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Bound State Solution of the Klein-Gordon Equation for Modified Echart plus Inverse Square Molecular Potential with an Improved New Approximation Scheme to the Centrifugal Term.

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ABSTRACT

In this research work, the Klein-Gordon equation for Modified Eckart plus Inverse square potentials using the generalized parametric form of Nikiforov-Uvarov method was studied. Energy eigenvalues and the corresponding unnormalized wave function expressed in terms of Jacobi polynomial was obtained. It was discovered that the two special cases of this potential comprises of the Eckart potential and the Inverse Square potential.

Keywords: Parametric Nikiforov-Uvarov method, new approximation scheme, Eckart, plus Inverse square potential.

1.0 INTRODUCTION

In the last decade, a lot of articles have focused on the analytical and approximate solutions of the Schrodinger, Klein-Gordon, and Dirac equations. This is because the solutions of these wave equations contain all the necessary information for the quantum system under consideration. As is well known, the

Schrodinger wave equation is used to describe non-relativistic spinless particles, the Klein-Gordon equation for relativistic spin-zero particles, the Duffin-Kemmer-Petiau equation for relativistic spin-zero and spin-one particles, and the Dirac equation for relativistic spin-half particles. Many potential models have been studied using these wave equations, such as the Kratzer potential, Morse potential, Rosen-Morse potential, Manning-Rosen potential, Deng-Fan potential, and Poschl-Teller potential among others. See for equations [1-8] for details. This paper will discuss the relativistic effects, when a particle moves in the potential consisted Modified Echart plus Inverse square potential (MEISP) which is given as:

$$V(s) = \frac{V_0 S}{(1-S)^2} + \frac{AC_O}{K^2} + \frac{AC_1}{K^2(1-S)} + \frac{AC_2}{K^2(1-S)^2} \quad (1)$$

Solutions of bound states of the Klein–Gordon equation with vector potentials are obtained, the normalized angular wave function and radial wave function are presented, simultaneously, energy spectrum equations are also obtained. The paper is organized as follows: Section 1 has the introduction, the NU method is reviewed in section 2. In section 3, the Klein-Gordon equation with MEISP is solved using the NU method. Finally, we give a brief discussion in section 4 before the conclusion in section 5 and then the references also given.

2.0 GENERALIZATION OF NIKIFOROV-UVAROV METHOD

The main equation which is closely associated with the method is given in the following form (Nikiforov and Uvarov, 1988).

$$\psi''(S) + \frac{\tilde{\iota}(S)}{\sigma(S)}\tilde{\iota}'(S) + \frac{\boldsymbol{\sigma}(S)}{\sigma^2(S)}\psi(S) = 0 \quad (2)$$

Where σ (s) and $\boldsymbol{\sigma}(s)$ are polynomials at most second-degree, $\tilde{\iota}(s)$ is a first-degree polynomial and $\psi(s)$ is a function of the hypergeometric-type.

In order to find the exact solution to Eq. (2), we set the wave function as:

$$\psi(x) = \phi(s)\, X\,(s) \quad (3)$$

And on substituting Eq. (3) into Eq. (2), then Eq. (3) reduces to hypergeometric-type,

$$\sigma(S)X''(s) + \tau(S)X'(S) + \lambda X(S) = 0 \quad (4)$$

Where the wave function $\emptyset$ (s) is defined as the logarithmic derivative

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)'} \quad (5)$$

Where π (s) is at most first-order polynomial.

The hypergeometric-type function ∅ (s) polynomial solutions are given by the Rodrigues relation

$$\phi(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s)\rho(s)] \tag{6}$$

Where B_n is the Normalization constant and the weight function $\rho(s)$ most satisfy the condition

$$\frac{d}{ds}[\sigma^n(s)\rho(s)] = \tau(s)\rho(s) \tag{7}$$

Where;

$$\tau(s) = \breve{\imath}(s) + 2\pi(s) \tag{8}$$

In order to accomplish the condition imposed on the weight function $\rho(s)$, it is necessary that the classical or polynomials $\tilde{\imath}(s)$ be equal to zero to some point of an interval (a , b) and its derivative at this interval at $\sigma(s)>0$ will be negative, that is;

$$\frac{d\tau(s)}{ds} < 0 \tag{9}$$

Therefore, the function $\pi(s)$ and the parameter λ required for the NU method are defined as follows:

$$\pi(s) = \sqrt{\left(\frac{\sigma' - \breve{\imath}}{2}\right)^2 - \sigma + K\boldsymbol{\sigma}} \tag{10}$$

