APROXIMATE ANALYTICAL SOLUTION OF SCHRODINGER EQUATION FOR COULOMBIC POTENTIAL WITH COSINE-COSEC AND EXPONENTIAL TERM

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Abstract: We solved Schrödinger equation for proposed Coulombic potential with cosine-cosec and exponential term (CP-CCET) in this research article. We obtained energy eigenvalues and wave functions for this CP-CCET using generalized parametric Nikiforov-Uvarov (NU) method . From solution of CP-CCET, We deduced and investigated few potentials and its energy eigenvalues. Obtained eigenvalues and wave functions are applicable to find dynamical properties of physical and chemical quantum mechanical systems.

Keyword: *Schrödinger equation, cosine – cosec potential, Coulombic potential, eigenvalues.*

1. Introduction

Numbers of methods are developed to solve the non relativistic and relativistic equations. The solutions of quantum wave equations including Schrodinger, Klein-Gordon, Dirac, Duffin-Kemmer Petiau (DKP) and spinless-Salpeter equations have been an attractive research subject for both physicists and applied mathematicians [1-8]. The Schrödinger equation is second order differential equation and it is important to solve quantum mechanical problems. Solution of these type equations gives the wave functions and eigenvalues for the given physical or chemical quantum mechanical systems. we can understand the properties and behavior of the quantum mechanical systems From the solutions. Transforming Schrödinger equation into the known ordinary differential equation whose solutions are available in terms of special functions such as associated Laguerre polynomials, hypergeometric functions etc. is one of the old method. Second method is Qiang Dong proper quantization rule [9,10], the exact quantization rule method [11], factorization techniques like supersymmetric method [12,13], the asymptotic iteration method [14-16], the Nikiforov-Uvarov (NU) method [17] and the Lie algebraic method [18] for exact solution of the Schrödinger equation.

The exponential-hyperbolic potentials under investigations are commonly used to model inter-atomic and inter-molecular forces [11,19]. Among such potentials Rosen-Morse, Scarf potential and Poschl-Teller are studied extensively and work are presented in the literatures [20-45]. Various methods have been adopted in solving the Schrödinger equation with exponential-hyperbolic potentials. Some of these exponential-hyperbolic potentials are exactly solvable or semi-exactly solvable and their bound state solutions have been reported in different literatures [11, 35,36, 42].

We proposed CP-CCET as

$$V(r) = -\frac{A+B\cosh(s\,\alpha r)\,e^{-\alpha r}+C\,cosech\alpha r\,e^{\alpha r}}{r} - G\,e^{-2\alpha r} \qquad (1)$$

where A, B, C, G are depth of potentials and $s,\ \alpha$ are parameters.

Other potentials are deduced from proposed potential. In section two, theory of generalized NU method presented. In third section, we obtained the solutions of Schrödinger equation for proposed potential. Result and discussion in forth section and concluded our work in the last section.

2.THEORY OF GENERALIZED NIKIFOROV-UVAROV (NU) METHOD

NU method [17] is very good method, it is a applicable to solve the second order differential equation, such as the Schrodinger, Klein-Gordon and Dirac equation for different kind of potentials [46-51]. This method is based on the solutions second order linear differential equation with special orthogonal functions. Using proper variable to transform second-order differential equation into particular form in which can be solved using NU method, the differential equation of the form

$$\frac{d^2\Psi_n}{dg^2} + \frac{\tilde{\tau}(g)}{\sigma(g)}\frac{d\Psi_n}{dg} + \frac{\tilde{\sigma}(g)}{\sigma^2(g)}\Psi_n(g) = 0 \qquad (2.1)$$

Where $\tilde{\tau}(g)$ is first degree polynomial, $\tilde{\sigma}(g)$ and $\sigma(g)$ are mostly second degree polynomial. $\psi_n(g)$ hyper geometric type function.

