

ANALYTICAL SOLUTIONS OF THE KLEIN-GORDON EQUATION IN THE PRESENCE OF COULOMB-ECKART POTENTIAL

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Abstract

The Nikiforov-Uvarov (NU) method is employed to calculate the approximate analytical solutions of the Klein-Gordon equation with a newly proposed potential known as the Coulomb-Eckart potential. The new potential is a combination of the Coulomb potential and the Eckart potential. The energy equation, eigenvalues and energy spectra of HCl, LiH and CH diatomic molecules were obtained. Also, the ro-vibrational energy for different energy states were computed. By varying some potential parameters, energy equations of some other potentials like the Hellmann potential and the Yukawa potential were obtained.

1. Introduction

The continuous interest in the study of the relativistic and non-relativistic wave equations in quantum mechanics had increased over the years because of its importance in physics today. The non-relativistic regime is described using the Schrödinger equation while the Klein-Gordon and the Dirac equation are used to describe the relativistic effect for spin 0 and spin-1/2 particles respectively when considering the relativistic effect. The solution of these waves can either be exact or approximate depending of the potential under consideration. Over the years, several traditional techniques have been developed to obtain these solutions. Examples include the Nikiforov-Uvarov (NU) method [1-3], the supersymmetric quantum mechanics and shape invariance method [4-9], asymptotic iteration method (AIM) [10-15], the variational method [16] and others. Most of these techniques can be used effectively for approximate solution i.e. when $l \neq 0$, for different physical potential models. However, for $l = 0$, the solution of these equations can be obtain with only few potentials such as Manning-Rosen potential [4,17,18], Hulthén potential [19, 20], Kratzer potential [21], Wood-Saxon potential [22, 23] and the Pöschl-Teller potential [24]. Thus, a lot of works have focus on the approximate solutions with some of these potential models. Some of the reported works are Yahya and Oyewumi [25], who solved the Klein-Gordon equation with the Pöschl-Teller-type potential. In their study, they obtained the thermodynamic properties for the Pöschl-Teller-type potential in the classical limit. Jia and Cao [26] obtained the molecular energy of spinless Morse potential under the Klein-Gordon equation. They also studied the vibrational transition frequencies using the methodology of supersymmetric and shape invariance approach. Recently, Ebomwonyi et al. [27], studied arbitrary l solutions of the Schrödinger equation in the presence of a new potential formed from a combination of Hellmann potential and Deng-Fan potential model. In the present work, we desire to study the approximate solution of the Klein-Gordon for a case when $V(r) = S(r)$ and the Schrödinger equations with a combined potential called the Coulomb-Eckart potential model. These potentials were individually studied under different in the past [28, 29]. However, a combination of these potential will give more applications and interesting results; and to the best of our knowledge, this combination is novel in the literature. The Coulomb-Eckart potential is of the form

$$V(r) = -\frac{A}{r} + \frac{Be^{-\delta r}}{1 - e^{-\delta r}} - \frac{4Ce^{-2ar}}{(1 - e^{-2ar})^2} \quad (1)$$

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where r is internuclear separation, α is the screening parameter related to the range of the potential, A , B and C are the potential strengths.

2. Parametric Nikiforov-Uvarov method

The Nikiforov-Uvarov (NU) method is based upon reducing the second-order linear differential equation to a hypergeometric type equation [30]. By introducing an appropriate transformation $s = s(x)$, we can then write an equation of the form

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

where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials of at most second degree two and $\bar{\tau}(s)$ is a polynomial of degree one at most. It is discovered that the conventional NU method has tedious and logical calculations. In order to simplify these calculations, Tezcan and Sever [31] in their study, derived the following equation from the conventional NU method [30-32]

$$\frac{d^2\psi(s)}{ds^2} + \left(\frac{\lambda_1 - \lambda_2 s}{s(1 - \lambda_3 s)}\right) \frac{d\psi(s)}{ds} + \left(\frac{-\zeta_1 s^2 + \zeta_2 s - \zeta}{s(1 - \lambda_3 s)}\right) \psi(s) = 0. \tag{3}$$

which they called parametric Nikiforov-Uvarov method. From the parametric NU method, the bound state energy condition is obtained as [31]