Where $\lambda = k + \pi'(s)$

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

$$\psi''(s) + \left[\frac{(C_1 - C_2S)}{S(1 - C_3S)}\right]\psi'(S) + \left[\frac{-\xi_1S^2 + \xi_2S - \xi_3}{S^2(1 - C_3S)^2}\right]\psi(s) = 0 \tag{11}$$

Equation (11) is solved by comparing it with Eq. (2) and the following polynomials are obtained:

$$\breve{\imath}(s) = (C_1 - C_2S), \boldsymbol{\sigma}(s) = S(1 - C_3S), \sigma(s) = -\xi_1s^2 + \xi_2s - \xi_3 \tag{12}$$

Now substituting Eq. (12) into Eq. (11), we find

$$\boldsymbol{\sigma}(s)C_4 + C_5S \pm \sqrt{[(C_6 - C_3K_{\pm})S^2 + (C_7 + K_{\pm})S + C_8]} \tag{13}$$

Where

$$C_4 = \frac{1}{2}(1 - C_1), C_5 = \frac{1}{2}(C_2 - 2C_3), C_6 = C_5^2 + \xi_1, C_7 = 2C_4C_5 - \xi_2, C_8 = C_4^2 + \xi_3, C_9 = C_3C_7 + C_3^2C_8 + C_{6,}C_{10} = C_1 + 2C_4 + 2\sqrt{}C_8\,C_4 \tag{14}$$

The resulting value of k in Eq. (13) is obtained from the condition that the function under the square root be square of a polynomials and it yields,

$$K_{\pm} = -(C_7 + 2C_3C_8) \pm 2\sqrt{C_9C_8} \tag{15}$$

Where $C_9 = C_3C_7 + C_3^2C_8 + C_6$

The new π (s) for k becomes

$$\pi(s) = C_4 + C_5S - \left[\left(\sqrt{C_9} + C_3\sqrt{C_8}\right)S - \sqrt{C_8}\right] \tag{16}$$

Using Eq. (8), we obtain

$$\tau(s) = C_1 + 2C_4 - (C_2 - 2C_5)s - 2\left[\left(\sqrt{C_9} + C_3\sqrt{C_8}\right)s - \sqrt{C_8}\right] \tag{17}$$

We obtain the energy equation as

$$(C_2 - C_3)n + C_3n^2 - (2n+1)C_5 + (2n+1)\left(\sqrt{C_9} + C_3\sqrt{C_8}\right) + C_7 + 2C_3C_8 + 2\sqrt{C_8C_9} = 0 \tag{18}$$

While the wave function is given as

$$\psi_4(s) = N_{n,1}S^{C_{12}}(1 - C_3S)^{-C_{12}-\frac{C_{13}}{C_3}}P_n^{\left(C_{10}-1,\frac{C_{11}}{C_3}-C_{10}-1\right)}(1 - 2C_3S) \tag{19}$$

Where P_n is the orthogonal polynomials.

Given that = $P_n{}^{(\alpha,\beta)} = \sum_{r=0}^{n} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(\alpha+r+1)\Gamma(n+\beta-r+1)(n-r)!r!}\left(\frac{x-1}{2}\right)^{r}\left(\frac{x+1}{2}\right)^{n-r}$ (20)

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

$$P_n{}^{(\alpha,\beta)}(x) = \frac{1}{2^n n!}(x-1)^{-a}(x+1)^{\beta}\left(\frac{d}{dx}\right)^{n}\left((x-1)^{n+a}(x+1)^{n+\beta}\right) \tag{21}$$

3 SOLUTIONS OF THE RADIAL KLEIN-GORDON EQUATION

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

$$\frac{d^2R(r)}{dr^2} + [(E_2 - M_2) - (E + M)V(r)]\, R(r) = 0 \quad (22)$$

The Modified Eckart Potential is given as:

$$V(r) = \left(\frac{V_o e^{-ar}}{(1-e^{-ar})^2}\right) \quad (23)$$

The Inverse Square Potential: $V(r) = \frac{A}{R^2}$ (24)

