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L-state analytical solution of the Klein-Gordon equation with position dependent mass using modified Deng-Fan plus exponential molecular potentials via Nikiforov-Uvarov method

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ABSTRACT

The solutions of the Klein-Gordon equation with Modified Deng-Fan plus Exponential molecular potentials (MDFEPP) has been presented using the Pekeris-like approximation and parametric Nikiforov-Uvarov (NU) method. The bound state energy eigenvalues and the corresponding un-unnormalized eigen functions are obtained in terms of Jacobi polynomials.

***Keywords*:** Deng-Fan Potential, Exponential Molecular Potential, Klein-Gordon equation

1. INTRODUCTION

The Klein-Gordon equation (KGE) is a well-known relativistic wave equation that describes spin-zero particles. It is also known that the analytic solutions of the KGE are

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possible only in few cases such as harmonic and Coulomb potentials. The presence of a particle in a strong potential field necessitates a relativistic description of such a particle [1-3]. By considering a relativistic case, we can describe the motion of such a particle either by the Klein-Gordon equation or the Dirac equation depending upon the spin character of the particle [4-6].The Deng-Fan molecular potential is a simple modified Morse potential called the generalized Morse potential, which was proposed by Deng and Fan in 1957 [7] in an attempt to find a more suitable diatomic potential to describe the vibrational spectrum [8]. Although, this potential is qualitatively similar to the Morse potential but it has correct asymptotic behaviour as the internuclear distance approaches zero [9].The Deng-Fan potential model can be used to describe the motion of nucleons in the mean field produced by the interactions between nuclei [10].

Recently our group has attempted to study the bound state solutions of Klein-Gordon, Dirac and Schrodinger equations using combined or mixed potentials. Some of which includes Woods-Saxon plus Attractive Inversely Quadratic potential (WSAIQP) [11], Manning-Rosen plus a class of Yukawa potential (MRCYP) [12], generalied wood-saxon plus Mie-type potential (GWSMP) [13], and Kratzer plus Reduced Pseudoharmonic Oscillator potential (KRPHOP) [14]. In this study, exact l-state solutions of the Klein-Gordon equation with modified Deng-Fan plus exponential type molecular potentials (MDFEP) will be obtained using the Nikiforov-Uvarov method.

This study is organized as follows. Section 2 contains the overview of the Nikiforov-Uvarov method. In Section 3, the Klein-Gordon equation with Modified Deng-Fan plus exponential molecular potentials is solved by using the Nikiforov-Uvarov method. The relativistic energy equations and the corresponding unnormalized wavefunctions are obtained and finally, the conclusion is given in Section 4.

2. REVIEW OF PARAMETRIC NIKIFAROV-UVAROV METHOD

The NU method is based on the solutions of a generalized second order linear differential equation with special orthogonal functions. The Nikiforov-Uvarov method has been successfully applied to relativistic and nonrelativistic quantum mechanical problems and other field of studies as well [11-14]. The hypergeometric NU method has shown its power in calculating the exact energy levels of all bound states for some solvable quantum systems.

$$\Psi''_n(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'_n(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\Psi_n(s) = 0 \qquad (1)$$

where σ(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

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

Thus eqn. (1) can be solved by comparing it with equation (2) and the following polynomials are obtained

$$\tilde{\tau}(s) = (c_1 - c_2 s), \sigma(s) = s(1 - c_3 s), \overline{\sigma}(s) = -\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3 \quad (3)$$

The parameters obtainable from equation (3) serve as important tools to finding the energy eigenvalue and eigenfunctions. They satisfy the following sets of equation respectively

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

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

While the wave function is given as

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

where:

$$c_4 = \frac{1}{2}(1 - c_1), c_5 = \frac{1}{2}(c_2 - 2c_3), c_6 = c_5{}^2 + \epsilon_1, c_7 = 2c_4 c_5 - \epsilon_2, c_8 = c_4{}^2 + \epsilon_3,$$
$$c_9 = c_3 c_7 + c_3{}^2 c_8 + c_6, c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}, c_{11} = c_2 - 2c_5 + 2\left(\sqrt{c_9} + c3\sqrt{c_8}\right)$$
$$c_{12} = c_4 + \sqrt{c_8}, c_{13} = c_5 - \left(\sqrt{c_9} + c3\sqrt{c_8}\right) \quad (7)$$

and P_n is the orthogonal polynomials.

