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Yukawa-angle Dependent Potential and its Applications to Diatomic Molecules under Schrodinger wave Equation

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Abstract

In this paper, we have solved the Schrödinger wave equation with Yukawa plus novel angle dependent potential using powerful Nikiforov-Uvarov method and obtained the energy eigenvalues and corresponding wave functions in terms of Jacobi and Laguerre polynomials for the angular and radial part respectively. We have also presented the effect of angle dependent solution on radial solutions and also applied our results to obtain numerical values for some selected diatomic molecules. We also studied the behavior of our potential graphically for H_2 diatomic molecule.

Keywords: Noncentral potential, Diatomic molecules, Nikiforov-Uvarov method, Yukawa potential, Novel angle dependent potential.

Introduction

Noncentral potential has been studied in various fields of nuclear physics and quantum chemistry which could be used for the interaction between deformed pair of nuclei and ring shaped molecules like benzenes [1-5]. Yukawa potential is one of the short ranged potentials that have been studied in physics, they have coulombic behavior for small r and are exponentially damped for large r, and they have limited number of bound states characterized by the presence of the screening parameter α [6-10]. This model receives great attention due to the fact that it plays an important role in high energy and particle physics, atomic physics, chemical physics, gravitational plasma physics and solid state physics. In solid state physics and atomic physics, it is called the Thomas-Fermi or screened coulomb potential while in plasma physics it is known as the Debye-Huckel potential [11,12].

There have been continuous interest in the solutions of Schrödinger equation, Klein-Gordon and Dirac equations for some noncentral potential. These equations are solved by using different methods for both exact and approximate solvable potentials. Antia et al solved approximately the Schrödinger equation with Hulthen-Yukawa plus angle dependent potential using Nikiforov-Uvarov (NU) method [13]. Yasuk et al presented an alternative and simple method for the exact solution of the Klein-Gordon equation in the presence of noncental equal scalar and vector potential by using NU method [14]. Hamzavi and Rajabi solved exactly the Dirac Equation with coulomb plus a novel angle-dependent potential using NU method [15]. They also applied the Schrodinger wave equation to solve the novel angle dependent potential using NU method [16].

The novel angle dependent potential as introduced by Zhang and Huang Fu is [17].

$$V_\theta(\theta) = \frac{\gamma + \beta\cos^2\theta + \eta\cos^4\theta}{\cos^2\theta\sin^2\theta} \tag{1}$$

They solved the Dirac equation for oscillatory potential under a pseudospin symmetry unit. Therefore the motivation of this present work is to solve the Schrödinger equation with Yukawa plus novel angel dependent potential given as

$$V(r,\theta) = -\frac{V_0 e^{-\alpha r}}{r} + \frac{\hbar^2}{2\mu}\left(\frac{\gamma + \beta\cos^2\theta + \eta\cos^4\theta}{r^2\cos^2\theta\sin^2\theta}\right) \tag{2}$$

Our potential is suggested based on the motivation derived from the applications of Yukawa potential and ring-shaped potential. The former as already mentioned in the paper has a lot of applications in physics such as in atomic physics, chemical physics, plasma physics etc. The ring-shaped potential is to study the interaction between deformed pair of nuclei and ring-shaped molecules like benzene. With these, we suggested and studied these combined potential. The results would give a more unique applications to particles in this model.

By Taylor's series expansion

$$e^{-\alpha r} = 1 - \alpha r + \frac{(\alpha r)^2}{2!} - \frac{(\alpha r)^3}{3!} + \frac{(\alpha r)^4}{4!} + \ldots + O(\alpha) \tag{3}$$

We only use the series expansion to get rid of the exponential term since we wanted to work with a more direct form of the potential for easier application of our method for exact solution. And since the potential is a short range, we expanded it to truncate the higher terms of screening parameter, thus the first two terms are considered. This makes it applicable to diatomic molecules because they have short distance of separation between the atoms.

Applying this potential in Eq. (2) becomes

$$V(r,\theta) = -\frac{V_0}{r}(1-\alpha r) + \frac{\hbar^2}{2\mu}\frac{V_\theta(\theta)}{r^2} \tag{4}$$

where V_0 are the potential depths, α is the screening parameter, μ is the reduced mass and $\hbar$ is the reduced plank's constant , γ, β *and* η are arbitrary constants.

We shall obtain the solution of the radial and angle dependent part, present the effect of angle dependent solution on radial solutions and apply our results to some diatomic molecules such as H_2, CO, NO, N_2 and Ar_2.