Applying the transformation $S = e^{-ar}$, the new improved approximation is given as

$$\frac{1}{r^2} = \frac{1}{k^2}\left[C_0 C_1 \left(\frac{-e^{-ar}}{1-e^{-ar}}\right) + C_2 \left(\frac{-e^{-ar}}{1-e^{-ar}}\right)^2\right] \quad (25)$$

Where: $C_0 = 1 - \left(\frac{1+e^{-arb}}{2ab}\right)^2, C_1 = \ 2(e^{ar} = 1)^2$

The superposed potential can be represented as MEISP

$$V(s) = \frac{V_0 S}{(1-s)^2} + \frac{AC_0}{K^2} + \frac{AC_1}{K^2(1-s)} + \frac{AC_2}{K^2(1-s)^2} \quad (26)$$

Applying the new improved approximation and after lengthy algebra, we have $\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds} + \frac{1}{(1-s)^2 s^2}[(2\beta^2 - H)s^2 + (-4\beta^2 + Q - P + 2H)s + (2\beta^2 - H - Q - J]R(s) = 0$

(27)

Where

$$-\beta^2 = \left(\frac{E^2+M_0^2}{4\alpha^2}\right), Q = \left(\frac{\mu}{2k^2\alpha^2\hbar^2}\right)AC_1,$$

$$H = \left(\frac{\mu}{2\alpha^2\hbar^2}\right)AC_{0,}P = \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0, J = \left(\frac{\mu}{2k^2\alpha^2\hbar^2}\right)AC_2,$$

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

$$c_8 = 2\beta^2 - H - Q - J, c_9 = \frac{1}{4} - P - J, c_{10} = 1 + 2\sqrt{2B^2 - H - Q - J, c_{11} = 2 + 2\left(\sqrt{\frac{1}{4} - P - J} + \sqrt{2\beta^2 - H - Q - J}\right)}$$

(28)

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

$$\beta^2 = \left[\frac{(P+Q+2J) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}-P-J}}{(2n+1)+2\sqrt{\frac{1}{4}-P-J}}\right]^2 - (H+Q+J) \tag{29}$$

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

$$E^2 - M^2 - 4\alpha^2 \left\{\left[\frac{\left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0 + \left(\frac{\mu}{2K^2\alpha^2\hbar^2}\right)AC_1 + 2\left(\frac{\mu}{2K^2\alpha^2h^2}\right)AC_2\right) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}} - \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0 - \left(\frac{\mu}{2k^2\alpha^2\hbar^2}\right)A_{C2}}{(2n+1)+\sqrt{\frac{1}{4}} - \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0\left(\frac{\mu}{2K^2\alpha^2\hbar^2}\right)AC_2}\right]^2\right\} \tag{30}$$

4. EIGEN FUNCTION CONSIDERATION

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

$$\rho(s) = S^{c_{10}-1}(1-C_3S)^{\frac{c_{11}}{c_3}c_{10}-1} \tag{31}$$

Using equation (28), we get the weight function as

$$\rho(s) = S^u(1-S)^v \tag{32}$$

Where $U = \beta^2 - R - P - \lambda$, and $V = 2\sqrt{\frac{1}{4} - P - J}$

Also we obtain the wave function $X_n(s)$ as

$$X_n(s) = P_n^{(u,v)}(1-2s) \tag{33}$$

Where $P_n^{(u,v)}$ are Jacobi polynomials

Lastly, $\varphi(s) = s^{c_{12}}(1-C_3s)^{-c_{12}-\frac{c_{13}}{c_3}}$ (34)

Using equation (28) we get

$$\varphi(s) = s^{\frac{u}{2}}(1-2)^{\frac{1+v}{2}} \tag{35}$$

We obtain Radial wave function from equation (28)

$$R_n(s) = N_n\varphi(s)X_n(s) \tag{36}$$

As

$$R_n(s) = N_n s^{\frac{u}{2}}(1-s)^{\frac{1+v}{2}} P_n^{(u,v)}(1-2s) \quad (37)$$

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

5. DISCUSSION

In this subsection, we will consider some special cases of the potential in consideration.

