

Approximate solutions of the Wei Hua oscillator using the Pekeris approximation and Nikiforov–Uvarov method

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Abstract. The approximate analytical bound-state solutions of the Schrödinger equation for the Wei Hua oscillator are carried out in N -dimensional space by taking Pekeris approximation scheme to the orbital centrifugal term. Solutions of the corresponding hyper-radial equation are obtained using the conventional Nikiforov–Uvarov (NU) method.

Keywords. Nikiforov–Uvarov (NU) method; N -dimensional Schrödinger equation; approximate solution through Pekeris approximation.

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1. Introduction

The search for exact bound-state solutions of wave equations, relativistic or non-relativistic, has been an important research area in quantum mechanics because they contain all the information of the quantum system. It is well known that the exact solutions are possible only for a few sets of quantum systems such as the Coulomb, the harmonic oscillator, the pseudoharmonic potentials and others [1–5]. The analytical exact solutions of the wave equation with some exponential-type potentials are impossible for $l \neq 0$ states. So, the next best thing to do is to find approximate analytical solutions of a given potential by appropriate approximation techniques. Therefore, approximate schemes like the Pekeris approximation [6–8] and the approximation scheme suggested by Greene and Aldrich [9] have to be used to deal with the orbital centrifugal terms. Some of these exponential-type potentials include the Morse potential [10], the Hulthen potential [11], the Pöschl–Teller potential [12], the Woods–Saxon potential [13], the Kratzer-type and pseudoharmonic potential [14], the Rosen–Morse potentials [15], the Manning–Rosen potential [16] etc.

Recently, there has been a renewed interest in solving simple quantum mechanical systems within the framework of the Nikiforov–Uvarov (NU) method [17]. This algebraic technique is based on solving the second-order linear differential equations, which has

been used successfully to solve Schrödinger, Dirac, Klein–Gordon and Duffin–Kemmer–Petiau wave equation in the presence of some well-known central and non-central potentials [18–27]. The aim of this work is to present the approximate solutions of the Schrödinger equation with the Wei Hua [28] oscillator in N dimensions for $l \neq 0$ states using the conventional NU method.

This paper is organized as follows: After a brief introductory discussion of the NU method in §2 and that of the eigenvalues and eigenfunctions in N dimensions in §3, we obtain the eigenvalues and eigenfunctions for Wei Hua oscillator through the Pekeris approximation and NU method in §4 and finally conclusions have been drawn in §5.

2. Basic equations of Nikiforov–Uvarov method

The Nikiforov–Uvarov (NU) [17] method provides us an exact solution of non-relativistic Schrödinger equation for certain potentials. This method is based on solutions of general second-order linear differential equation with special orthogonal functions [29]. For a given real or complex potential, the Schrödinger equation is reduced to a generalized equation of hypergeometric type with an appropriate $s = s(x)$ coordinate transformation. Thus, it can be written in the following form:

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \quad (1)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second degree and $\tilde{\tau}(s)$ is a first-degree polynomial. Hence, the Schrödinger equation or the Schrödinger-like equations can be solved by means of this method for potentials we consider. To find a particular solution of eq. (1), we use the separation of variables with the transformation

$$\psi(s) = \phi(s)y(s). \quad (2)$$

It reduces eq. (1) to an equation of hypergeometric type,

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0 \quad (3)$$

and $\phi(s)$ in eq. (2) is defined as a logarithmic derivative in the following form and its solution can be obtained from

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}. \quad (4)$$

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

$$y(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} (\sigma^n \rho(s)), \quad (5)$$

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

$$\frac{d}{ds} (\sigma(s)\rho(s)) = \tau(s)\rho(s). \quad (6)$$

The function $\pi(s)$ and the parameter λ required for this method are defined as

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \quad (7)$$

and

$$\lambda = k + \pi'(s). \quad (8)$$

Here, $\pi(s)$ is a polynomial with the parameter s and the determination of k is essential for calculating $\pi(s)$. Thus, to find the value of k , the expression under the square root must be the square of a polynomial. Hence, the new eigenvalue equation for the Schrödinger or Schrödinger-like equation becomes

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n = 0, 1, 2, 3, \dots, \quad (9)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \quad (10)$$

and it will have a negative derivative.

