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I-state Solutions of the Relativistic and Non-Relativistic Wave Equations for Modified Hylleraas-Hulthen Potential Using the Nikiforov-Uvarov Quantum Formalism

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Abstract

An exact analytical and approximate solution of the relativistic and non-relativistic wave equations for central potentials has attracted enormous interest in recent years. By using the basic Nikiforov-Uvarov quantum mechanical concepts and formalism, the energy eigenvalue equations and the corresponding wave functions of the Klein–Gordon and Schrodinger equations with the interaction of Modified Hylleraas-Hulthen Potentials (MHHP) were obtained using the conventional Pekeris-type approximation scheme to the orbital centrifugal term.The corresponding unnormalized eigen functions are evaluated in terms of Jacobi polynomials.

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Introduction

Quantum mechanical Wavefunctions and their corresponding eigenvalues give significant information in describing various quantum systems[1-3]. Bound state solutions of relativistic and nonrelativistic wave equation arouse a lot of interest for decades. Schrodinger wave equations constitute nonrelativistic wave equation while Klein-Gordon and Dirac equations constitute the relativistic wave equations[1–5]. The quantum mechanical interacting potentials (MHHP) can be used to compute and predict the bound state energies for both homonuclear and

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heteronuclear diatomic molecules. Other potentials that have been used to investigate bound state solutions are as follows: Coulomb, Poschl-Teller, Yukawa, Hulthen, Hylleraas, pseudoharmonic, Eckart and many other potential combinations[6–13]. The aforementioned potentials are studied with some specific quantum mechanical methods and concepts like the following:Wentzel, Kramers, and Brillouin known as the WKB approximation, asymptotic iteration method, Nikiforov-Uvarov method, formular method, supersymmetric quantum mechanics approach, exact quantization, and many more[14–24].

In theoretical physics, the shape form of a potential plays a significant role, particularly when investigating the structure and natureof the interaction between systems. Therefore, our aim, in this present work, is to investigate approximate bound state solutions of the Klein-Gordon and Schrodinger equations with newly proposed Modified Hylleraas-Hulthen potential (MHHP) using the conventional parametric Nikiforov-Uvarov (NU) method. The solutions of this equation will definitely give us a wider and deeper knowledge of the properties of molecules moving under the influence of the mixed interacting potentials which is the goal of this paper. The parametric NU method is very convenient and does not require the truncation of a series like the series solution method which is more difficult to useThis article is divided into five sections. Section 1 is the introduction; Section 2 is the brief introduction of Nikiforov-Uvarov quantum mechanical concept. In Section 3, we presented the angular solutions to Klein-Gordon and Schrodinger wave equations using the proposed potential and obtained both the energy eigenvalue and their corresponding normalized. We gave a brief discussion and conclusion in sections 4 and 5 respectively.

Theory of Parametric Nikiforov-Uvarov Method

The parametric form is simply using parameters to obtain explicitly energy eigenvalues and it is still based on the solutions of a generalized second order linear differential equation with special orthogonal functions. The NU is based on solving the second order linear differential equation by reducing to a generalized equation of hyper-geometric type. This method has been used to solve the Schrödinger, Klein–Gordon and Dirac equation for different kind of potentials[24-31]. The second-order differential equation of the NU method has the form.

$$\Psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi_n'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\Psi_n(s) = 0 \quad \text{....(1)}$$

Where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials at most second degree and $\tilde{\tau}(s)$ is first degree polynomials. The parametric generalization of the N-U method is given by the generalized hypergeometric-type equation

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

Thus eqn. (2) can be solved by comparing it with equation (3) and the following polynomials are obtained

$$\tilde{\tau}(s) = (c_1 - c_2 s),\ \sigma(s) = s(1-c_3 s),\ \bar{\sigma}(s) = -\epsilon_1 s_2 + \epsilon_2 s - \epsilon_3 \quad \text{....(3)}$$