The general form of the Schrodinger-like equation for the potential is written as [52],

$$\frac{d^2\Psi_n}{dg^2} + \frac{b_1 - b_2 g}{g(1-b_3 g)}\frac{d\Psi_n}{dg} + \frac{-\chi_1 g + \chi_2 g - \chi_3}{g^2(1-b_3 g)^2}\Psi_n(g) = 0 \qquad (2.2)$$

Comparing Eqs 2.1 with 2.2,

$$\tilde{\tau}(g) = b_1 - b_2 g\ ,\quad \sigma(g) = g(1-b_3 g),\quad \tilde{\sigma}(g) = -\chi_1 g + \chi_2 g - \chi_3 \qquad (2.3)$$

Using NU method [17]

$$\tilde{\tau}(g) = b_4 + b_5 g \pm [(b_6 - (b_3 K^{\pm})g^2 + (b_7 + K^{\pm})g + b_8]^{\frac{1}{2}}$$

Where

$b_4 = (1 - b_1)/2$, $b_5 = (b_2 - 2b_3)/2$, $b_6 = b_5^2 + \chi_1$, $b_7 = 2\,b_4\,b_5 - \chi_2$,

$$b_8 = b_4^2 + \chi_3,\quad b_9 = b_3 b_7 + b_3^2 b_8 + b_6 \qquad (2.4)$$

And

$$K^{\pm} = -(b_7 + 2\,b_3\,b_8) \pm \sqrt{b_8 b_9} \qquad (2.5)$$

Now as per NU method, function $\pi(g)$ and parameters $\tau(g),\ \lambda,\ \lambda_n$ are defined as follow

$$\pi(g) = b_4 + b_5 g - [(\sqrt{b_9} + b_3\sqrt{b_8})g - \sqrt{b_8}], \text{ for } K^- = -(b_7 + 2\, b_3\, b_8) - \sqrt{b_8 b_9} \quad (2.6)$$

$$\tau(g) = \tilde{\tau}(g) + 2\,\pi(g) = b_1 + 2b_4 - (b_2 - 2b_5)g - [(\sqrt{b_9} + b_3\sqrt{b_8})g - \sqrt{b_8}] \quad (2.7)$$

The physical condition for bound state solution is $\frac{d\tau(g)}{dg}$ must be negative.

$$\lambda = K + \frac{d\pi(g)}{dg} \quad (2.8)$$

The eigenvalues equation becomes

$$\lambda = \lambda_n = -n\tau'(g)K + \frac{n(n-1)}{2}\,\sigma''(g) \quad (2.9)$$

Using 2.3 to 2.7 in 2.8 and 2.9, the eigenvalues equation becomes

$$(b_2 - b_3)n + b_3 n^2 - (2n+1)b_5 + (2n+1)(\sqrt{b_9} + b_3\sqrt{b_8}) + b_7 + 2\, b_3\, b_8 + 2\sqrt{b_8 b_9} = 0 \quad (2.10)$$

The exact solutions of Eq. 2.1 can be written using NU method as,

Consider $\psi_n(g)$ as,

$$\psi_n(g) = x_n(g) y_n(g) \quad (2.11)$$

Where $x_n(g)$ and $y_n(g)$ are hypergeometric type functions defined as,

$$\frac{1}{x_n(g)}\frac{dx_n(g)}{dg} = \frac{\pi(g)}{\sigma(g)} \quad (2.11a)$$

$$y_n(g) = \frac{B_n}{\rho(g)}\frac{d^n(\sigma^n(g)\rho(g))}{dg} \quad (2.12)$$

B_n Normalization constant and $\rho(g)$ weight function which satisfy the below condition

$$\frac{d(\sigma\rho)}{dg} = \tau(g)\rho(g), \quad \frac{dw(g)}{dg} = w(g)\frac{\tau(g)}{\sigma(g)} \quad (2.13)$$

Here, $w(g) = \sigma(g)\rho(g)$

$\rho(g)$ is obtained from Eq. 2.13 as,

$$\rho(g) = g^{b_{10}-1}(1 - b_3)^{\frac{b_{11}}{b_3} - b_{10} - 1} \quad (2.14)$$

So, Eq. 2.12 written as,

$$y_n(g) = P_n^{\left(b_{10}-1, \frac{b_{11}}{b_3} - b_{10} - 1\right)}(1 - 2b_3 g) \quad (2.15)$$

Where

$$b_{10} = b_1 + 2b_4 + 2\sqrt{b_8}\,, \quad b_{11} = b_2 - 2b_5 + 2\left(\sqrt{b_9} + b_3\sqrt{b_8}\right) \tag{2.16}$$

$P_n^{(\alpha,\beta)}$ are the Jacobi polynomials.