Given that $$P_n{}^{(\alpha,\beta)} = \sum_{r=0}^{n} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(\alpha+r+1)\Gamma(n+\beta-r+1)(n-r)!r!} \left(\frac{x-1}{2}\right)^r \left(\frac{x+1}{2}\right)^{n-r} \quad (8)$$

This can also be expressed in terms of the Rodriguez's formula

$$P_n{}^{(\alpha,\beta)}(x) = \frac{1}{2^n n!}(x-1)^{-\alpha}(x+1)^{-\beta}\left(\frac{d}{dx}\right)^n \left((x-1)^{n+\alpha}(x+1)^{n+\beta}\right)$$

3. SOLUTIONS OF THE RADIAL PART OF THE l-STATE KLEIN-GORDON EQUATION WITH MDFEP POTENTIALS

The l-state Klein-Gordon Equation with vector V(r), potential in atomic units (ħ = c = 1) [14] is given as

$$\frac{d^2 R(r)}{dr^2} + \left[(E^2 - M^2) - 2(E+M)V(r) + \frac{l(l+1)}{r^2}\right]R(r) = 0 \quad (9)$$

The Modified Deng-Fan Potential is given as

$$V(r) = -\left(A_1 + \frac{A_2}{(1-S)} + \frac{A_3}{(1-S)^2}\right) \quad (10)$$

where: A_1, A_2 and A_3 are constant that depends on the dissociation energy.
where: $S = e^{-\alpha r}$ is taking as transformation equation.

The Exponential molecular Potential is given as,

$$V(r) = -V_o S \tag{11}$$

The superposed or combined potentials can be represented as

$$V(r) = -\left(A_1 + \frac{A_2}{(1-S)} + \frac{A_3}{(1-S)^2} + V_o S\right) \tag{12}$$

For a position dependent mass (PDM), $M(x) = M_o + V(r)$
Substitute eq. (12) into eq. (9) we have:

$$\frac{d^2 R(r)}{dr^2} + \left[(E^2 - M^2) + 2(E+M)\left(A_1 + \frac{A_2}{(1-S)} + \frac{A_3}{(1-S)^2} + V_o S\right) + \frac{l(l+1)}{r^2}\right] R(r) = 0 \tag{13}$$

Applying the pekeris-type approximation to eq. (13) we obtained:

$$\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds} + \frac{1}{(1-s)^2s^2}[(\beta^2 + B)s^2 + (V_o + K - A_2 - 2B - 2\beta^2)s + (A_2 + A_3 + B + \beta^2)]R(s) = 0 \tag{14}$$

where:

$\beta^2 = \left(\frac{E^2+M_o^2}{4\alpha^2}\right)$, $B = \left(\frac{E+M_o}{2\alpha^2}\right) A_1$, $k = l(l+1)$

$$c_1 = c_2 = c_3 = 1, c_4 = 0, c_5 = -\frac{1}{2}, c_6 = \frac{1}{4} + \beta^2 + B, c_7 = V_o + K - A_2 - 2B - 2\beta^2,$$

$$c_8 = A_2 + A_3 + B + \beta^2, c_9 = \frac{1}{4} + A_3 + V_o + K, c_{10} = 1 + 2\sqrt{A_2 + A_3 + B + \beta^2},$$

$$c_{11} = 2 + 2\left(\sqrt{\frac{1}{4} + A_3 + V_o + K} + \sqrt{A_2 + A_3 + B + \beta^2}\right),$$

$$c_{12} = \sqrt{A_2 + A_3 + B + \beta^2}, c_{13} = -\frac{1}{2} - \left(\sqrt{\frac{1}{4} + A_3 + V_o + K} + \sqrt{A_2 + A_3 + B + \beta^2}\right),$$

$$\varepsilon_1 = \beta^2 + B,$$
$$\varepsilon_2 = A_2 + 2B + 2\beta^2 - K - V_o, \varepsilon_3 = A_2 + A_3 + B + \beta^2$$

