

Bound- State Solution of Klein-Gordon Equation with Combined Potentials Using Nikiforov-Uvarov Method

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Abstract

We apply Pekeris approximation to the centrifugal term to find an approximate solution to Klein-Gordon equation with the combined potential using conventional Nikiforov-Uvarov method. The proposed combined potential is relevant in studying diatomic molecules. We obtained energy-eigen value and normalized wave functions using confluent hypergeometric functions. Numerical computations of the resulting energy were obtained using Fortran programming.

Keywords: Nikiforov-Uvarov method, Klein-Gordon equation, combined potential

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1.0 Introduction

Quantum mechanics is basically divided into two broad classes: The relativistic and non- relativistic. Klein-Gordon equation is non-relativistic wave equations that described spin-zero particles otherwise called the bosons while its counterpart Dirac equation described spin1/2 particles. Klein-Gordon equations though having negative probabilities provides bound state solutions with considerable potentials. Klein-Gordon equation can described particles at low and significantly high speed and that makes it be relevant in particle physics, high energy physics and molecular dynamics among others. However, because of its enormous applications especially in chemical and physical sciences, a lot authors developed a keen interest in studying Klein-Gordon equation. [1-5].

Different analytical techniques have been adopted by different authors in studying both relativistic and non –relativistic wave equations. Among them are: Nikiforov-Uvarov method [6-9], factorization method [10-12], super-symmetric quantum mechanics approach [13-15],asymptotic iteration method [16-18]

However, these techniques are applicable for selected potentials, few among them are : Rosen-Morse, Hulthen, pseudo harmonic, Poschl-Teller, kratzerfues and Mie-Type potential, Eckart potential, P-T symmetric Hulthen potential [19-28]. The study of the proposed potential is very essential in investigating the interaction existing between diatomic molecules.

The main aim of this paper is to present and study combined potential (Hulthen-yukawa inversely quadratic potential) This article is organized as follows: section 1 is the introduction, section 2 gives a brief discussion of parametric Nikiforov-Uvarov method. The method used in this article reproduces accurate analytical solutions for many differential equations with significant application in physics, for example it can be used for equation of Hermite, Laguerre and Jacobi. Section 3 gives the radial solution of one dimensional Klein-Gordon equation with the combined potential. Section 4 present analytical solutions of the normalized wave function using confluent hypergeometric function. Finally, section 5 gives the numerical computation of the resulting energy as applied to oxygen molecule. The combined potential is given by

$$V(r) = -\frac{V_0 e^{-2\alpha r}}{(1-e^{-2\alpha r})} - \frac{Ae^{-\alpha r}}{r} + \frac{B}{r^2} + C \quad (1)$$

A, B and C are real constants and r is the intermolecular distance. The potential is useful in molecular dynamics.

The first term is the Hulthen potential which is a short range potential, the third term is the inversely quadratic potential which is a long range potential that decays faster relative to the intermolecular distance, while the second term is the Yukawa potential which is attractive in nature.

2.0 Review of Parametric Nikiforov-Uvarov method

The NU method is based on reducing second order linear differential equation to a generalized equation of hyper-geometric

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type .This method provides solution in terms of special orthogonal functions as well as corresponding energy eigen value. The parametric formalization of NU is applicable and valid for central and non- central potential. Here the hypergeometric differential equation is given by

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

The energy eigen-value can be calculated using the equation

$$c_2 n - (2n+1)c_5 + (2n+1)\left(\sqrt{c_9} + c_3\sqrt{c_8}\right) + n(n-1)c_3 + c_7 + 2c_3c_8 + 2\sqrt{c_8c_9} = 0 \quad (3)$$

While the wave function can be calculated using equation (4)

$$\Psi(s) = \phi(s)\chi_n(s) = N_n s^{c_{12}} (1 - c_3 s)^{c_{13}} P_n^{(c_{10}, c_{11})}(1 - 2c_3 s) \quad (4)$$

Equations (1),(2) and (3) has parametric constant that can be determine using the following parametric coefficients

$$\begin{cases} c_4 = \frac{1}{2}(1 - c_1), \\ c_5 = \frac{1}{2}(c_2 - 2c_3), \\ c_6 = c_5^2 + \xi_1 \\ c_7 = 2c_4c_5 - \xi_2 \\ c_8 = c_4^2 + \xi_3 \end{cases} \quad (5)$$

Meanwhile, c_1, c_2 and c_3 are parametric coefficients obtained by comparing the resulting differential equation to equation (2). Other parametric coefficients are

$$\begin{aligned} c_9 &= c_3c_7 + c_3^2c_8 + c_6 \\ c_{10} &= c_1 + 2c_4 + 2\sqrt{c_8} \\ c_{11} &= c_2 - 2c_5 + 2(\sqrt{c_9} + c_3\sqrt{c_8}) \\ c_{12} &= c_4 + \sqrt{c_8} \\ c_{13} &= c_5 - (\sqrt{c_9} + c_3\sqrt{c_8}) \end{aligned} \quad (6)$$