As per NU method, the second part of the Eq. 2.11,

$$x_n(g) = g^{b_{12}}\,(1 - b_3 g)^{-b_{12} - \frac{b_{13}}{b_3}} \tag{2.17}$$

$$b_{12} = \; b_4 + \sqrt{b_8}\,, \quad b_{13} = b_5 - \left(\sqrt{b_9} + b_3\sqrt{b_8}\right) \tag{2.18}$$

Total wave function written as,

$$\psi_n(g) = N_n\, g^{b_{12}}\,(1 - b_3 g)^{-b_{12} - \frac{b_{13}}{b_3}} P_n^{\left(b_{10}-1, \frac{b_{11}}{b_3} - b_{10} - 1\right)}(1 - 2b_3 g) \tag{2.19}$$

3 BOUND STATE SOLUTIONS OF SCHRODINGER EQUATION WITH CP-CCET

3.1 Eigenvalues Equation of Schrodinger Equation for CP-CCET

Applying the Pekeris-like approximation [51,53] to the $cosech\alpha r$ term as,

$$\frac{1}{r^2} = \frac{\alpha^2}{(1-e^{-2\alpha r})^2} \Rightarrow \frac{1}{r} = \frac{\alpha}{1-e^{-2\alpha r}} \tag{3.1a}$$

$$cosh\alpha r = \frac{e^{\alpha r} + e^{-\alpha r}}{2} \quad ;\, s=1 \tag{3.1b}$$

$$cosech\alpha r\; e^{\alpha r} = \frac{2\, e^{\alpha r}}{e^{\alpha r} - e^{-\alpha r}} = \frac{2}{1-e^{-2\alpha r}} = \frac{2}{r\,\alpha} \tag{3.1c}$$

$$V(r) = -\frac{A + \frac{B}{2}(1+e^{-2\alpha r})}{r} - \frac{2C}{\alpha\, r^2} - G\, e^{-2\alpha r} \tag{3.2}$$

The radial Schrödinger equation given as [54]

$$\frac{d^2U_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dU_{nl}(r)}{dr} + \frac{2\mu}{\hbar^2}\left(E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right)U_{nl}(r) = 0 \tag{3.3}$$

From Eq. 3.2,

$$\frac{d^2U_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dU_{nl}(r)}{dr} + \frac{1}{r^2}$$

$$\times\left(\frac{2\mu}{\hbar^2}(E + G\, e^{-2\alpha r})r^2 + \frac{2\mu}{\hbar^2}\left[A + \frac{B}{2}\,(1 + e^{-2\alpha r})\right]r - \left[l(l+1) - \frac{2C}{\alpha}\right]\right)U_{nl}(r) = 0 \tag{3.4}$$

$$\frac{d^2U_{nl}(r)}{dr^2}+\frac{2}{r}\frac{dU_{nl}(r)}{dr}+\frac{1}{r^2}\times(-\beta^2r^2+\gamma r-\delta)U_{nl}(r)=0 \quad (3.5)$$

β^2, γ and δ are dimensional parameters defined as,

$$-\beta^2=\frac{2\mu}{\hbar^2}(E+G\,e^{-2\alpha r}), \gamma=\frac{2\mu}{\hbar^2}\left[A+\frac{B}{2}\,(1+e^{-2\alpha r})\right], \delta=\left[l(l+1)-\frac{2C}{\alpha}\right]=l'(l'+1) \quad (3.6)$$

$$l'=\frac{1}{2}\left(-\frac{1}{2}\pm\frac{1}{2}\sqrt{1+\frac{8c}{\alpha}-4\,l(1+l)}\right) \quad (3.6a)$$

From Eq. 3.4 and 2.4 and using Eq. 2.4,

$b_1=2,\ b_2=b_3=0,$

$b_4=(1-b_1)/2=\frac{1}{2}$, $b_5=(b_2-2b_3)/2=0$, $b_6=b_5^2+\chi_1=\beta^2$, $b_7=2\,b_4\,b_5-\chi_2=\gamma$

$$b_8=b_4^2+\chi_3=\frac{1}{4}+\delta,\ \ b_9=b_3b_7+b_3^2b_8+b_6=\beta^2 \quad (3.7)$$

Using Eq. 3.7 in 2.6, we obtain [55],

$$\pi(r)=\frac{1}{2}\pm\frac{1}{2}\sqrt{\frac{1}{4}+\beta^2r^2-\gamma\,r+\delta+K\,r}$$

$$\pi(r)=-\frac{1}{2}\pm\frac{1}{2}\sqrt{4\beta^2r^2+4(\mathrm{K}-\gamma)\,r+4\delta+1} \quad (3.8)$$