3. Eigenvalues and eigenfunctions in N dimensions

In this article, we use NU method to deal with the N -dimensional ($N \geq 3$) Schrödinger equation and obtain the eigenstate and eigenvalue for the anharmonic oscillators. The extension sought by us, although straightforward, is quite instructive because laws of physics in N spatial dimensions may often lead to insights concerning laws of physics in lower dimensions [30–32].

Consider the motion of a particle of mass m in an N -dimensional Euclidian space. The time-independent Schrödinger equation for any integral dimension is given by [30–32]

$$\left(-\frac{\hbar^2}{2m}\Delta_N^2 + V_N \right) \Psi = E\Psi. \quad (11)$$

Here, the wave function Ψ belongs to the energy eigenvalue E and Δ_N^2 and V_N stand for the N -dimensional Laplacian and potential respectively. Investigation of physical processes based on eq. (11) is a well-studied problem and many authors proceed by using the standard central potential $V(r)$ in place of V_N . Here r represents the N -dimensional radius $(\sum_i^N x_i^2)^{1/2}$. Going over to a spherical coordinate system with $N - 1$ angular variables and one radial coordinate we can write

$$\Psi = \psi_{n,l}^{(N)} Y_l^M(\theta_i), \quad (12)$$

where $Y_l^M(\cdot)$ represents contributions from the hyperspherical harmonics that arise in higher dimensions. The eigenvalues and eigenfunctions for generalized angular momentum operators in N -dimensional polar coordinates are determined [33] using the results known from the factorization method [34]. However, from eqs (11) and (12) we have l th partial-wave radial Schrödinger equation

$$\frac{d^2\psi_{n,l}^{(N)}}{dr^2} + \frac{N-1}{r} \frac{d\psi_{n,l}^{(N)}}{dr} + \frac{2m}{\hbar^2} \left(E_{n,l}^{(N)} - V(r) - \frac{\hbar^2}{2m} \frac{l(l+N-2)}{r^2} \right) \psi_{n,l}^{(N)} = 0. \quad (13)$$

Here, the superscript (N) on the radial function $\psi_{n,l}^{(N)}$ and the energy eigenvalue $E_{n,l}^{(N)}$ merely stand for the dimensionality of the problem and the subscript n refers to a quantum number, the interpretation of which depends on the choice of $V(r)$. Introducing a new function

$$R_{n,l}^{(N)}(r) = r^{(N-1)/2} \psi_{n,l}^{(N)}(r),$$

eq. (13) takes the form

$$\frac{d^2 R_{n,l}^{(N)}(r)}{dr^2} + \frac{2m}{\hbar^2} (E_{n,l}^{(N)} - V_{\text{eff}}(r)) R_{n,l}^{(N)}(r) = 0 \quad (14)$$

where the effective potential

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2}{2m} \frac{l(l + N - 2)}{r^2} = V(r) + V_l(r).$$

4. Pekeris approximation and Nikiforov–Uvarov method for approximate solutions of the Wei Hua oscillators

For Wei Hua oscillator, the Schrödinger equation can be solved for the s-wave, i.e., for the angular momentum quantum number $l = 0$ only. However, for the general solution, one needs to include the Pekeris approximation to obtain analytical solutions to the Schrödinger equation. Also, it is often necessary to determine the l -wave solutions. The approximation is based on the expansion of the centrifugal barrier in a series exponentials depending on the nuclear distance, until the second order. By construction, this approximation is valid only for lower vibrational energy states. Therefore, for a Pekeris approximation, we can take care of the rotational term in the following way.

