Approximate Solution of the N-Dimensional Radial Schrodinger Equation for Kratzer plus Reduced Pseudoharmonic Oscillator Potential within the framework of NU-Method.

[1]B. I. Ita., [2]B. E. Nyong., [1]H. Louis., [1]T. O. Magu., [2]N. O. Alobi and [1]N. A. Nzeata-Ibe

[1]Physical/Theoretical Chemistry Research Group, Department of Pure and Applied Chemistry, University of Calabar, Calabar, Cross River State, Nigeria.

[2]Department of Chemical Sciences, Cross River University of Technology, Calabar, Cross River State, Nigeria.

Corresponding author's email: tommylife4u@yahoo.com **Phone No**: +2347067024323

ABSTRACT

We solved approximately the bound state solution of the N-dimensional radial Schrodinger Equation for kratzer plus reduced harmonic oscillator. We obtained explicitly the energy eigenvalues and the corresponding eigen functions expressed in terms of the Jacobi polynomials

Keywords: Schrodinger Equation, Kratzer, Reduced Pseudoharmonic oscillator potential, Nikiforov-Uvarov.

1. INTRODUCTION

It is interesting way any l −state solution of the Schrödinger equation can be obtained for several diatomic molecules within a given potential [1-5]. The Schrödinger equation reveals that the Eigen function of the system can furnish us with information regarding the behavior of such a system. Hence, if the system is exactly solvable for a given potential, the wave function can describe such system completely [6]. The exact solution to Schrödinger equation plays a major role in quantum mechanical systems; meanwhile this solution is only possible for several selected potentials and approximation methods are frequently used to arrive at the solution. With $l = 0$, exact analytic solution of the Schrodinger equation is obtained for some potential. When $l \neq 0$, the Schrödinger equation can only be solved approximately for certain potentials [7,8]. In recent times, the study of exponential-type potential has attracted a lot of interest to different authors [9-20]. These potentials under investigation are Hulthen potential [13], Yukawa potential [14], Manning- Rosen potential [15], Woods-Saxon potential [16], Eckart potential [17], Mie-type [7,18] potential and others. Various methods have been employed to obtain the exact or approximate solution of the Schrödinger equation for exponential-type potentials. These methods include the supersymmetric(SUSY) and shape invariance method [21,22], the variational method [23], standard method [9,24], path integral approach[25], the asymptotic iteration method (AIM)[26,27], Exact quantization rule (EQR)[15,28], hypervarial perturbation [29], series method[30], shifted 1/N expansion [31,32], the algebraic approach [33], the Nikiforov-Uvarov Method [34] and others. The NU method has been used in calculating the bound states for some solvable quantum systems.

Ita, [7] and Okon*et. al.*,[18] solved the Mie-type potential and obtained the exact analytic solution for the energy term of the kratzer type potential under certain conditions. Meanwhile, the kratzerpotential is amongst the most attractive physical potentials as it contains a degeneracy-removing inverse square term beside the common coulomb term.It appears in a wide class of physical and chemical sciences including the atomic and molecular physics providing quite motivating results [26,28,33,36-40,43].

(*Kocak*, 2006) obtained the bound state solution of the kratzerpotential[35]. (*Saad et. al.*, 2008) obtained the bound state energy spectrum of kratzer-type potential by using the Asymptotic Iteration Method(AIM) [36]. (*Cheng and Dai*, 2007) obtained the exact solution for a newly proposed potential called the ringed-shaped modified kratzer potential which have its application to ring-shaped organic molecules like cyclic polyenes and benzenes [37,38]. (Berkdemir et. al., 2006) proposed a new potential which is called the modified kratzer type of molecular potential$V(r) = De\left(r - {r_e}/{r}\right)^2$, where$De$ is the dissociation energy and r_e is the equilibrium internuclear separation [39]. *Sadeghiand Pourhassan*, obtained the exact solution to the non-central modified kratzer potential plus ring-shaped like potential [40].Much work has been achieved in the area of obtaining both bound state and approximate solutions for kratzer potential as well as pseudo-harmonic and pseudo-coulombic like potential in the literature [41-47]. However, not much has been achieved in the area of solving the N-Dimensional radial Schrödinger equation for any angular momentum quantum number “l" with kratzer plus reduced pseudoharmonic oscillator potential defined as $V(r) = \frac{V_1 e^{-\alpha r}}{(1-e^{-\alpha r})} + \frac{B}{r^2}$ using NU method. The purpose of this paper is to solve the N-Dimensional Schrodinger Equation for the above mentioned mixed potential.