The Generalized Parametric NIKIFOROV-UVAROV (NU) Method

The NU method was presented by Nikiforov and Uvarov [18] and has been employed to solve second order differential equations such as the Schrödinger wave equation (SWE), Klein-Gordon equation (KGE), Dirac equation (DE) etc. This method is not a variational method. The SWE

$$\psi''(r) + [E - V(r)]\psi(r) = 0 \tag{5}$$

can be solved by transforming it into a hypergeometric type equation through using the transformation, $s = s(r)$ and its resulting equation is expressed as

$$\psi''(s) + \frac{\bar{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \tag{6}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ must be polynomials of at most second degree and $\bar{\tau}(s)$ is a polynomial with at most first degree and $\psi(s)$ is a function of the hypergeometric type.

The parametric generalization of the NU method is given by the generalized hypergeometric-type equation as [19]

$$\psi''(s) + \frac{(c_1 - c_2 s)}{s(1-c_3 s)}\psi'(s) + \frac{1}{s^2(1-c_3 s)^2}\left[-\xi_1 s^2 + \xi_2 s - \xi_3\right]\psi(s) = 0. \tag{7}$$

Parametric form of Nikiforov-Uvarov method gives a more direct and reliable solutions to a second order differential equations which are transformed into hypergeometric equations compare to others. Equation (7) is solved by comparing it with Eq. (6) and the following polynomials are obtained:

$$\tilde{\tau}(s) = (c_1 - c_2 s),\ \sigma(s) = s(1-c_3 s),\ \tilde{\sigma}(s) = -\xi_1 s^2 + \xi_2 s - \xi_3. \tag{8}$$

According to the NU method, the energy eigenvalues equation and eigen functions respectively satisfy the following sets of equation

$$c_2 n - (2n+1)c_5 + (2n+1)\left(\sqrt{c_9} + c_3\sqrt{c_8}\right) + n(n-1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0, \tag{9}$$

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

where

$$c_4 = \frac{1}{2}(1-c_1),\ c_5 = \frac{1}{2}(c_2 - 2c_3),\ c_6 = c_5^2 + \xi_1,\ c_7 = 2c_4 c_5 - \xi_2,\ c_8 = c_4^2 + \xi_3,$$
$$c_9 = c_3 c_7 + c_3^2 c_8 + c_6,\ c_{10} = c_1 + 2c_4 + 2\sqrt{c_8},\ c_{11} = c_2 - 2c_5 + 2\left(\sqrt{c_9} + c_3\sqrt{c_8}\right),$$
$$c_{12} = c_4 + \sqrt{c_8},\ c_{13} = c_5 - \left(\sqrt{c_9} + c_3\sqrt{c_8}\right) \tag{11}$$

and $P_n^{(\alpha,\beta)}(s)$ is the orthogonal Jacobi polynomial.

In some problem $c_3 = 0$. For this type of problems we have

$$\lim_{c_3 \to 0} P_n^{\left(c_{10}-1, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1-2c_3 s) = L_n^{c_{10}-1}(c_{11} s) \tag{12}$$

And

$$\lim_{c_3 \to 0}(1-c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} = e^{c_{13} s} \tag{13}$$

And the solution given in Eq(10) becomes [20]

$$\psi(s) = N_{nl} s^{c_{12}} e^{c_{13} s} L_n^{c_{10}-1}(c_{11} s) \tag{14}$$

Where $L_n^{\alpha}(s)$ is the Laguerre polynomial.

Factorization Method

In spherical coordinate the Schrödinger equation with noncentral potential of Eq. (4) can be written as follows [21]

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$
$$\times\psi(r,\theta,\varphi) + \left(-\frac{V_0}{r}(1-\alpha r) + \frac{\hbar^2}{2\mu}\frac{V_\theta(\theta)}{r^2}\right)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi). \tag{15}$$

The total wave function in Eq. (15) can be defined as

$$\psi(r,\theta,\varphi) = \frac{R(r)}{r}Y(\theta,\varphi) \tag{16}$$

and by decomposing the spherical wave function in Eq. (15) using Eq. (16) the following equations are obtained:

$$\frac{d^2R(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2}\left(E + \frac{V_0}{r}(1-\alpha r)\right) - \frac{\lambda}{r^2}\right]R(r) = 0, \tag{17}$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}Y(\theta,\varphi)\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}Y(\theta,\varphi) + [\lambda - V_\theta(\theta)]Y(\theta,\varphi) = 0 \tag{18}$$

Substituting $Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$ into Eq. (18) yields:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left(\lambda - \frac{m^2}{\sin^2\theta} - V_\theta(\theta)\right)\Theta(\theta) = 0, \tag{19}$$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2}+m^2\Phi(\varphi)=0, \tag{20}$$

where $\lambda=l(l+1)$ and m^2 are the separation constants. The solution of Eq.(20) is well known [22]. Equations (17) and (19) are the radial and angular parts of Schrödinger equation respectively which are subject for discussion in the preceding section.

