}{\kappa}\frac{e^{-r/\kappa}}{1 - e^{-r/\kappa}}\right) - \frac{\ell(\ell+1)}{r^2}\right]U(r) = 0. \tag{165}$$

This equation is similar to the s-wave SE for the Hulthen potential, except for the additional term $\frac{\ell(\ell+1)}{r^2}$, which is commonly mentioned as a centrifugal term. To solve Eq.(165), we can think about an approximation regarding with the centrifugal term as follows (Greene & Aldrich, 1976; Qiang & Dong, 2007)

$$\frac{\ell(\ell+1)}{r^2} \approx \frac{\ell(\ell+1)e^{-r/\kappa}}{\kappa^2(1-e^{-r/\kappa})^2}. \tag{166}$$

The present approximation is just valid for the short-range potentials (i.e., large κ and small ℓ) but not for the long-range potentials (i.e., small κ and large ℓ). Nevertheless it provides good results, which are in agreement with the previously reported numerical integration method (Lucha & Schöberl, 1999). Moreover, in order to improve the accuracy of this approximation, a different approximation scheme has been recently proposed for the centrifugal term (Ikhdair, 2009; 2011). Readers are strongly encouraged to review these studies.

After replacing the term $\ell(\ell+1)/r^2$ by its approximation $\frac{\ell(\ell+1)e^{-r/\kappa}}{\kappa^2(1-e^{-r/\kappa})^2}$ and the transformation $s = e^{-r/\kappa}$ (and also $U(r) \to \psi(s)$), Eq.(165) becomes

$$\frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{d\psi(s)}{ds} + \frac{1}{s^2(1-s)^2}[-(\alpha+\beta)s^2 + (2\alpha+\beta-\gamma)s - \alpha]\psi(s) = 0 \tag{167}$$

where

$$\begin{aligned} \alpha &= -\frac{2\mu E\kappa}{\hbar^2}, \\ \beta &= \frac{2\mu K\kappa}{\hbar^2}, \\ \gamma &= \ell(\ell+1). \end{aligned} \tag{168}$$

By comparing Eq.(167) with the main equation that comes from the NU method, Eq.(4), we can define the following polynomials

$$\begin{aligned} \tilde{\tau}(s) &= 1-s, \\ \sigma(s) &= s(1-s), \\ \tilde{\sigma}(s) &= -(\alpha+\beta)s^2 + (2\alpha+\beta-\gamma)s - \alpha. \end{aligned} \tag{169}$$

Inserting these polynomials into Eq.(18), we have

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2}\sqrt{[1+4(\alpha+\beta-k)]s^2 - 4(2\alpha+\beta-\gamma-k)s + 4\alpha} \tag{170}$$

The discriminant of the expression under the square root in the above equation has to be set equal to zero. Therefore, it becomes

$$\Delta = 16(2\alpha+\beta-\gamma-k)^2 - 16[1+4(\alpha+\beta-k)]\alpha = 0, \tag{171}$$

and the two roots of k are obtained

$$k_{\pm} = \beta - \gamma \pm \sqrt{\alpha(1+4\gamma)}. \tag{172}$$

Substituting the double roots of $k_\pm$ into Eq.(170), the four possible forms of the $\pi(s)$ for either k_+ or k_- are derived as follows

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2} \begin{cases} \left[\left(2\sqrt{\alpha} - \sqrt{1+4\gamma}\right) s - 2\sqrt{\alpha}\right] \text{ for } k_+ = \beta - \gamma + \sqrt{\alpha(1+4\gamma)} \\ \left[\left(2\sqrt{\alpha} + \sqrt{1+4\gamma}\right) s - 2\sqrt{\alpha}\right] \text{ for } k_- = \beta - \gamma - \sqrt{\alpha(1+4\gamma)}. \end{cases} \tag{173}$$