By changing the coordinates

$$x = \frac{r - r_0}{r_0}, \quad (15)$$

the centrifugal potential is expanded in the Taylor series around the point $x = 0 (r = r_0)$

$$V_l = \frac{\hbar^2}{2m} \frac{l(l + N - 2)}{r^2} = \gamma(1 + x)^{-2} = \gamma(1 - 2x + 3x^2 - 4x^3 + \dots) \quad (16)$$

and we define an equivalent potential such that

$$\tilde{V}_l = \gamma(D_0 + D_1 f_1(x) + D_2 f_2(x) + \dots), \quad (17)$$

where $f_1(x)$, $f_2(x)$, ... are functional forms of the potential and

$$\gamma = \frac{\hbar^2}{2m} \frac{l(l + N - 2)}{r_0^2}. \quad (18)$$

According to Pekeris approximation

$$V_l = \tilde{V}_l \quad (19)$$

and the constants D_0 , D_1 and D_2 are determined by comparing equal powers of x of eqs (16) and (17). Now we take the potential \tilde{V}_l instead of the true rotational potential V_l and

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solve the Schrödinger equation for $l \neq 0$ in eq. (14) with the effective potential after Pekeris approximation

$$V_{\text{eff}}(r) = V(r) + \tilde{V}_l(r). \quad (20)$$

Now we shall apply the NU method to find the approximate solutions of Schrödinger equation for the Wei Hua oscillator [28]

$$V(r) = D \left(\frac{1 - \exp(-c_1(r - r_0))}{1 - a \exp(-c_1(r - r_0))} \right)^2, \quad (21)$$

which gives description of anharmonic vibrations of diatomic molecules and where only s-wave bound state solutions are possible/available. Here, D represents the dissociation energy of the system. With the dimensionless coordinate $x = (r - r_0)/r_0$, $\alpha = c_1 r_0$ and according to the Pekeris approximation, we replace the potential V_l with the expression

$$V_l = \tilde{V}_l = \gamma \left(D_0 + D_1 \left(\frac{1 - \exp(-\alpha x)}{1 - a \exp(-\alpha x)} \right)^2 \right). \quad (22)$$

Comparing equal power of x up to the second order from eqs (16) and (22), we obtain the constants

$$D_0 = 1, \quad D_1 = \frac{3}{\alpha^2(1 + 2a + 3a^2)}. \quad (23)$$

Now taking the potential \tilde{V}_l instead of the true rotational potential V_l , eq. (14) takes the following form for the Wei Hue oscillator:

$$\frac{d^2 R_{n,l}^{(N)}(x)}{dx^2} + \frac{2m}{\hbar^2} \left((E_{n,l}^{(N)} - \gamma D_0) - (V_0 + \gamma D_1) \left(\frac{1 - \exp(-\alpha x)}{1 - a \exp(-\alpha x)} \right)^2 \right) R_{n,l}^{(N)}(x) = 0. \quad (24)$$

With the dimensionless coordinate $s = ae^{-\alpha x}$, one can rewrite eq. (24) as

$$\frac{d^2 R_{n,l}^{(N)}(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR_{n,l}^{(N)}(s)}{ds} + \frac{1}{s^2(1-s)^2} (-c_0^2 + c_2 s^2 - c_3 s) R_{n,l}^{(N)}(s) = 0, \quad (25)$$

which is a hypergeometric-type equation. Here, the dimensional parameters are

$$-c_0 = \frac{2m}{\hbar^2 \alpha^2} (E_{n,l}^{(N)} - \gamma D_0 - V_0 - \gamma D_1), \quad (26)$$

$$c_2 = \frac{2m}{\hbar^2 \alpha^2} (E_{n,l}^{(N)} - \gamma D_0 - \frac{1}{a^2} (V_0 + \gamma D_1)) \quad (27)$$

and

$$c_3 = \frac{2m}{\hbar^2 \alpha^2} (E_{n,l}^{(N)} - \gamma D_0 - \frac{1}{a} (V_0 + \gamma D_1)). \quad (28)$$

After comparing eq. (25) with eq. (1), we obtain the corresponding polynomials as

$$\tilde{\tau}(s) = 1 - s, \quad \sigma(s) = s(1 - s), \quad \tilde{\sigma}(s) = -c_0^2 - c_3 s + c_2 s^2. \quad (29)$$

Substituting these polynomials into eq. (7), we obtain $\pi(s)$ as

$$\pi(s) = -\frac{s}{2} \pm \sqrt{s^2 \left(\frac{1}{4} - c_2 - k \right) + (k + c_3)s + c_0^2}. \quad (30)$$