Solutions of the Radial Schrödinger Equation

For eigenvalues and corresponding eigen functions of the radial part of the Schrödinger equation from Eq.(17) we have;

$$\frac{d^2R(r)}{dr^2}+\left[\frac{2\mu}{\hbar^2}\left(E+\frac{V_0}{r}-V_0\alpha\right)-\frac{\lambda}{r^2}\right]R(r)=0. \tag{21}$$

Using the following dimensionless quantities

$$\varepsilon=\frac{2\mu E}{\hbar^2}, A'=\frac{2\mu V_o}{\hbar^2},\ B'=A'\alpha \tag{22}$$

We have

$$\frac{d^2R(s)}{ds^2}+\frac{1}{s}\frac{dR(s)}{ds}+\frac{1}{s^2}\left[-(\varepsilon+B')s^2+(A')s-\lambda\right]R(s)=0, \tag{23}$$

Comparing Eq.(23) with Eq.(7) and making use of Eq.(11), the following parameters are obtained:

$$\begin{aligned}
&c_1=1;\ \ c_2=c_3=0,\\
&\xi_1=\varepsilon+B';\ \ \xi_2=A';\ \ \ \xi_3=\lambda\\
&c_4=-\frac{1}{2};\ c_5=0;\ \ c_6=\varepsilon+B'\\
&c_7=-A';\ \ c_8=\lambda+\frac{1}{4};\ c_9=\varepsilon+B';\ \ c_{10}=1+2\sqrt{\lambda+\frac{1}{4}}\\
&c_{11}=2\sqrt{\varepsilon+B'};\ c_{12}=-\frac{1}{2}+\sqrt{\lambda+\frac{1}{4}};\ c_{13}=-\sqrt{\varepsilon+B'}
\end{aligned} \tag{24}$$

Substituting Eq.(24) into Eq. (9) and solving the resulting equation explicitly, the energy eigenvalues for the radial part of the Schrödinger equation is obtained as

$$E_{nl}=V_0\alpha-\frac{2\mu}{\hbar^2}\frac{V_0^2}{\left[(2n+1)+2\sqrt{\lambda+\frac{1}{4}}\right]^2}. \tag{25}$$

The corresponding radial wave function for this system is obtained as:

$$R(r)=N_n r^{-\frac{1}{2}+\nu}e^{-\sqrt{\varepsilon+B'}r}L_n^{2\nu}\left(2\sqrt{\varepsilon+B'}r\right) \tag{26}$$

where $\nu=\sqrt{\lambda+\frac{1}{4}}$ and N_n is a normalization constant.

Solutions of the Polar (Angular) Part

The eigenvalues and the eigen functions of the polar part of the Schrödinger equation in this case can be obtained by making use of Eq.(19). Thus, we have

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\theta\right)+\left[\lambda-\frac{m^2}{\sin^2\theta}-\frac{\gamma+\beta\cos^2\theta+\eta\cos^4\theta}{\cos^2\theta\sin^2\theta}\right]\Theta(\theta)=0 \tag{27}$$

Using the transformation, $q=\cos^2\theta$, Eq. (28) reduces to

$$\frac{d^2\Theta(s)}{ds^2}+\frac{(1-3s)}{2s(1-s)}\frac{d\Theta(s)}{ds}+\frac{1}{4s^2(1-s)^2}\left[-(\lambda+\eta)s^2+(\lambda-m^2-\beta)s-\gamma\right]\Theta(s)=0 \tag{28}$$