In order to obtain a physical solution we have to ensure that the polynomial $\tau(s) = \tilde{\tau}(s) + 2\pi(s)$ must satisfy a negative derivative. For this reason, we select the $\pi(s)$;

$$\pi(s) = -\frac{s}{2} - \frac{1}{2}\left[\left(2\sqrt{\alpha} + \sqrt{1+4\gamma}\right) s - 2\sqrt{\alpha}\right], \tag{174}$$

for $k_- = \beta - \gamma - \sqrt{\alpha(1+4\gamma)}$. The following track in this selection is to achieve the condition $\tau'(s) < 0$. Therefore $\tau(s)$ is written

$$\tau(s) = 1 - 2s - \left[\left(2\sqrt{\alpha} + \sqrt{1+4\gamma}\right) s - 2\sqrt{\alpha}\right], \tag{175}$$

and then its negative derivative becomes

$$\tau'(s) = -(2 + 2\sqrt{\alpha} + \sqrt{1+4\gamma}) < 0. \tag{176}$$

We can also write down the $\lambda = k_- + \pi'(s)$ and $\lambda_n = -n\tau'(s) - n(n-1)\sigma''(s)/2$, keeping in our mind that $\lambda = \lambda_n$;

$$\lambda = \beta - \gamma - \frac{1}{2}(1 + 2\sqrt{\alpha})\left(1 + \sqrt{1+4\gamma}\right) = n\left[1 + 2\sqrt{\alpha} + n + \sqrt{1+4\gamma}\right], \qquad n = 0, 1, 2, ... \tag{177}$$

After bring back α, β and γ which are defined in Eq.(168) and simple manipulations, we have the energy spectrum of the Hulthen potential (Agboola, 2011)

$$E = -\frac{\hbar^2}{2\mu}\left[\frac{(K\mu/\hbar^2)}{n+\ell+1} - \frac{n+\ell+1}{2\kappa}\right]^2. \tag{178}$$

If we take into account the limitation of $\kappa \to \infty$, we have $E_n = -\frac{\mu}{2\hbar^2}[K/(n+\ell+1)]^2$. This is the energy spectrum of the Coulomb potential we have investigated in Section 4.2.
We can now apply the relationships given by Eq.(7) and Eq.(27) through Eq.(28) to obtain the wavefunction $\psi(s)$. Therefore, the relevant polynomials are given

$$\phi(s) = s^{\sqrt{\alpha}}(1-s)^{\ell+1}, \tag{179}$$

$$\rho(s) = s^{2\sqrt{\alpha}}(1-s)^{2\ell+1}, \tag{180}$$

$$y_n(s) = B_n s^{-2\sqrt{\alpha}}(1-s)^{-(2\ell+1)} \frac{d^n}{ds^n}\left[s^{n+2\sqrt{\alpha}}(1-s)^{n+2\ell+1}\right] \equiv P_n^{(2\sqrt{\alpha},\, 2\ell+1)}(1-2s). \tag{181}$$

So the wavefunction $\psi(s)$ is written as

$$\psi(s) = N_{n\ell} s^{\sqrt{\alpha}} (1-s)^{\ell+1} P_n^{(2\sqrt{\alpha},\, 2\ell+1)}(1-2s), \tag{182}$$

where $N_{n\ell}$ is the normalization constant and $P_n^{(2\sqrt{\alpha},\, 2\ell+1)}(1-2s)$ is the Jacobi polynomials (Szego, 1934). As a reminder notice, the relationship between the $\psi(s)$ and the $R(r)$ is $\psi(s) \equiv rR(r)$ with the transformation of $s = e^{-r/\kappa}$.

5. Conclusion

An exact solution of the SE is not a practical manner, except for the simplest of potential energy functions. In most cases of practical interest, we can just settle for an approximate solution. To overcome various types of problems in quantum mechanics, we have to apply several methods or approximations to solve the SE appropriately. One of this method is introduced by A. F. Nikiforov and V. B. Uvarov. The solution range of this method is limited by the hypergeometric-type second-order differential equations. We know that the time-independent SE has the second-order differential equation in the *Schrödinger picture* as well. Therefore, in this book chapter we confined our attention to this equation and its exact or approximate solutions for the selected potentials such as Harmonic oscillator, Coulomb, Kratzer, Morse and Hulthen potentials. The solution meant that we have obtained the energy spectrum and the corresponding wavefunction of a particle subject to one of these potentials.

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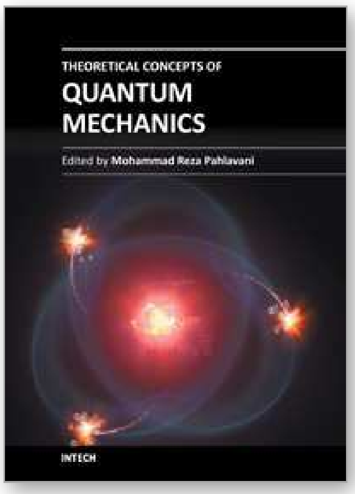

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