$$n\lambda_2 - (2n + 1)\lambda_5 + (2n + 1)(\sqrt{\lambda_9} + \lambda_3\sqrt{\lambda_8}) + n(n - 1)\lambda_3 + \lambda_7 + 2\lambda_3\lambda_8 + 2\sqrt{\lambda_8\lambda_9} = 0, \tag{4}$$

with the wave function as

$$\psi_{n,l}(s) = N_{n,l} s^{\lambda_{12}} (1 - \lambda_3 s)^{-\lambda_{12} - \frac{\lambda_{13}}{\lambda_3}} P_n^{\left(\lambda_{10} - 1, \frac{\lambda_{11} - \lambda_{10} - 1}{\lambda_3}\right)} (1 - 2\lambda_3 s), \tag{5}$$

where the parameters in Eq. (4) and Eq. (5) are given as follows

$$\left. \begin{aligned} \lambda_4 &= \frac{1 - \lambda_1}{2}, \lambda_5 = \frac{\lambda_2 - 2\lambda_3}{2}, \lambda_6 = \lambda_5^2 + \zeta_1, \lambda_7 = 2\lambda_4\lambda_5 - \zeta_2, \lambda_8 = \lambda_4^2 + \zeta_3, \\ \lambda_9 &= \lambda_3(\lambda_7 + \lambda_3\lambda_8) + \lambda_6, \lambda_{10} = \lambda_1 + 2\lambda_4 - 2\sqrt{\lambda_8}, \lambda_{11} = \lambda_2 - 2\lambda_5 + 2(\sqrt{\lambda_9} - \lambda_3\sqrt{\lambda_8}), \\ \lambda_{12} &= \lambda_4 - \sqrt{\lambda_8}, \lambda_{13} = \lambda_5 - (\sqrt{\lambda_9} - \lambda_3\sqrt{\lambda_8}) \end{aligned} \right\}. \tag{6}$$

3. Bound state solution

3.1 Solution to the Klein-Gordon equation

The Klein-Gordon equation with scalar potential $S(r)$ and vector potential $V(r)$ of a particle of mass M with relativistic energy E is given as

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + (S(r) + M)^2 - (E - V(r))^2 \right] \varphi(r) \tag{7}$$

Eq. (7) has a potential $2V$ in the nonrelativistic limit. Substituting Eq. (1) into Eq. (7), we have

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \left(-\frac{A}{r} + \frac{Be^{-\delta r}}{1 - e^{-\delta r}} - \frac{4Ce^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} + M \right)^2 + \left(E - \left(V(r) = -\frac{A}{r} + \frac{Be^{-\delta r}}{1 - e^{-\delta r}} - \frac{4Ce^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right) \right)^2 \right] \varphi(r) \tag{8}$$

Due to the centrifugal term $\frac{l(l+1)}{r^2}$ in Eq. (8), we need to apply a suitable approximation scheme to deal with the centrifugal term. For a short potential range, we apply the following Greene-Aldrich [33] approximate type

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1 - e^{-\delta r})^2} \tag{9}$$

Where we have taken $\delta = 2\alpha$

Substituting Eq. (9) into Eq. (8), we have

$$\left[\frac{d^2}{dr^2} - \frac{4l(l+1)\alpha^2}{(1 - e^{-2\alpha r})^2} - \frac{2A(M + E)2\alpha}{1 - e^{-2\alpha r}} + \frac{2B(M + E)e^{-2\alpha r}}{1 - e^{-2\alpha r}} - \frac{8C(M + E)e^{-2\alpha r}}{1 - e^{-2\alpha r}} + M^2 - E^2 \right] \varphi(r) = 0 \tag{10}$$

In order to use the parametric Nikiforov-Uvarov method, it is important we define a variable of the form $s = e^{-2\alpha r}$ and substitute it into Eq. (10) to have

$$\left[\frac{d^2}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d}{ds} + \frac{1}{s^2(1-s^2)} \{-\kappa_1 s^2 + \kappa_2 s - \kappa_3\} \right] R(s) = 0, \tag{11}$$

where

$$\kappa_1 = \frac{B(E+M)}{2\alpha^2} + \frac{E^2 - M^2}{4\alpha^2}, \kappa_2 = \frac{B(E+M)}{2\alpha^2} - \frac{2C(E+M)}{\alpha^2} + \frac{A(E+M)}{\alpha} + \frac{E^2 - M^2}{2\alpha^2}, \kappa_3 = \frac{A(E+M)}{\alpha} + \frac{E^2 - M^2}{4\alpha^2} + l(l+1). \tag{12}$$