This paper is organized as follows. In Section 2, we review the Nikiforov-Uvarov (NU) method and the factorization of the Schrodinger Equation (SE) briefly. Section 3 is devoted to the exact solutions of the Schrodinger Equation for the quantum system by the NU method. Finally, the relevant results are discussed in Section 4

2.1 NIKIFOROV-UVAROV METHOD

The NU method is based on solving a second-order linear differential equation by reducing it to a generalized equation of hypergeometric-type. The NU method has been used to solve the Schrodinger, Dirac, and Klein-Gordon wave equations for a certain kind of potential. In this method, the second-order differential equation can be written in the following form:

$$\Psi''_n(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'_n(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\Psi_n(s) = 0 \qquad (1)$$

Where σ(s) and $\bar{\sigma}$(s) are polynomials at most second degree and $\tilde{\tau}$(s) is first degree polynomials. To make the application of the NU method simpler and direct without needing to check the validity of solution, we presenta shortcut for the method. At first we write the general formof the Schrodinger-like equation (1) ina moregeneralized form as

$$\Psi''(s) + \frac{c_1 - c_2 s}{s(1 - c_3 s)}\Psi'(s) + \frac{1}{s^2(1 - c_3 s)^2}[-\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3]\Psi(s) = 0 \qquad (2)$$

Satisfying the wave functions$\psi_n(s) = \varphi(s) y_n(s)$ (3)

Comparing Eq. (2) with its counterpart in (1), we obtain the following identifications:

$$\tilde{\tau}(s) = (c_1 - c_2 s)$$
$$\sigma(s) = s(1 - c_3 s) \quad (4)$$
$$\bar{\sigma}(s) = -\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3$$

Following the NU method, we obtain the bound-state energy condition

$$c_2 n - (2n+1)c_5 + (2n+1)(\sqrt{c_9} + c3\sqrt{c_8}) + n(n-1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0 \quad (5)$$

resulting also in

$$\varphi(s) = s^{c12}(1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}}, \quad (6)$$

$$y_n(s) = P_n^{\left(c_{10} - 1, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1 - 2c_3 s), \quad (7)$$

so that the wave function becomes

$$R_n(s) = N_{n,l} S^{c_{12}} (1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{\left(c_{10} - 1, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1 - 2c_3 s) \quad (8)$$

Where

$$c_4 = \frac{1}{2}(1 - c_1),\ c_5 = \frac{1}{2}(c_2 - 2c_3),\ c_6 = c_5{}^2 + \epsilon_1,\ c_7 = 2c_4 c_5 - \epsilon_2,\ c_8 = c_4{}^2 + \epsilon_3,$$
$$c_9 = c_3 c_7 + c_3{}^2 c_8 + c_6,\quad c_{10} = c_1 + 2c_4 + 2\sqrt{c_8} c_{11} = c_2 - 2c_5 + 2(\sqrt{c_9} + c3\sqrt{c_8}),$$
$$c_{12} = c_4 + \sqrt{c_8},\ c_{13} = c_5 - (\sqrt{c_9} + c3\sqrt{c_8}) \quad (9)$$

and P_n is the orthogonal polynomials.

Given that $P_n^{(\alpha,\beta)}(x) = \sum_{r=0}^{n} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(\alpha+r+1)\Gamma(n+\beta-r+1)(n-r)!r!} \left(\frac{x-1}{2}\right)^r \left(\frac{x+1}{2}\right)^{n-r}$ (10)

This can also be expressed in terms of the Rodriguez's formula

$$P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n n!}(x-1)^{-\alpha}(x+1)^{-\beta}\left(\frac{d}{dx}\right)^n \left((x-1)^{n+\alpha}(x+1)^{n+\beta}\right) \quad (11)$$

2.2 FACTORIZATION METHOD

In spherical coordinate, the Schrödinger equation with the potential $V(r)$ is given as

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\Psi(r,\theta,\varphi) + V(r)\Psi(r,\theta,\varphi) = E\Psi(r,\theta,\varphi) \quad (12)$$

