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SOLUTIONS OF THE SCHRÖDINGER EQUATION WITH INVERSELY QUADRATIC YUKAWA PLUS WOODS-SAXON POTENTIAL USING NIKIFOROV-UVAROV METHOD

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ABSTRACT

The solutions of the Schrödinger equation with inversely quadratic Yukawa plus Woods-Saxon potential (IQYWSP) have been presented using the parametric Nikiforov-Uvarov (NU) method. The bound state energy eigenvalues and the corresponding un-normalized eigen functions are obtained in terms of Jacobi polynomials. Also, a special case of the potential has been considered and its energy eigen values obtained. The result of the work could be applied to molecules moving under the influence of IQYWSP potential as negative energy eigenvalues obtained indicate a bound state system.

Keywords

Schrödinger equation, inversely quadratic Yukawa potential, Woods-Saxon potential, Nikiforov-Uvarov method, Laguerre polynomials

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In non-relativistic quantum mechanics, one of the interesting problems is to obtain exact solutions of the Schrödinger equation. In order to do this, a real potential is normally chosen to derive the energy eigenvalues and the eigen functions of the Schrödinger equation. [1] These solutions describe the particle dynamics in non-relativistic quantum mechanics. Many authors have studied the bound states of the Schrödinger equation using different potentials and methods. [2-10] Some of these potentials play very important roles in many fields of Physics such as Molecular Physics, Solid State and Chemical Physics. [11] The Woods-Saxon potential, either in its spherical or deformed form, has been used more in nuclear numerical calculations. [12 – 16] Dudek et al [17] have also used the Woods-Saxon potential to study the behaviour of valence electrons in metallic systems. The details of the Woods-Saxon potential are described by free parameters such as depth, width and slope of the potential, which have been fitted to experimental observation.[1] The inversely quadratic Yukawa potential was first studied in 2012 by Hamzavi et al [18] when they obtained approximate spin and pseudospin solutions to the Dirac equation with the potential including a tensor interaction. Since, then several papers on the potential have appeared in the literature. [19-21].

The purpose of the present paper is to solve the Schrödinger equation for the mixed potential IQYWSP using the parametric NU method. The paper is organized as follows: After a brief introduction in section 1, the NU method is reviewed in section 2. In section 3, we solve the radial Schrödinger equation using the NU method. Finally, we discuss our results in section 4 and a brief conclusion is then advanced in section 5.

Nikiforov-Uvarov Method

The Nikiforov-Uvarov (NU) method is based on the solutions of a generalized second-order linear differential equation with special orthogonal functions. [22] The Schrödinger equation and Schrödinger-like equations of the type as:

$$\psi''(r) + [E - V(r)]\psi(r) = 0, \tag{1}$$

can be solved by this method. This can be done by transforming equation (1) into an equation of hypergeometric type with appropriate coordinate transformation $s = s(r)$ to get

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

To solve equation (2) we can use the parametric NU method. The parametric generalization of the NU method is expressed by the generalized hypergeometric type equation [23]

$$\psi''(s) + \frac{(c_1 - c_2 s)}{s(1 - c_3 s)}\psi'(s) + \frac{1}{s^2(1 - c_3 s)^2}[-\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3]\psi(s) = 0, \tag{3}$$

where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials atmost second degree, and $\bar{\tau}(s)$ is a first degree polynomial. The eigen functions (equation 4) and corresponding eigenvalues (equation 5) to the equation become

$$\psi(s) = N_n s^{c_{12}}(1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{\left(c_{10} - 1, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1 - 2c_3 s), \tag{4}$$

$$(c_2 - c_3)n + c_3 n^2 - (2n+1)c_5 + (2n+1)\left(\sqrt{c_9} + c_3\sqrt{c_8}\right) + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0, \tag{5}$$

Where

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

$$c_{13} = c_5 - \left(\sqrt{c_9} + c_3\sqrt{c_8}\right), \tag{6}$$

N_n is the normalization constant and $P_n^{(\alpha,\beta)}$ are the Jacobi polynomials.