Comparing Eq. (11) with Eq. (3), we obtain the following parametric constants

$$\begin{aligned} \lambda_1 = \lambda_2 = \lambda_3 = 1, \lambda_4 = 0, \lambda_5 = -\frac{1}{2}, \lambda_6 = \frac{1}{4} + \kappa_1, \lambda_7 = -\kappa_2, \lambda_8 = \kappa_3, \\ \lambda_9 = -\kappa_2 + \kappa_3 + \kappa_1 + \frac{1}{4}, \lambda_{10} = 1 + 2\sqrt{\kappa_3}, \lambda_{11} = 2(1 - \sqrt{\lambda_8} + \sqrt{\lambda_9}), \\ \lambda_{12} = -\sqrt{\kappa_3}, \lambda_{13} = -\frac{1}{2} - \sqrt{\lambda_9} + \sqrt{\lambda_8}. \end{aligned} \tag{13}$$

Using these parametric constants in Eq. (13) in Eq. (4), the energy equation is obtained as

$$\frac{1}{4\alpha^2} \left((E^2 - M^2) + 2A\alpha(E+M) - 4\alpha^2 L \right) = \left[\frac{\left((n + \frac{1}{2}) \sqrt{\frac{8C}{\alpha^2}(E+M) - (2l+1)^2} + n(n-1) + \left(\frac{A}{2\alpha} + \frac{2C}{\alpha^2} - \frac{B}{2\alpha^2} \right) (E+M) - 2L - \frac{1}{2} \right)^2}{2n+1 + \sqrt{\frac{8C}{\alpha^2}(E+M) - (2l+1)^2}} \right] \tag{14}$$

3.2 Solution to the Schrödinger equation

In order to obtain the solution of the Schrödinger-like equation in the nonrelativistic limit with the Coulomb-Eckart potential in Eq. (1), we write the radial Schrödinger equation of the form [29]

$$\left[\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} \left\{ E - V(r) - \frac{L\hbar^2}{2\mu r} \right\} \right] R(r) = 0, \tag{15}$$

where $L = l(l+1)$, μ is the reduced particle mass, E is the non-relativistic energy and $V(r)$ is the interacting potential.

Now substituting the Eq. (1) and Eq. (9) into Eq. (15), we have

$$\left[\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} \left\{ E + \frac{2\alpha A}{(1 - e^{-2\alpha r})} - \frac{B e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \frac{4C e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} - \frac{L\hbar^2 4\alpha^2}{2\mu(1 - e^{-2\alpha r})^2} \right\} \right] R(r) = 0. \tag{16}$$

Using the same transformation as in the Klein-Gordon equation and substitute it into Eq. (16) we, have

$$\left[\frac{d^2}{ds^2} + \frac{(1-s)d}{s(1-s)} \frac{d}{ds} + \frac{1}{s^2(1-s)^2} \{-A_1 s^2 + A_2 s - A_3\} \right] R(s) = 0, \tag{17}$$

where

$$A_1 = \frac{-\mu E - \mu B}{2\alpha^2 \hbar^2}, \tag{18}$$

$$A_2 = \frac{-\mu(2E + B + 2A\alpha - 4C)}{2\alpha^2 \hbar^2}, \tag{19}$$

$$A_3 = L - \frac{\mu(B + E)}{2\alpha^2 \hbar^2}. \tag{20}$$

On comparing Eq. (17) with Eq. (3), we obtain

$$\left. \begin{aligned} \theta_1 = \theta_2 = \theta_3 = 1, \theta_4 = 0, \theta_5 = -\frac{1}{2}, \theta_6 = \frac{1}{4} + A_1, \theta_7 = -A_2, \theta_8 = A_3, \\ \theta_9 = \frac{1}{4} \left((1 + 2l)^2 - \frac{8\mu C}{\alpha^2 \hbar^2} \right), \theta_{10} = 1 + 2\sqrt{A_3}, \theta_{11} = 2(1 + \sqrt{\theta_9} + \sqrt{A_3}), \\ \theta_{12} = \sqrt{A_3}, \theta_{13} = -\frac{1}{2} - \sqrt{\theta_9} - \sqrt{A_3} \end{aligned} \right\} \tag{21}$$