Using the common ansatz for the wave function as

$$\Psi(r,\theta,\varphi) = \frac{R(r)}{r} Y_{l,m}(\theta,\varphi) \quad (13)$$

And substituting eq. (13) into eq. (12), we obtain the following set of equation

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[(E - V) - \frac{\lambda\hbar^2}{2\mu r^2}\right] R_{nl} = 0 \quad (14)$$

$$\frac{d^2\Theta(\theta)}{d\theta^2}+cot\theta\frac{d\Theta(\theta)}{d\theta}\left(\lambda-\frac{m^2}{sin^2\theta}\right)\Theta(\theta)=0 \quad (15)$$

$$\frac{d^2\Phi(\varphi)}{d\theta^2}+m^2\Phi(\varphi)=0 \quad (16)$$

Where m^2 and $\lambda=l(l+N-2)$ are the separation constant.

Eqn. (16) is spherical harmonic functions whose solutions are well known.

3. BOUND STATE SOLUTION OF THE RADIAL PART OF SCHRÖDINGER EQUATION WITH KRPHP POTENTIAL

N-dimensional Schrodinger Equation with vector V(r), potential in atomic units (ħ = c = 1) is given as

$$\frac{d^2R_{nl}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[(E-V)-\frac{l(l+N-2)\hbar^2}{2\mu r^2}\right]R_{nl}=0 \quad (14)$$

The Pseudoharmonic potential is given as

$$V(r)=Ar^2+\frac{B}{r^2}+C \quad (17)$$

For Reduced Pseudoharmonic Potential (RPHP) also called inversely quadratic Coulombic-like Potential, we assume $A=C=0$, therefore our Potential becomes

$$V(r)=\frac{B}{r^2} \quad (18)$$

For the Kratzer Potential, $V(r)=\frac{V_1e^{-\alpha r}}{(1-e^{-\alpha r})}$ (19)

Applying the transformation $S=e^{-\alpha r}$ and pekeris-type approximation

The superposed potential can be represented as

$$V(s)=\frac{V_1s}{(1-s)}+\frac{4B\alpha^2s}{(1-s)^2} \quad (20)$$

Applying the pekeris-type approximation $\frac{1}{r^2}=\frac{4\alpha^2}{(1-s)^2}$ and after lengthy algebra, we have

$$\frac{d^2R(s)}{ds^2}+\frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds}+\frac{1}{(1-s)^2s^2}[(2\beta^2+H)s^2+(-H-4\beta^2)s+(2\beta^2-2P-\lambda)]R(s)=0 \quad (21)$$

Where

$$-\beta^2=\left(\frac{\mu E}{4\alpha^2\hbar^2}\right),\ H=\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1,\ P=\left(\frac{\mu}{\hbar^2}\right)B,\ \lambda=l(l+N-2) \quad (22)$$

$$c_1=c_2=c_3=1, c_4=0, c_5=-\frac{1}{2}, c_6=\frac{1}{4}+2\beta^2+H, c_7=-4\beta^2-H,$$

$c_8 = 2\beta^2 - 2P - \lambda, c_9 = \frac{1}{4} - \lambda - 2P, c_{10} = 1 + 2\sqrt{2\beta^2 - 2P - \lambda}, c_{11} = 2 + 2\left(\sqrt{\frac{1}{4} - \lambda - 2P} + \sqrt{2\beta^2 - 2P - \lambda}\right), c_{12} = \sqrt{2\beta^2 - 2P - \lambda}\,, c_{13} = -\frac{1}{2} - \left(\sqrt{\frac{1}{4} - \lambda - 2P} + \sqrt{2\beta^2 - 2P - \lambda}\right), \varepsilon_1 = 2\beta^2 + H, \varepsilon_2 = 4\beta^2 + H, \varepsilon_3 = 2\beta^2 + 2P - \lambda$ (23)

Using the eigenvalue equation, the energy eigen spectrum of KRPHOP is found to be

$$\beta^2 = \left[\frac{(4P+2\lambda+H)-\left(n^2+n-\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-\lambda-2P}}{\left(n+\frac{1}{2}\right)+2\sqrt{\frac{1}{4}-\lambda-2P}}\right]^2 - (2P - \lambda) \quad (24)$$