The parameters obtainable from equation (4) serve as important tools to finding the energy eigenvalue and eigenfunctions. They satisfy the following sets of equation respectively

$$c_2 n - (2n+1)c_5 + (2n+1)(\sqrt{c_9} + c_3\sqrt{c_8}) + n(n-1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{(c_8 c_9)} = 0 \quad \text{....(4)}$$

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

While the wave function is given as

$$\Psi_n(s) = N_{n,l} S^{c_{12}} (1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{\left(c_{10} - 1, \frac{c_{11}}{c_3} - c_{10} - 1\right)} (1 - 2c_3 s) \quad \text{....(6)}$$

Where

$c_4 = 1/2\,(1 - c_1)$, $c_5 = 1/2\,(c_2 - 2c_3)$, $c_6 = c_5^2 + \epsilon_1$, $c_7 = 2c_4 c_5 - \epsilon_2$, $c_8 = c_4^2 + \epsilon_3$,

$c_9 = c_3 c_7 + c_3^2 c_8 + c_6$, $c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}$, $c_{11} = c_2 - 2c_5 + 2(\sqrt{c_9} + c3\sqrt{(c_8)})$

$c_{12} = c_4 + \sqrt{c_8}$, $c_{13} = c_5 - (\sqrt{c_9} + c3\sqrt{c_8})$ ....(7)

and P_n is the orthogonal polynomials.

Solutions of the Wave Equations

Solutions of the Klein-Gordon Equation

The Klein-Gordon Equation[29] with vector V(r), potential in atomic units (ħ = c = 1) is given as

$$\frac{d^2 R(r)}{dr^2} + \left[(E^2 - M^2) - 2(E+M)V(r) + \frac{l(l+1)}{r^2}\right] R(r) = 0 \quad ....(8)$$

Where E,M,l and V(r) are the Energy, reduced mass, angular momentum and potential

The Modified Hylleraas Potential

The Modified Hylleras Potential as proposed by ref.[32] is given as:

$$V(s) = -\frac{V_o}{b}\left(\frac{a-s}{1-s}\right) \quad .....(9a)$$

wherea and b are Hyllera as potential screening parameterswhile V_ois the potential depth and S is the transformation, thus

$$S = e^{-2\alpha r} \quad .....(9b)$$

Eqn. (9b) is the relationship between S and r, the so-called transformation!

The Hulthen Potential

The Hulthen potential is one of the important short-range potentials, which behaves like a Coulomb potential for small values of r and decreases exponentially for large values ofr [33]. The Hulthen potential in it simplest form is given as:

$$V(s) = -\frac{V_o s}{(1-s)} \quad ....(10)$$

Where V_o and S are the potential depth and the transformation parameter respectively.

The Modified Hylleraas-Hulthen Potential

The Modified Hylleraas-Hulthen potential is our newly proposed interacting potential which is formed by combining eqns.(9) and (10) to get eqn.(11) given as:

$$V(s) = -\frac{V_o s}{(1-s)} + \frac{V_o}{b}\left(\frac{a-s}{1-s}\right) \quad ....(11)$$

Where all the parameters have their usual meaning Substitute eqn. (11) into eqn. (8) gives:

$$\frac{d^2 R(r)}{dr^2} + \left[(E^2 - M^2) - 2(E+M) - \frac{V_o s}{(1-s)} + \frac{V_o}{b}\left(\frac{a-s}{1-s}\right) + \frac{l(l+1)}{r^2}\right] R(r) = 0 \quad ....(12)$$

Applying the Pekeris-like approximation given as 1/ $\frac{1}{r^2} = \frac{4\alpha^2}{(1-s)^2}$ [25-31], to eq. (12) enable us completely solve eq. (8).