Now substituting the appropriate parametric constants in Eq. (21) into Eq. (4), the nonrelativistic energy equation for the Coulomb-Eckart potential is obtained as

$$E = \frac{2\alpha^2 \hbar^2}{\mu} \left[\ell(\ell+1) - \frac{\left(\frac{\mu(4C + 2\alpha A - B)}{2\alpha^2 \hbar^2} - 2\ell(\ell+1) - n(n+1) - \frac{1}{2} - \left(n + \frac{1}{2} \right) \sqrt{(1+2\ell)^2 - \frac{8\mu C}{\alpha^2 \hbar^2}} \right)^2}{1 + 2n + \sqrt{(1+2\ell)^2 - \frac{8\mu C}{\alpha^2 \hbar^2}}} \right] - 2\alpha A \quad (22)$$

Table 1: Eigenvalues for $S = V$ for different values of A, B, C

state	α	A=3,B=2,C=1	B=3,C=2,A=1	C=3,A=2,B=1
2p	0.20	-0.121573037	1.596974043	4.984537368
	0.25	-0.246720366	1.624127558	4.978625478
	0.30	-0.363398574	1.657963870	4.975411249
3p	0.20	0.213878422	2.082085681	5.636945503
	0.25	0.169641448	2.224864947	5.781081216
	0.30	0.128749939	2.370101913	5.922107193
3d	0.20	0.025865441	1.741322672	5.072496125
	0.25	-0.021735002	1.850123256	5.115069275
	0.30	-0.043422302	1.985866087	5.171178676
4p	0.20	0.593179477	2.612922085	6.329231686
	0.25	0.651121652	2.894666417	6.645895549
	0.30	0.711457496	3.179277529	6.958763198
4d	0.20	0.343592799	2.213527357	5.720139919
	0.25	0.362751334	2.426451131	5.908640340
	0.30	0.396922423	2.656923872	6.103087016
4f	0.20	0.270800284	1.968924914	5.208860058
	0.25	0.376177899	2.216949678	5.330623926
	0.30	0.571857003	2.538014138	5.487800922

Table 2: Energy spectra for HCl, LiH and CH for 2p to 4f states; $\hbar c = 1973.29eV\text{\AA}$, $\mu_{HCl} = 0.9801045amu$, $\mu_{LiH} = 0.8801221amu$, $\mu_{CH} = 0.929931amu$, $2B = A = 2 = -2C$.

$\mu_{HCl} =$

state	α	HCl	LiH	CH
2p	0.10	3.306050903	3.507385413	3.402421902
	0.15	5.387403793	5.880970851	5.624331604
	0.20	8.578879671	9.478067148	9.010895426
3p	0.10	1.483263394	1.632546315	1.554374747
	0.15	3.090964529	3.480121112	3.277708186
	0.20	5.618459629	6.328062076	5.959465221
3d	0.10	8.456705783	9.221052317	8.823892712
	0.15	16.75546869	18.50518821	17.59646044
	0.20	28.61378177	31.74110263	30.11719323
4p	0.10	1.243370524	1.450429206	1.342467664
	0.15	3.456891290	3.948961455	3.693484310
	0.20	6.685976721	7.556229436	7.104608190
4d	0.10	5.388504535	5.939705114	5.653093141
	0.15	11.39664223	12.67160740	12.00941455
	0.20	20.02753155	22.30707360	21.12342071
4f	0.10	16.56907552	18.23954454	17.37194455
	0.15	34.94067213	38.72825884	36.76153418
	0.20	60.90013035	67.64852340	64.14467373

Table 3: Comparison of ro-vibrational Hellmann energy $(-E_{n\ell})$ for 2s, 2p, 3s, 3p and 3d with $\hbar = 2\mu = 1$, $B = \delta$ and $A = 2$.

state	δ	Present	Hamzavi et al.[34]	Onate et al.[35]
2s	0.001	0.064001	0.063243	0.064250
	0.005	0.070025	0.067106	0.071256
	0.010	0.077600	0.071689	0.080025
2p	0.001	0.063750	0.063495	0.063999
	0.005	0.068756	0.067377	0.069975
	0.010	0.075025	0.072020	0.077400
3s	0.001	0.029280	0.028283	0.029611
	0.005	0.035334	0.031993	0.036951
	0.010	0.043003	0.036142	0.046136
3p	0.001	0.029168	0.028765	0.029499
	0.005	0.034756	0.032480	0.036356
	0.010	0.041803	0.036645	0.044869
3d	0.001	0.028945	0.028767	0.029274
	0.005	0.033617	0.032526	0.035184
	0.010	0.039469	0.036814	0.042403