(i) If we set $V_0 = 0$ in equation (23), the eigen energy spectrum of equation reduces to (34) Which is the energy spectrum for inverse square potential using the new approximation scheme.

$$E^2 - M^2 = -4\alpha^2 \left\{ \left[\frac{\left(\left(\frac{\mu}{2K^2\alpha^2\hbar^2}\right)AC_1 + 2\left(\frac{\mu}{2K^2\alpha^2\hbar^2}\right)AC_2\right) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}}\left(\frac{\mu}{2k^2\alpha^2\hbar^2}\right)AC2}{(2n+1)+\sqrt{\frac{1}{4}-\left(\frac{\mu}{2\alpha^2\hbar^2}\right)AC_2}} \right]^2 \right\} \quad (34)$$

(ii) If we set $A = 0$ in equation (24), the eigen energy spectrum of equation (29) reduces to (35) Which is the energy spectrum for modified Echart potential under the new approximation scheme

$$E^2 - M^2 = -4\alpha^2 \left\{ \left[\frac{\left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0\right) - \left(n^2+n-\frac{1}{2}\right) - (2n+1)\sqrt{\frac{1}{4}}\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0}{(2n+1)+\sqrt{\frac{1}{4}-\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_0}} \right]^2 \right\} \quad (35)$$

6. NUMERICAL ANALYSIS

In this subsection, we discussed the behavior of our calculated Eigen energy values and the superposed potential (MEISP) at different values of the screening parameters. **Figure I** shows the variation of the eigen energy with screening parameter. It can be observed that eigen energy increases with increasing screening parameter. **Figure II** shows the relationship between the superposed potential with the internuclear distance. The plot has a repulsive behavior within the potential energy diagram. **Table I and II** depicts the numerical result of the eigen energy and superposed potential at different screening parameters.