Again, applying the transformation $s=e^{-2\alpha r}$ to get the form that NU method is applicable, equation (8) gives a generalized hypergeometric-type equation as

$$\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds} + \frac{1}{(1-s)^2 s^2}[(\beta^2 - B - H)s^2 + (B + H + K + P - 2\beta^2)s + (\beta^2 - P)]R(s) = 0 \quad ....(13)$$

Where

$$\beta^2 = \left(\frac{E^2+M_o^2}{4\alpha^2}\right), B = \left(\frac{E+M_o}{2\alpha^2}\right)V_o, k = l(l+1), P = \left(\frac{E+M_o}{2b\alpha^2}\right)V_o a, H = \left(\frac{E+M_o}{2b\alpha^2}\right)V_o \quad ....(14)$$

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

$$c_8 = \beta^2 - P, c_9 = \frac{1}{4} + K, c_{10} = 1 + 2\sqrt{\beta^2 - P}, c_{11} = 2 + 2\left(\sqrt{\frac{1}{4} + K} + \sqrt{\beta^2 - P}\right), c_{12} = \sqrt{\beta^2 - P}, c_{13} = -\frac{1}{2} - \left(\sqrt{\frac{1}{4} + K} + \sqrt{\beta^2 - P}\right), \varepsilon_1 = \beta^2 - B - H, \varepsilon_2 = 2\beta^2 - B - H - K - p, \varepsilon_3 = \beta^2 - P \quad ....(15)$$

Now using equations (6), (14) and (15) we obtain the energyeigen spectrum of the newly proposed interacting potential (MHHP) given as:

$$\beta^2 = \left[\frac{-(P+H+B+K) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}+K}}{(2n+1)+2\sqrt{\frac{1}{4}+K}}\right]^2 + P \quad ...(16)$$

The above equation can be solved explicitly and the energyeigen spectrum of the Klein-Gordon equation with MHHP becomes

$$E^2 - M^2 = -4\alpha^2\left\{\left[\frac{-\left(\left(\frac{E+M_o}{2b\alpha^2}\right)V_o a + \left(\frac{E+M_o}{2b\alpha^2}\right)V_o + \left(\frac{E+M_o}{2\alpha^2}\right)V_o + l(l+1)\right) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}+(l(l+1))}}{(2n+1)\sqrt{\frac{1}{4}+(l(l+1))}}\right]\right\} - \left(\frac{E+M_o}{2b\alpha^2}\right)V_o a \quad ....(17)$$

Solutions of the Schrodinger Equation

The l-State Schrodinger Equation[27] with vector V(r), potential is given as

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[(E - V(r)) + \frac{l(l+1)\hbar^2}{2\mu r^2}\right] R(r) = 0 \quad ....(18)$$

Where E,V(r),μ and l are the energy, potential, reduced mass and angular momentum respectively Substitute eqn. (11) into eqn. (18) we have

$$\frac{d^2R(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[\left(E+\left(\left(\frac{V_0 s}{1-s}\right)+\frac{V_0}{b}\left(\frac{a-s}{1-s}\right)\right)\right)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r)=0 \quad \text{....(19)}$$

Applying the Pekeris-like approximation given as $\frac{1}{r^2}=\frac{4\alpha^2}{(1-s)^2}$ [25-31], to eq. (19) enable us completely solve eq. (18).

Again, applying the transformation $s=e^{-2\alpha r}$ to get the form that NU method is applicable, equation (18) gives a generalized hypergeometric-type equation as

$$\frac{d^2R(s)}{ds^2}+\frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds}+\frac{1}{(1-s)^2s^2}[(2\beta^2-B+H)s^2+(B+K-H-P-4\beta^2)s+(2\beta^2+P)]R(s)=0 \quad \text{....(20)}$$