The value under the square root of Eq. (3.8) must be the square root of polynomial which is mostly first degree polynomial and this is possible when its determiner is zero i.e $b^2-4ac=0$. So we obtain

$$(4(\mathrm{K}-\gamma))^2-16\beta^2(4\delta+1)=0 \quad (3.9)$$

Using Eq. 2.5 in the solution of Eq. 3.9, we obtain

$$K^{\pm}=-\gamma\pm\beta\sqrt{4\delta+1} \quad (3.10)$$

Four possible values of $\pi(r)$ corresponds to $K^{\pm}$,

$$\pi(r)=-\frac{1}{2}\pm\begin{cases}\beta\,r-\frac{1}{2}\sqrt{4\delta+1} & \text{for } K^-=-\gamma-\beta\sqrt{4\delta+1}\\ \beta\,r+\frac{1}{2}\sqrt{4\delta+1} & \text{for } K^+=-\gamma+\beta\sqrt{4\delta+1}\end{cases} \quad (3.11)$$

Acceptable solution as per NU method,

$$\pi(r)=-\frac{1}{2}-\beta\,r+\frac{1}{2}\sqrt{4\delta+1} \quad \text{for } K^-=-\gamma-\beta\sqrt{4\delta+1} \quad (3.12)$$

$\frac{d\tau(r)}{dr}$ must be negative to generate eigenvalues and corresponding wave functions. Therefore $\tau(r)$ satisfies these condition from Eq. 2.7,

$$\tau(r) = 1 - 2\beta r + \sqrt{4\delta + 1}$$

$$\frac{d\tau(r)}{dr} = -2\beta \tag{3.13}$$

And

$$\frac{d\pi(r)}{dr} = -\beta \tag{3.14}$$

From Eqs. (2.9) and (2.10), we obtain

$$\beta^2 = \left[\frac{\gamma}{2n+1+\sqrt{4\delta+1}}\right]^2 \tag{3.15}$$

$$-\frac{2\mu}{\hbar^2}(E + G\, e^{-2\alpha r}) = \left[\frac{A+\frac{B}{2}(1+e^{-2\alpha r})}{2n+1+\sqrt{4\delta+1}}\right]^2$$

$$E_{nl} = -G\, e^{-2\alpha r} - \frac{\mu}{2\hbar^2}\left[\frac{A+\frac{B}{2}(1+e^{-2\alpha r})}{n+l'+1}\right]^2 \tag{3.16}$$

Eq. 3.16 is energy spectrum for CP-CCET

Where
$l' = \frac{1}{2}\left(-\frac{1}{2} \pm \frac{1}{2}\sqrt{1 + \frac{8c}{\alpha} - 4\, l(1+l)}\right)$ and N_n is normalization constant

3.2 Wave function for the Schrodinger equation with CP-CCET

As per NU method, for $b_3 \to 0$, from Eqs. (2.12), (2.14) and (2.15) $y_n(r)$ obtained as,

$$y_n(r) = P_n^{\left(b_{10}-1, \frac{b_{11}}{b_3} - b_{10} - 1\right)}(1 - 2b_3 r)$$

But

$$\lim_{b_3 \to 0} P_n^{\left(b_{10}-1, \frac{b_{11}}{b_3} - b_{10} - 1\right)}(1 - 2b_3 r) = L_n^{b_{10}}(b_{11} r)$$

Therefore

$$y_n(r) = L_n^{b_{10}-1}(b_{11} r) \tag{3.17}$$

Second part of the wave function $x_n(r)$ obtained as

$$\lim_{b_3 \to 0} (1 - b_3 r)^{-b_{12} - \frac{b_{13}}{b_3}} = e^{b_{13} r}$$

So,

$$x_n(r) = r^{b_{12}} (1 - b_3 r)^{-b_{12} - \frac{b_{13}}{b_3}} = r^{b_{12}} e^{b_{13} r} \tag{3.18}$$

Now total radial wave function from Eqs. 3.17 and 3.18,

$$U_{nl}(r) = N_n r^{b_{12}} e^{b_{13} r} L_n^{b_{10}}(b_{11} r)$$

$$U_{nl}(r) = N_n r^{-\frac{1}{2}+\frac{1}{2}\sqrt{4l'(l'+1)+1}} e^{-\beta r} L_n^{1+\sqrt{4l'(l'+1)+1}}(2\beta r) \tag{3.19}$$

Therefore equation 3.19 is wave function for CP-CCET.