The discriminant of the above expression under the square root has to be zero. Hence, the expression becomes the square of a polynomial of first degree. When the required arrangements are done with respect to the constant k , its double roots are derived as

$$k_{\pm} = -c_3 - 2c_0^2 \pm 2c_0 \left(\frac{1}{A} - \frac{1}{2} \right), \quad (31)$$

where

$$\frac{1}{A} - \frac{1}{2} = \sqrt{\frac{2m(V_0 + \gamma D_1)}{\hbar^2 \alpha^2} \left(\frac{1}{a} - 1 \right)^2 + \frac{1}{4}}. \quad (32)$$

Substituting k_- into eq. (30), the following possible solution is obtained for $\pi(s)$ as

$$\pi_-(s) = c_0(1 - s) - \frac{s}{A}. \quad (33)$$

It is clearly seen that the eigenvalues are found with a comparison of eqs (8) and (9). We select the polynomial $\pi_-(s)$ for which the function $\tau(s)$ in eq. (10) has a negative derivative. Therefore, the function $\tau(s)$ satisfies these requirements, with

$$\tau(s) = 1 - s - 2 \left(c_0 + \frac{1}{A} \right) s + 2c_0. \quad (34)$$

From eqs (8) and (9), we get

$$\lambda = 2 \frac{2m(V_0 + \gamma D_1)}{\hbar^2 \alpha^2} \left(\frac{1}{a} - 1 \right) - \frac{2c_0}{A} - \frac{1}{A} \quad (35)$$

and also

$$\lambda = \lambda_n = n \left(n + \frac{2}{A} \right) + 2nc_0. \quad (36)$$

From eqs (35) and (36), we get quantized eigenvalue as

$$E_{n,l}^{(N)} = V_0 + \frac{l(l + N - 1)}{r_0^2} \left(1 + \frac{3}{\alpha^2(1 + 2a + 3a^2)} \right) - \alpha^2 \frac{\hbar^2}{2m} \left(\frac{n(n + \frac{2}{A}) + \frac{1}{A} - 2 \frac{2m}{\hbar^2} \left(\frac{V_0}{\alpha^2} + \frac{3\gamma}{\alpha^4(1 + 2a + 3a^2)} \right) \left(\frac{1}{a} - 1 \right)^2}{2(n + \frac{1}{A})} \right). \quad (37)$$

If we take the limit $l = 0$ in $N = 3$ dimensional space, we obtain the s-wave result.

Let us now find the corresponding eigenfunctions for this potential. Due to the NU-method, the polynomial solutions of the hypergeometric function $y(s)$ depend on the determination of the weight function $\rho(s)$ which is calculated as

$$\rho(s) = s^{2c_0} (1 - s)^{(2/A) - 1}. \quad (38)$$

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Substituting into the Roddiques relation given in eq. (6), the eigenfunctions are obtained in the following form:

$$y_n(s) = B_n s^{-2c_0} (1-s)^{-\left(\frac{2}{A}-1\right)} \frac{d^n}{ds^n} \left(s^{n+2c_0} (1-s)^{n+(2/A)-1} \right), \quad (39)$$

where B_n is the normalization constant. The polynomial solutions of $y_n(s)$ in eq. (39) are expressed in terms of the Jacobi polynomials as

$$y_n(s) = B_n n! P_n^{2c_0, (2/A)-1}(1-2s). \quad (40)$$

By substituting $\pi_-(s)$ and $\sigma(s)$ into eq. (5) and solving the differential equation, the other part of the wave function is found as

$$\phi_n(s) = s^{c_0} (1-s)^{1/A}. \quad (41)$$

Combining the Jacobi polynomials and $\phi_n(s)$, we get wave functions as

$$R_{n,l}^{(N)}(s) = A_n s^{c_0} (1-s)^{1/A} P_n^{2c_0, (2/A)-1}(1-2s), \quad (42)$$

where A_n is the normalization constant.