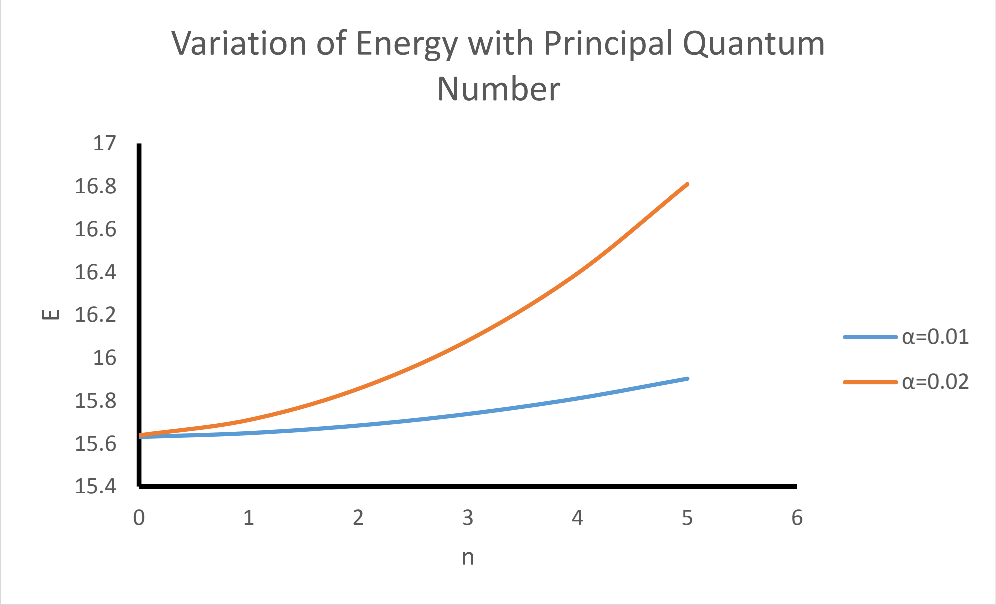

Figure I: Plot of eigen energy versus Principal Quantum Number

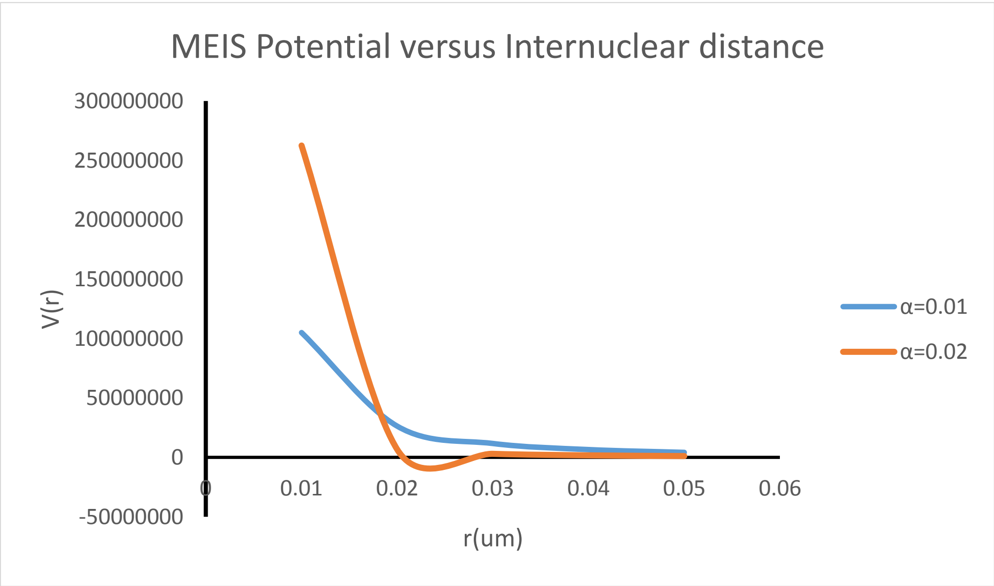

Figure II: Variation of Potential with internuclear distance

Table 6.1: Eigen energy at different Screening Parameter

E_l		
n	α=0.01	α=0.02
1	15.64899551	15.71069848
2	15.68466633	15.85621798
3	15.73857948	16.08133291

4	15.81123382	16.39499224
5	15.90331266	16.81052189

Table 6.2: Potential Values at different Screening Parameter

R(um)	V(r)	
	α=0.01	α=0.02
0.01	105020002.30	262660002.26
0.02	26260002.260	6567502.2630
0.03	11673335.600	2920002.2400
0.04	6567502.2630	1643126.8520
0.05	4204002.2630	1052001.8420

7. CONCLUSION

In this paper, we investigated the solutions of the Klein-Gordon equation for the Modified Eckart plus Inverse square potentials using a new approximation method for the centrifugal term via parametric Nikiforv-Uvarov method. The eigenvalues of the potential reduced to that of well-known potentials viz Echart potential in (35) and Inverse square potential in (34), when we make appropriate choices of the parameters. Finally, we also obtained the numerical result of our eigen energy spectrum.

REFERENCES

W. A. Yahya, K. J. Oyewumi, C. O. Akoshile and T. T. Ibrahim (2010). Bound state solutions of the relativistic Dirac equation with equal scalar and vector Eckart potential using Nikiforov-Uvarov method. *JVR*. 3:27-34.

W. A. Yahya and K. J. Oyewumi(2013). Information-theoretic and complexity measures of the Mie-type potential. *Journal of Mathematical Physics*. 54:(22).

W. A. Yahya, B. J. Falaye, O. J. Oluwadare, and K. J. Oyewumi. (2013). Thermodynamic properties and the approximate solutions of the Schrödinger equation with the shifted Deng-Fan potential model. Int. J. Mod. Phys. E 22 (8),135-145.

J. Y. Liu, J. F. Du, and C. S. Jia. (2013). Molecular spinless energies of the improved Tietz potential energy model. *European Physical Journal Plus,* 128-139. doi: 10.1140/epjp/i2013-13139-4.

T. Chen, S. R. Lin, and C. S. Jia, Eur. Phys. J. Plus 128, 69 (2013).

J. Y. Liu, X. T. Hu, and C. S. Jia, Can. J. Chem. 91, 1 (2013). doi: 10.1139/cjc-2013-0396.

H. M. Tang, G. C. Liang, L. H. Zhang, F. Zhao, and C. S. Jia, Can. J. Chem. 92, 201 (2014). doi: 10.1139/cjc 2013-0466.

Y. F. Cheng and T. Q. Dai, Chinese J. Phys. 45(5), 480 (2007).