Consider $u = \frac{1}{2}\sqrt{4l'(l'+1)+1}$ and $v = 2\beta r$, we obtain radial wave function as,

$$U_{nl}(r) = N_{n,l} (2\beta)^{\frac{1}{2}-u} v^{-\frac{1}{2}+u} e^{-\frac{v}{2}} L_n^{1+2u}(v) \tag{3.20}$$

Where $N_{n,l}$ is normalization constant

4. RESULTS AND DISCUSSIONS

We deduced few potential from CP-CCET such as MGESC potential and MGESC potential [55] plus inverse square potential

4.1 The More General Exponential Screened Coulomb (MGESC) potential

Adjusting $A = C = 0, \frac{B}{2} = V_0$, and $G = \alpha V_0$, from Eq.1, we obtain

$$V(r) = -\frac{V_0}{r} - \frac{V_0 e^{-2\alpha r}}{r} - \alpha V_0 \tag{4.1}$$

Eq 4.1 is MGESC potential [55]

From Eqs. 3.16 and 3.20, the energy spectrum and wave functions respectively as,

$$E_{nl} = -\alpha V_0 e^{-2\alpha r} - \frac{\mu}{2\hbar^2}\left[\frac{V_0 (1+e^{-2\alpha r})}{n+l+1}\right]^2 \tag{4.2}$$

$$U_{nl}(r) = N_{n,l} (2\beta)^{\frac{1}{2}-u} v^{-\frac{1}{2}+u} e^{-\frac{v}{2}} L_n^{1+2u}(v) \tag{4.3}$$

Where $u = \frac{1}{2}\sqrt{4l(l+1)+1}$ and $v = 2\beta r$ $\quad \beta = \sqrt{-\frac{2\mu}{\hbar^2}(E_{nl} + \alpha V_0 e^{-2\alpha r})}$ (4.4)

Eqs. 4.2, 4.3 and 4.4 are exactly same obtained by Ita, B. I et al [55]

4.2 Eigenvalues equation for Schrodinger equation with More General Exponential Screened Coulomb

(MGESC) Potential plus Inverse Square Potential

Setting $A = 0$, $\frac{B}{2} = V_{0,}, C = V_1$ and $G = \alpha\, V_0$, in Eq. 3.2, we obtained MGESC Potential plus Inverse Square potential as,

$$V(r) = -\frac{V_0}{r} - \frac{V_0 e^{-2\alpha r}}{r} - \alpha\, V_0 - \frac{V_1}{r^2} \tag{4.5}$$

From Eqs. 3.16 and 3.20, the energy spectrum and wave functions respectively for MGESC plus Inverse Square Potential as,

$$E_{nl} = -\alpha\, V_0 e^{-2\alpha r} - \frac{\mu}{2\hbar^2}\left[\frac{V_0 + V_0 e^{-2\alpha r}}{n + l' + 1}\right]^2 \tag{4.6}$$

$$U_{nl}(r) = N_{n,l}\,(2\beta)^{\frac{1}{2}-u} v^{-\frac{1}{2}+u}\; e^{-\frac{v}{2}}\, L_n^{1+2u}(v) \tag{4.7}$$

Where $= \frac{1}{2}\sqrt{4l'(l'+1)+1}$, $v = 2\beta\, r$, $\beta = \sqrt{-\frac{2\mu}{\hbar^2}(E_{nl} + \alpha\, V_0\, e^{-2\alpha r})}$

$l' = \frac{1}{2}\left(-\frac{1}{2} \pm \frac{1}{2}\sqrt{1 + \frac{8V_1}{\alpha} - 4\, l(1+l)}\right)$ and $= N_{n,l}$ is normalization constant.

5. CONCLUSIONS

In this research article, we obtained eigenvalues and wave functions for Coulombic potential with cosine-cosec and exponential term using generalized NU method with appropriate coordinate transformation. By choosing appropriate values of parameters A, B, C, G, α and s, we can obtain eigenvalues and wave functions for quantum mechanical systems. We recover MGESC potential and MGESC potential plus inverse square potential from CP-CCET potential. From the solution of CP-CCET, we find different dynamical properties of the different quantum mechanical systems. Our result is applicable in nuclear physics and quantum chemistry such as diatomic molecular vibration.

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