Where

$$\beta^2=\left(\frac{\mu E}{4\alpha^2\hbar^2}\right), B=\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o, k=l(l+1), P=\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o a, H=\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o \quad \text{....(21)}$$

$$c_1=c_2=c_3=1, c_4=0, c_5=-\frac{1}{2}, c_6=\frac{1}{4}+2\beta^2-B+H, c_7=-4\beta^2+B-P-H+K, c_8=2\beta^2+P, c_9=\frac{1}{4}+K, c_{10}=1+2\sqrt{2\beta^2+P}, c_{11}=2+2\left(\sqrt{\frac{1}{4}+K}+\sqrt{2\beta^2+P}\right), c_{12}=\sqrt{2\beta^2+P}, c_{13}=-\frac{1}{2}-\left(\sqrt{\frac{1}{4}+K}+\sqrt{2\beta^2+P}\right), \varepsilon_1=2\beta^2-B+H, \varepsilon_2=4\beta^2-B+P-K+H, \varepsilon_3=2\beta^2+P \quad \text{....(22)}$$

Similarly, using equations (6), (21) and (22) we obtain the energyeigen spectrum of the newly proposed interacting potential (MHHP) for Schrodinger equation given as:

$$\beta^2=\left[\frac{(P+H)-(B+K)-\left(n^2+n-\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}+K}}{(2n+1)+2\sqrt{\frac{1}{4}+K}}\right]^2-P \quad \text{....(23)}$$

The above equation can be solved explicitly and the energyeigen spectrum of Schrodinger equation with MHHP becomes

$$E=\frac{4\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o a+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o\right)-\left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o+l(l+1)\right)-\left(n^2+n-\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}+l(l+1)}}{(2n+1)+2\sqrt{\frac{1}{4}+l(l+1)}}\right]\right\}-\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_o a \quad \text{....(24)}$$

Wave Functions

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

$$\rho(s)=s^u(1-qs)^v \quad \text{....(25)}$$

Where
$u=\beta^2$ -B-H-K-p, and $v=2\sqrt{(\beta^2-P)}$

$$X_n(s)=p_n^{(u,v)}(1-2s), \quad \text{....(26)}$$

$$\phi(s)=s^{u/2}(1-s)^{1+v/2} \quad \text{....(27)}$$

Using equation (6) we get the function $\chi(s)$ as

$$\chi(s)=P_n^{(U,V)}(1-2s), \quad \text{....(28)}$$

Where $P_n^{(U,V)}$ are Jacobi polynomials
Lastly,

$$\phi(s)=s^{c12}(1-c_3 s)-c_{12}-c_{13}/c_3 \quad \text{....(29)}$$

And using equation (6) we get

$$\phi(s)=s^{U/2}(1-s)^{V-1/2}, \quad \text{....(30)}$$

We then obtain the radial wave function from the equation

$$R_n(s)=N_n\phi(s)\chi_n(s),$$

As

$$R_n(s)=N_n s^{U/2}(1-s)^{(V-1)/2}P_n^{(U,V)}(1-2s), \quad \text{....(31)}$$

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

Discussion

In this section, we are going to consider certain case of potential evaluation to enable check the behavior of the obtained bound state solutions:

When $V_o=0$, eqn. (24) is reduced to l-state solution of the Schrodinger equation with no potential interaction:

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

Similarly, eqn (17) is also reduced to l-state solution of the Klein-Gordon equation in the absence of interacting potential

$$E^2 - M^2 = -4\alpha^2 \left\{ \left[\frac{-(l(l+1)) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}+(l(l+1))}}{(2n+1)\sqrt{\frac{1}{4}+(l(l+1))}} \right] \right\} \quad ....(33)$$

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Conclusion

In this paper, we solved explicitly the Klein-Gordon and Schrodinger equations for the modified Hylleraas plus Hulthen potential for arbitrary states by using the parametric form of the Nikiforov-Uvarov method. By using the Pekeris-type approximation for the centrifugal term, we obtained approximately the energy eigenvalues and the unnormalized wave function expressed in terms of the Jacobi polynomials for arbitrary wave states. It is hope that the results we obtained in this research work could enlarge and enhance the application of the Hylleraas-Hulthen potentials (which is our newly proposed potentials) in the relevant fields of physics and atomic spectroscopy.

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