Solutions of the Radial Schrödinger Equation

The radial Schrödinger equation is given as [23]

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{\lambda\hbar^2}{2\mu r^2}\right]R_{nl}(r), \tag{7}$$

Where $\lambda = l(l+1)$ and $V(r)$ is the potential energy function. The inversely quadratic Yukawa potential (IQYP) is given as [18]

$$V(r) = -\frac{V_0' e^{-2\alpha r}}{r^2}, \tag{8}$$

The Woods-Saxon potential (WSP) is given as [1]

$$V(r) = -\frac{V_o}{1 + e^{2\alpha r}}, \tag{9}$$

Where V_0 and V_0' are the potential depths of the WSP and IQYP respectively and α is an adjustable positive parameter. The sum of these potentials known as IQYWSP is given as

$$V(r) = -\frac{V_o}{1 + e^{2\alpha r}} - \frac{V_0'}{r^2 e^{2\alpha r}}, \tag{10}$$

Making the transformation $s=-e^{-2\alpha r}$ equation (10) becomes

$$V(s,r)=\frac{V_0 s}{1-s}+\frac{V_0' s}{r^2}, \tag{11}$$

Again, applying the transformation $s=-e^{-2\alpha r}$ to get the form that NU method is applicable, equation (7) gives a generalized hypergeometric-type equation as

$$\frac{d^2R(s)}{ds^2}+\frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds}+\frac{1}{(1-s)^2s^2}\left[-\beta^2s^2+\left(2\beta^2+A\right)s-\left(\beta^2-B\right)\right]R(s)=0, \tag{12}$$

Where

$$\lambda=0,-\beta^2=\frac{\mu E}{2\alpha^2\hbar^2},A=\frac{\mu V_0}{2\alpha^2\hbar^2}-\frac{2\mu V_0'}{\hbar^2},B=-\frac{\mu V_0}{2\alpha^2\hbar^2},\frac{1}{r^2}\approx\frac{4\alpha^2}{(1+e^{-2\alpha r})^2}\approx\frac{4\alpha^2}{(1-s)^2}, \tag{13}$$

Comparing equation (12) with equation (3) yields the following parameters

$$c_1=c_2=c_3=1,c_4=0,c_5=-\frac{1}{2},c_6=\frac{1}{4}+\beta^2,c_7=-2\beta^2-A,c_8=\beta^2-B,c_9=\frac{1}{4}-(A+B),c_{10}=1+2\sqrt{\beta^2-B},c_{11}=2+2\left(\sqrt{\frac{1}{4}-A-B}+\sqrt{\beta^2-B}\right),c_{12}=\sqrt{\beta^2-B},c_{13}=-\frac{1}{2}-\left(\sqrt{\frac{1}{4}-A-B}+\sqrt{\beta^2-B}\right),\epsilon_1=\beta^2,\epsilon_2=2\beta^2+A,\epsilon_3=\beta^2-B, \tag{14}$$

Now using equations (5), (13) and (14) we obtain the energy eigen spectrum of the IQYWSP as

$$\beta^2=\left[\frac{2B+A-\left(n^2+n+\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}-A-B}}{(2n+1)+2\sqrt{\frac{1}{4}-A-B}}\right]^2+B, \tag{15}$$

Equation (15) can be solved explicitly and the energy eigen spectrum of IQYWSP becomes

$$E=-\frac{2\alpha^2\hbar^2}{\mu}\left\{\left[\frac{-\frac{2\mu V_0'}{\hbar^2}-\frac{\mu V_0}{2\alpha^2\hbar^2}-\left(n^2+n+\frac{1}{2}\right)\sqrt{\frac{1}{4}-\frac{2\mu V_0'}{\hbar^2}}}{(2n+1)+2\sqrt{\frac{1}{4}-\frac{2\mu V_0'}{\hbar^2}}}\right]^2\right\}, \tag{16}$$

We now calculate the radial wave function of the IQYWSP as follows

The weight function $\rho(s)$ is given as [23]

$$\rho(s)=s^{c_{10}-1}(1-c_3s)^{\frac{c_{11}}{c_3}-c_{10}-1}, \tag{17}$$

Using equation (14) we get the weight function as

$$\rho(s)=s^{\omega}(1-s)^{\vartheta}, \tag{18}$$

Where $\omega=2\sqrt{\beta^2-B}$ and $\vartheta=2+2\sqrt{\frac{1}{4}-A-B}$

Also we obtain the wave function $\chi(s)$ as [23]