Using the eigenvalue equation, the energy eigen spectrum of MDFEP is found to be

$$\beta^2 = \left[\frac{2A_3 + A_2 - K - V_o - \left(n^2 + n - \frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4} + A_3 + V_o + K}}{(2n+1) + 2\sqrt{\frac{1}{4} + A_3 + V_o + K}}\right]^2 - A_2 - A_3 - B \tag{15}$$

The above equation can be solved explicitly and the energy eigen spectrum of MDFEP becomes

$$E^2 - M^2 = -4\alpha^2 \left\{\left[\frac{2A_3+A_2-V_o-(l(l+1))-\left(n^2+n-\frac{1}{2}\right)-(2n+1)\sqrt{\frac{1}{4}+(l(l+1))+V_o+A_3}}{(2n+1)\sqrt{\frac{1}{4}+(l(l+1))+V_o+A_3}}\right]\right\}^2 - \left(\frac{E+M_o}{2\alpha^2}\right)A_1 - (A_2+A_3) \tag{16}$$

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

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

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

Using equation (14) we get the weight function as

$$\rho(s) = s^U(1-s)^V, \tag{18}$$

where: $U = 2\sqrt{A_2+A_3+B+\beta^2}$, and $V = \sqrt{\frac{1}{4}+\left(l(l+1)\right)+V_o+A_3}$

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

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

Using equation (12) we get the function $\chi(s)$ as

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

where: $P_n^{(U,V)}$ are Jacobi polynomials

Lastly,

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

and using equation (12) we get

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

We then obtain the radial wave function from the equation

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

As

$$R_n(s) = N_n s^{U/2}(1-s)^{(V-1)/2} P_n^{(U,V)}(1-2s), \qquad (24)$$

where: n is a positive integer and N_n is the normalization constant.

4. DISCUSSION

Special case of potential

Case 1: Putting $\boldsymbol{A_1 = A_2 = A_3 = 0}$, Eq. (16) is reduced to bound state Klein-Gordon equation with exponential molecular potential.

$$E^2 - M^2 = -4\alpha^2 \left\{ \left[\frac{V_o - (l(l+1)) - \left(n^2 + n - \frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4} + (l(l+1)) + V_o}}{(2n+1)\sqrt{\frac{1}{4} + (l(l+1)) + V_o}} \right] \right\}^2 \qquad (25)$$

Case 2: When $\boldsymbol{V_0 = 0}$, Eq. (16) is reduced to bound state solution of Klein-Gordon equation with Modified Deng-Fan Molecular potential.

$$E^2 - M^2 = -4\alpha^2 \left\{ \left[\frac{2A_3 + A_2 - (l(l+1)) - \left(n^2 + n - \frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4} + (l(l+1)) + A_3}}{(2n+1)\sqrt{\frac{1}{4} + (l(l+1)) + A_3}} \right] \right\}^2 - \left(\frac{E + M_o}{2\alpha^2}\right) A_1 - (A_2 + A_3) \qquad (26)$$

Eq. (26) is similar to eq. (26) obtained in ref. [15]

5. CONCLUSION

In this paper, we have investigated the numerical l-state analytical solutions of the Klein-Gordon equation with modified Deng-Fan plus exponential molecular potentials (MDFEP) by using the Nikiforov- Uvarov (NU) method. The approximate analytical bound state energy eigenvalues and the corresponding unnormalized wave functions have been obtained. Interestingly, the Schrödinger and Dirac equation with the arbitrary angular momentum values for this potential can be solved by this method. The resulting eigen energy equations can be used to study the spectroscopy of some selected diatomic atoms and molecules.

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