Discussion

Table 1 shows the energy eigenvalues for different values of the potential strengths, A , B and C . It can be seen that as the screening parameter increases across the states, the energy eigenvalue decreases for $2p$, $3p$ and $3d$. However, the reverse is the case in $4p$, $4d$ and $4f$. It is also observed in Table 1 that energy increases linearly with the potential strength C . In Table 2, we present the energy spectrum for three diatomic molecules. It is also observed that as the screening parameter increases, the energy also increases.

In Table 3, the ro-vibrational energies for $2p$, $3s$, $3p$ and $3d$ states were computed and it can be observed that our results compare favourably with the works of Hamzavi et al, 2013 and Onate et al., 2017.

One very important and interesting feature of our proposed potential is that, the results of other potentials can be deduced from it. For instance, when we put $A = 0$, the potential reduced to Eckart potential

$$V(r) = -\frac{A}{r} + \frac{Be^{-\delta r}}{1 - e^{-\delta r}} - \frac{4Ce^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}, \tag{23}$$

and the energy equation becomes

$$E = \frac{2L\alpha^2\hbar^2}{\mu} - \frac{2\alpha^2\hbar^2}{\mu} \left[\frac{\left(\frac{-4\mu C + \mu B}{2\alpha^2\hbar^2} + 2L + n(n+1) + \left(n + \frac{1}{2}\right) \sqrt{\left((1+2l)^2 - \frac{8\mu C}{\alpha^2\hbar^2} \right) - \frac{1}{2}} \right)^2}{2n+1 + \sqrt{\left((1+2l)^2 - \frac{8\mu C}{\alpha^2\hbar^2} \right) - \frac{1}{2}}} \right]. \tag{24}$$

Similarly, when we put $C = 0$, the potential turns to Hellmann potential

$$V(r) = -\frac{A}{r} + \frac{Be^{-\delta r}}{1 - e^{-\delta r}}, \tag{25}$$

with energy equation as

$$E = \frac{2L\alpha^2\hbar^2}{\mu} - 2A\alpha - \frac{2\alpha^2\hbar^2}{\mu} \left[\frac{\left(\frac{-2\mu\alpha A + \mu B}{2\alpha^2\hbar^2} + 2L + n(n+1) + \left(n + \frac{1}{2}\right) (1+2l) - \frac{1}{2} \right)^2}{2(1+n+l)} \right]. \tag{26}$$

Putting $B = C = 0$, the potential becomes Coulomb like potential

$$V(r) = -\frac{A}{r} \tag{27}$$

with energy equation as

$$E = \frac{2L\alpha^2\hbar^2}{\mu} - 2A\alpha - \frac{2\alpha^2\hbar^2}{\mu} \left[\frac{\frac{\mu\alpha A}{\alpha^2\hbar^2} + 2L + n(n+1) + \left(n + \frac{1}{2}\right)(1+2l) - \frac{1}{2}}{2(1+n+l)} \right]^2. \quad (28)$$

Putting $A = C = 0$, the potential turns to a Yukawa like potential

$$V(r) = \frac{Be^{-\delta r}}{1 - e^{-\delta r}} \quad (29)$$

and the energy equation becomes

$$E = \frac{2L\alpha^2\hbar^2}{\mu} - \frac{2\alpha^2\hbar^2}{\mu} \left[\frac{\frac{\mu B}{2\alpha^2\hbar^2} + 2L + n(n+1) + \left(n + \frac{1}{2}\right)(1+2l) - \frac{1}{2}}{2(1+n+l)} \right]^2. \quad (30)$$

Conclusion

The solutions of the Coulomb-Eckart potential (a combination of the Coulomb potential and the Eckart potential) for the Klein-Gordon equation have been obtained via the Nikiforov-Uvarov method. The energy equation and the eigenvalues for different values of the potential strengths were obtained. The energy spectra of HCl, LiH and CH diatomic molecules for $2p$ to $4f$ states were also obtained. Also, the ro-vibrational energies for different states that we computed compare favourably and are in agreement with other works in literature. The Hellmann potential and the Yukawa potential were recovered from the energy equation by adjusting the potential parameters.

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