The above equation can be solved explicitly and the energy eigen spectrum of KRPHOP becomes

$$E = \frac{2\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(4\left(\frac{\mu}{\hbar^2}\right)B+2l(l+N-2)+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1\right)-\left(n^2+n+\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-l(l+N-2)-2\left(\frac{\mu}{\hbar^2}\right)B}}{\left(n+\frac{1}{2}\right)+2\sqrt{\frac{1}{4}-l(l+N-2)-2\left(\frac{\mu}{\hbar^2}\right)B}}\right]^2\right\} - \left(2\left(\frac{\mu}{\hbar^2}\right)B - l(l+N-2)\right)$$
(25)

Eigen function consideration

The weight function $\rho(s)$ is given as

$$\rho(s) = s^{c_{10}-1}(1 - c_3 s)^{\frac{c_{11}}{c_3} - c_{10} - 1} \quad (26)$$

Using equation (23)on eqn. (26), we get the weight function as

$$\rho(s) = s^u(1 - s)^v \quad (27)$$

Where $u = 2\sqrt{2\beta^2 - 2P - \lambda}$, and $v = 2\sqrt{\frac{1}{4} - \lambda - 2P}$

Also we obtain the wave function $X_n(s)$ as

$$X_n(s) = p_n^{(u,v)}(1 - 2s), \quad (28)$$

Where $p_n^{(u,v)}$are Jacobi polynomials

Lastly, $\varphi(s) = s^{c_{12}}(1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}}$ (6)

Using equation (23) we get

$$\varphi(s) = s^{u/2}(1 - s)^{1+v/2} \quad (29)$$

We obtain Radial wavefunction from equation (3)

$$R_n(s) = N_n\varphi(s)X_n(s) \quad (30)$$

as

$$R_n(s) = N_n s^{u/2}(1 - s)^{1+v/2} P_n^{(u,v)}(1 - 2s) \quad (31)$$

Where n is a positive integer and N_n is the normalization constant.

4. DISCUSSION

In this section, we discuss the special potential eigenvalue energy of our superposed potentials (KRPHOP)

4.1. When$\boldsymbol{V_1 = 0}$in equation (20), the eigenvalue spectrum in equation (25) is reduced to a Reduced Pseudoharmonic Oscillator Potential given as

$$E = \frac{2\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(4\left(\frac{\mu}{\hbar^2}\right)B+2l(l+N-2)\right)-\left(n^2+n+\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-l(l+N-2)-2\left(\frac{\mu}{\hbar^2}\right)B}}{\left(n+\frac{1}{2}\right)+2\sqrt{\frac{1}{4}-l(l+N-2)-2\left(\frac{\mu}{\hbar^2}\right)B}}\right]^2\right\}-\left(2\left(\frac{\mu}{\hbar^2}\right)B-l(l+N-2)\right) \qquad (32)$$

4.2. When$\boldsymbol{B = 0}$ in equation (20), the eigenvalue spectrum in equation (25) is reduced to a Kratzer type Potential given as

$$E = \frac{2\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(2l(l+N-2)+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1\right)-\left(n^2+n+\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-l(l+N-2)}}{\left(n+\frac{1}{2}\right)+2\sqrt{\frac{1}{4}-l(l+N-2)}}\right]^2\right\}-\left(l(l+N-2)\right) \qquad (33)$$

4.3. When$\boldsymbol{\lambda = 0}$in equation (25), the eigenvalue spectrum is reduced to a pure Schrodinger equation for Kratzer and Pseudoharmonic oscillator potential given as

$$E = \frac{2\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(4\left(\frac{\mu}{\hbar^2}\right)B+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1\right)-\left(n^2+n+\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-2\left(\frac{\mu}{\hbar^2}\right)B}}{\left(n+\frac{1}{2}\right)+2\sqrt{\frac{1}{4}-2\left(\frac{\mu}{\hbar^2}\right)B}}\right]^2\right\}-\left(2\left(\frac{\mu}{\hbar^2}\right)B\right) \qquad (34)$$

5. CONCLUSION

In this study, we investigate the solution of the Schrodinger equation for theKratzerplusReducedPseudoharmonic potential by using thepeketris type approximation for the centrifugal term. We obtain the energy eigenvalue and the corresponding un-normalized wavefunction using Nikiforov-Uvarov Method.Futhermore, special conditions of potential have been presented by variation of some parameters associated with each potential.

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