$$\chi(s)=P_n^{c_{10}-1,\frac{c_{11}}{c_3}-c_{10}-1}(1-2c_3s), \tag{19}$$

Using equation (14) we get the function $\chi(s)$ as

$$\chi(s)=P_n^{(\omega,\vartheta)}(1-2s), \tag{20}$$

Where $P_n^{(\omega,\vartheta)}$ are Jacobi polynomials

Lastly,

$$\varphi(s)=s^{c_{12}}(1-c_3s)^{-c_{12}-\frac{c_{13}}{c_3}}, \tag{21}$$

And using equation (14) we get

$$\varphi(s)=s^{\omega/2}(1-s)^{\vartheta-1/2}, \tag{22}$$

We then obtain the radial wave function from the equation [23]

$$R_n(s)=N_n\varphi(s)\chi_n(s), \tag{23}$$

As

$$R_n(s) = N_n s^{\omega/2}(1-s)^{\vartheta-1/2} P_n^{(\omega,\vartheta)}(1-2s), \tag{24}$$

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

DISCUSSION

We have solved the radial Schrödinger equation and obtained the energy eigen values for the inversely quadratic Yukawa plus Woods-Saxon potential (IQYWSP) in equation (16). If $V_0' = 0$ in equation (10), the potential turns back into the Woods-Saxon potential and equation (16) yields the energy eigen values of the Woods-Saxon potential as

$$E = -\frac{\hbar^2}{2a^2\mu}\left[\left(\frac{\mu a^2 V_0}{\hbar^2(n+1)}\right)^2 + \left(\frac{n+1}{2}\right)^2 + \frac{\mu a^2 V_0}{\hbar^2}\right], \tag{25}$$

Where we have used $\frac{1}{a} = 2\alpha$

Equation (25) is similar to equation (22) of the reference [1] obtained for the Woods-Saxon potential in the Schrödinger formalism. Table 1 reveals that bound state energy eigenvalues are obtained which increase in magnitude with increase in the principal quantum number, n as well as the increase in the screening parameter which is plausible. We suggest that our results can be applied to understanding molecules moving under the IQYWSP potential. Fig. 1 represents the plot of IQYWSP and its approximation. The fact that the plots overlap is indicative that our approximation is correct.

CONCLUSION

We have obtained the energy eigen values and the corresponding un-normalized wave function using the parametric NU method for the Schrödinger equation with IQYWSP. A special case of the potential has also been considered.

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Table 1. Energy spectrum for different values of α for IQYWSP

n	Energy Spectrum		
	α = 0.5	α = 0.2	α = 0.4
1	-0.01426	-0.00034	-0.005699765
2	-0.08903	-0.00224	-0.036209583
3	-0.23544	-0.00598	-0.096103554
4	-0.45673	-0.01164	-0.186692537
5	-0.75429	-0.01925	-0.30853781
6	-1.12882	-0.02883	-0.461919373
7	-1.58071	-0.0404	-0.646992419

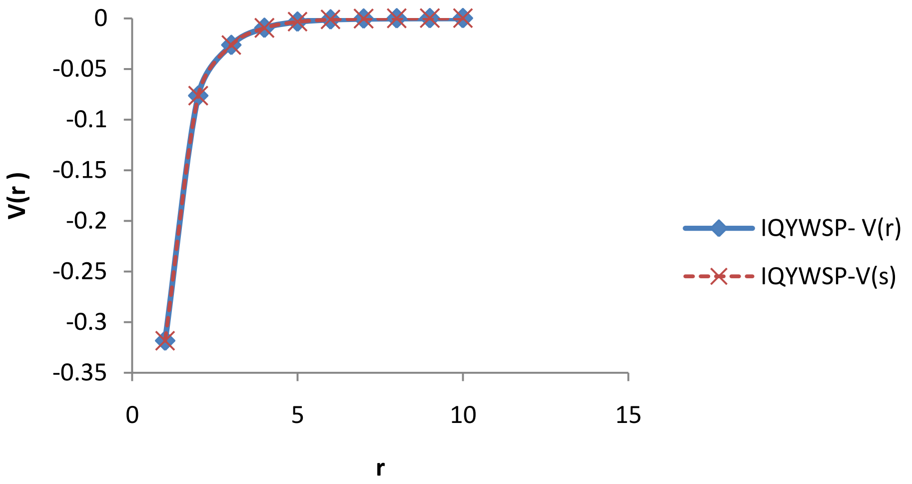

Fig. 1: Plot of IQYWS, V (r) and Approximated IQYWS, V(s) potential against r. The potentials overlap which shows the accuracy of the approximation