Comparing Eq.(28) with Eq.(7), the following parameters are obtained

$$\begin{aligned}
&c_1=\frac{1}{2};\ c_2=\frac{3}{2};\ c_3=1\\
&\xi_1=\frac{1}{4}(\lambda+\eta);\ \xi_2=\frac{1}{4}(\lambda-m^2-\beta);\ \xi_3=\frac{\gamma}{4},\\
&c_4=\frac{1}{4};\ c_5=-\frac{1}{4};\ \ c_6=\frac{1}{16}+\frac{1}{4}(\lambda+\eta)\\
&c_7=-\frac{1}{8}-\frac{1}{4}(\lambda-m^2-\beta);\ c_8=\frac{1}{16}+\frac{\gamma}{4};\ c_9=\frac{1}{4}(m^2+\gamma+\beta+\eta)\\
&c_{10}=1+\sqrt{\gamma+\frac{1}{4}};c_{11}=2+\left(\sqrt{m^2+\gamma+\beta+\eta}+\sqrt{\gamma+\frac{1}{4}}\right)\ c_{12}=\frac{1}{4}+\frac{1}{2}\sqrt{\gamma+\frac{1}{4}}\\
&c_{13}=-\frac{1}{4}-\frac{1}{2}\left(\sqrt{m^2+\gamma+\beta+\eta}+\sqrt{\gamma+\frac{1}{4}}\right)
\end{aligned} \tag{29}$$

Substituting Eq. (29) into Eq. (9) gives the relation for λ as

$$\begin{aligned}
\lambda=4\left(n+\frac{1}{2}\right)^2+2(2n+1)\left(\sqrt{m^2+\gamma+\beta+\eta}+\sqrt{\gamma+\frac{1}{4}}\right)\\
+2\sqrt{(m^2+\gamma+\beta+\eta)\left(\gamma+\frac{1}{4}\right)}+m^2+2\gamma+\beta,
\end{aligned} \tag{30}$$

where $\lambda=l(l+1)$.

The corresponding wave function of the angle dependent part is obtained as

$$\Theta(s)=N_m s^{\frac{1}{4}+\frac{1}{2}\sqrt{\gamma+\frac{1}{4}}}(1-s)^{\frac{1}{2}\sqrt{m^2+\gamma+\beta+\eta}}\times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(1-2s) \tag{31}$$

Equation (31) can further be written as

$$\Theta(\theta)=N_m(\cos\theta)^{\frac{1}{2}+\sqrt{\gamma+\frac{1}{4}}}(\sin\theta)^{\sqrt{m^2+\gamma+\beta+\eta}}\times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(-\cos 2\theta) \tag{32}$$

where N_m is a normalization constant.

Effect of Angle Dependent Part on Radial Solutions

The total energy of the Yukawa plus angle dependent potential is obtained by considering the effect of the angle dependent part on the radial part. Substituting Eq.(30) into Eq.(25) yields the energy spectra for this system as

$$E_{nlm} = V_0\alpha - \frac{2\mu}{\hbar^2}\frac{V_0^2}{\left[(2n+1)+2\delta\right]^2} \tag{33}$$

where

$$\delta = \sqrt{\begin{array}{l} 4\left(n+\frac{1}{2}\right)^2 + 2(2n+1)\left(\sqrt{m^2+\gamma+\beta+\eta}+\sqrt{\gamma+\frac{1}{4}}\right) \\ +2\sqrt{\left(m^2+\gamma+\beta+\eta\right)\left(\gamma+\frac{1}{4}\right)}+m^2+2\gamma+\beta+\frac{1}{4} \end{array}}$$

Finally, the total wave function for the system can be written as

$$\begin{aligned}\psi(r,\theta,\phi) = \frac{N_{nm}}{\sqrt{2\pi}} r^{-\frac{1}{2}+v} e^{im\phi-\sqrt{\varepsilon+B'}r} L_n^{2v}\left(2\sqrt{\varepsilon+B'}r\right) \\ \times(\cos\theta)^{\frac{1}{2}+\sqrt{\gamma+\frac{1}{4}}}(\sin\theta)^{\sqrt{m^2+\gamma+\beta+\eta}} \\ \times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(-\cos 2\theta)\end{aligned} \tag{34}$$

where N_{nm} is the normalization constant.