To compute the normalization constant A_n , it is easy to show using $\psi_{nl}^{(N)}(r) = r^{-(N-1)/2} R_{nl}^{(N)}(r)$ that

$$\int_0^\infty |\psi_{nl}^{(N)}(r)|^2 r^{N-1} dr = \int_{r_0}^\infty |R_{nl}^{(N)}(r)|^2 dr = \frac{1}{c_1} \int_0^1 |R_{nl}^{(N)}(s)|^2 \frac{ds}{s} = 1, \quad (43)$$

where we have also used the substitution $s = ae^{-c_1(r-r_0)}$. Putting eq. (42) into eq. (39) and using the following definition of the Jacobi polynomial [35]

$$P_n^{(a,b)}(x) = \frac{\Gamma(n+a+1)}{n!\Gamma(1+a)} {}_2F_1\left(-n, a+b+n+1; 1+a; \frac{1-x}{2}\right), \quad (44)$$

we arrived at

$$A_n^2 \left(\frac{\Gamma(n+2c_0+1)}{n!\Gamma(1+2c_0)} \right)^2 \int_0^1 s^{2c_0-1} (1-s)^{2/A} \times \left({}_2F_1\left(-n, 2c_0 + \frac{2}{A} + n; 1+2c_0; s\right) \right)^2 ds = c_1, \quad (45)$$

where F is the hypergeometric function. Using the following series representation of the hypergeometric function

$${}_pF_q(a_1, a_2, \dots; b_1, b_2, \dots; s) = \sum_{n=0}^{\infty} \frac{(a_1)_n \dots (a_p)_n s^n}{(b_1)_n \dots (b_q)_n n!} \quad (46)$$

we have

$$A_n^2 \left(\frac{\Gamma(n + 2c_0 + 1)}{n! \Gamma(1 + 2c_0)} \right)^2 \sum_{k=0}^n \sum_{j=0}^n \frac{(-n)_k (n + 2c_0 + \frac{2}{A})_k}{k! (1 + 2c_0)_k} \times \frac{(-n)_j (n + 2c_0 + \frac{2}{A})_j}{j! (1 + 2c_0)_j} \int_0^1 s^{2c_0+k+j-1} (1-s)^{2/A} ds = c_1. \quad (47)$$

Hence, by the definition of the beta function, eq. (47) becomes

$$A_n^2 \left(\frac{\Gamma(n + 2c_0 + 1)}{n! \Gamma(1 + 2c_0)} \right)^2 \sum_{k=0}^n \sum_{j=0}^n \frac{(-n)_k (n + 2c_0 + \frac{2}{A})_k}{k! (1 + 2c_0)_k} \times \frac{(-n)_j (n + 2c_0 + \frac{2}{A})_j}{j! (1 + 2c_0)_j} B\left(2c_0 + k + j, \frac{2}{A} + 1\right) = c_1. \quad (48)$$

Using the relation $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$ and the Pochhammer symbol $(a)_n = \Gamma(a + n)/\Gamma(a)$, eq. (48) can be written as

$$A_n^2 \left(\frac{\Gamma(n + 2c_0 + 1)}{n! \Gamma(1 + 2c_0)} \right)^2 \sum_{k=0}^n \frac{(-n)_k (2c_0)_k (n + 2c_0 + \frac{2}{A})_k}{(1 + 2c_0 + \frac{2}{A})_k k! (1 + 2c_0)_k} \times \sum_{j=0}^n \frac{(-n)_j (2c_0 + k)_j (n + 2c_0 + \frac{2}{A})_j}{(1 + 2c_0 + \frac{2}{A} + k)_j j! (1 + 2c_0)_j} = \frac{c_1}{B(2c_0, \frac{2}{A} + 1)}. \quad (49)$$

Equation (49) can be used to compute the normalization constants for $n = 0, 1, 2, \dots$. In particular for the ground state, $n = 0$, we have

$$A_0 = \sqrt{\frac{c_1}{B(2c_0, \frac{2}{A} + 1)}}. \quad (50)$$

5. Conclusion

In this paper, we obtain the approximate solutions of the N -dimensional Schrödinger equation for Wei Hua oscillator, within the framework of Pekeris approximation to the centrifugal term. For solving the N -dimensional Schrödinger equation, the NU method has been used to obtain the energy eigenvalues and eigenfunctions. The energy eigenvalues obtained has been found to agree with the three-dimensional case when $N = 3$. It is important to note that the approximation is valid only for small values of the screening parameter c_1 of the Wei Hue oscillator. Hence, the results obtained are parameter-dependent.

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