Application to Diatomic Molecules

Diatomic molecular potential is very important to describe the intramolecular and intermolecular interactions and atomic pair correlations in quantum mechanics [23,24]. We shall apply the exact solution of Schrödinger equation for some selected diatomic molecules for the s-wave by setting $V_0 = D_e r_e$ in Eq.(33).

$$E_{nlm} = D_e r_e \alpha - \frac{2\mu}{\hbar^2}\frac{\left(D_e r_e\right)^2}{\left[(2n+1)+2\delta\right]^2} \tag{35}$$

Where D_e is the dissociation energy (interaction energy between two atoms in a molecular system) and r_e is the distance of separation between the atoms. Setting $\gamma = \beta = \eta = 1$ and making use of Table 1 we obtain numerical values for our total energy eigenvalue. The values for $\gamma = \beta = \eta = 1$ are used arbitrarily for uniformity. However, depending on the purpose and interest one may use any different value for these potential parameters. The potential is a short range potential and the range of values for α must be small. That is why we chose range of 0.01-0.05 as seen in Table 2. But one can still extend the table to other range say 0.06……..0.09. α must lie in the range 0< α <1.

Table 1: Potential parameters of some selected diatomic molecules [24]

Diatomic Molecules	$D_e(eV)$	$r_e\left(\overset{o}{A}\right)$	$\mu\left(\overset{o}{A}\right)$
H_2	4.7446	0.7416	0.5039
C_O	10.845	1.1282	6.8606
N_O	8.0437	1.1508	7.4684
N_2	11.938	1.0940	7.0034
Ar_2	1.6720	2.5300	53.934

In Table 3, we compare the results for the diatomic molecules under Yukawa-angle dependent potential (our work) with those of exponential-cosine screened Coulomb plus Morse potential of ref.[25] for the values of α=0.01. From the table, though the numerical values for the two works are extremely different and quite obvious but both are physically interesting. Both of them have negative values indicating a case of bound state particle interaction. The different in the values is due to the fact that we are comparing two physically different potential systems.

Table 3: Comparison of energy eigenvalues of diatomicmolecules for α=0.01

Diatomic molecules	$E_{nlm}(eV)$	
	Present work	ref.[25]
H2	-0.1310	-13.091031
CO	-10.183	-0.079024
NO	-8.8804	-0.034704
N_2	-12.191	-9.75887
Ar_2	-4.2942	-

From Figure 1, it shows that the potential for H_2 diatomic molecules decreases downward with increase in θ and this suggest a good condition for the bound state of this system.

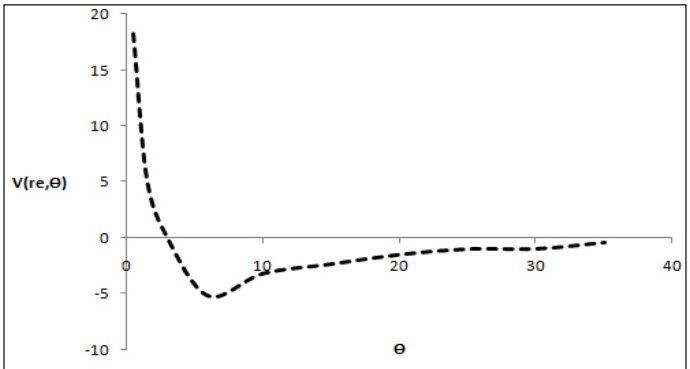

Figure 1: Variation of $V(r_e,\theta)$ with θ for H_2 diatomic molecule

Table 2: Energy eigenvalue for $0.01 \le \alpha \le 0.05$

	α	H_2	CO	NO	N_2	Ar_2
$E_{nlm}(eV)$	0.01	−6.1310	−10.183	−8.8804	−12.191	−4.2942
	0.02	−5.7632	−7.3483	−7.9872	−8.7922	−3.6548
	0.03	−5.5244	−6.7375	−6.8755	−7.3482	−3.3075
	0.04	−5.0912	−6.1143	−5.8349	−6.5159	−3.0981
	0.05	−4.9396	−4.9992	−5.0399	−6.0141	−2.9621

Conclusion

The exact bound state solutions of Schrödinger wave equation with Yukawa plus Novel angle dependent potential using Nikiforov-Uvarov method is obtained and the corresponding wave functions are expressed in terms of Jacobi polynomial $P_n^{(\alpha,\beta)}(s)$ and Laguerre polynomial $L_n^{\alpha}(s)$ for angular and radial solutions respectively. These results are used to study the interactions of the non-central potential for diatomic molecules. The Yukawa potential is often used to compute bound state normalization and energy levels of neutral atoms while the angle dependent potentials are used for the interaction between deformed pair of nuclei and ring shaped molecules. The results obtained would have many applications in chemical and molecular physics and the recently reported result of neutron-proton pair in heavy nuclei using perturbation theory [26]. Numerical data for some selected diatomic molecules are presented in Table 2 and Variation of the potential is presented for H_2 diatomic molecule in Figure 1.

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