3.0 Solution Of Klein-Gordon Equation

One dimensional Klein-Gordon equation with equal vector and scalar potential is given by

$$\frac{d^2 R(r)}{dr^2} + \left[E_{nl}^2 - m^2 - 2(E_{nl} + m)v(r) - \frac{\lambda}{r^2} \right] R(r) = 0 \quad (7)$$

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

Substituting equation (1) into (7) gives

$$\frac{d^2 R(r)}{dr^2} + \left[E_{nl}^2 - m^2 - 2(E_{nl} + m) \left(\frac{-V_0 e^{-2\alpha r}}{(1 - e^{-2\alpha r})} - \frac{A e^{-\alpha r}}{r} + \frac{B}{r^2} + C \right) - \frac{\lambda}{r^2} \right] R(r) = 0 \quad (8)$$

Using the transformation $s = e^{-2\alpha r}$ then,

$$\frac{d^2 R(r)}{dr^2} = 4\alpha^2 e^{-4\alpha r} \frac{d^2 R(r)}{ds^2} + 4\alpha^2 e^{-2\alpha r} \frac{dR(r)}{ds} \quad (9)$$

Substituting equation (9) into (8) gives

$$4\alpha^2 e^{-4\alpha r} \frac{d^2 R(r)}{ds^2} + 4\alpha^2 e^{-2\alpha r} \frac{dR(r)}{ds} \left[\begin{aligned} &E^2 - m^2 + \frac{2V_0 E e^{-2\alpha r}}{(1 - e^{-2\alpha r})} + \frac{2AE e^{-\alpha r}}{r} - \frac{2EB}{r^2} - 2EC \\ &+ \frac{2V_0 m e^{-2\alpha r}}{(1 - e^{-2\alpha r})} + \frac{2Am e^{-\alpha r}}{r} - \frac{2Bm}{r^2} - 2Cm - \frac{\lambda}{r^2} \end{aligned} \right] \quad (10)$$

Let's define standard pekeris approximation to the centrifugal term as

$$\frac{1}{r} = \frac{2\alpha e^{-\alpha r}}{(1-e^{-2\alpha r})} \Rightarrow \frac{1}{r^2} = \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} \quad (11)$$

Substituting equation (11) into (10) and expressing the exponential term in s-dimension gives

$$\frac{d^2 R(r)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR(r)}{ds} + \left\{ \begin{array}{l} \frac{1}{4\alpha^2} [E^2 - m^2 - 2v_0 E - 4A\alpha E - 2EC - 2v_0 m - 4A\alpha m - 2Cm] s^2 + \\ \frac{1}{4\alpha^2} [2m^2 - 2E^2 + 2v_0 E + 4A\alpha E - 8\alpha^2 EB + 4EC + 4A\alpha m - 8\alpha^2 Bm + 4cm - 4\alpha^2 \lambda + 2v_0 m] s \\ + \frac{1}{4\alpha^2} [E^2 - m^2 - 2EC - 2Cm] \end{array} \right\} R(s) = 0 \quad (12)$$

Comparing equation (12) to (2) gives

$$c_1 = c_2 = c_3 = 1 \quad (13)$$

$$\begin{aligned} \xi_1 &= -\frac{1}{4\alpha^2} [E^2 - m^2 - 2v_0 E - 4A\alpha E - 2EC - 2v_0 m - 4A\alpha m - 2Cm] \\ \xi_2 &= -\frac{1}{4\alpha^2} [2m^2 - 2E^2 + 2v_0 E + 4A\alpha E - 8\alpha^2 EB + 4EC + 4A\alpha m - 8\alpha^2 Bm + 4Cm - 4\alpha^2 \lambda + 2v_0 m] \\ \xi_3 &= -\frac{1}{4\alpha^2} [E^2 - m^2 - 2EC - 2Cm] \end{aligned} \quad (14)$$

Using equations (5) and (6), we obtained other parametric coefficients as follows:

$$\begin{aligned} c_4 &= 0 \\ c_5 &= -\frac{1}{2} \\ c_6 &= \frac{1}{4} - \frac{1}{4\alpha^2} [E^2 - m^2 - 2v_0 E - 4A\alpha E - 2EC - 2v_0 m - 4A\alpha m - 2Cm] \\ c_7 &= -\frac{1}{4\alpha^2} [2m^2 - 2E^2 + 2v_0 E + 4A\alpha E - 8\alpha^2 EB + 4EC + 4A\alpha m - 8\alpha^2 Bm + 4Cm - 4\alpha^2 \lambda + 2v_0 m] \\ c_8 &= -\frac{1}{4\alpha^2} [E^2 - m^2 - 2EC - 2Cm] \\ c_9 &= \frac{1}{4} + 2EB + 2Bm + \lambda \\ c_{10} &= 1 + 2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \\ c_{11} &= 2 + \sqrt{1 + 8EB + 8Bm + 4\lambda} + \frac{1}{\alpha} \sqrt{[m^2 - E^2 + 2EC + 2Cm]} \\ c_{12} &= \frac{1}{2\alpha} \sqrt{[m^2 - E^2 + 2EC + 2Cm]} \\ c_{13} &= -\frac{1}{2} \left[\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right] \end{aligned} \quad (15)$$

(a) CALCULATION OF ENERGY EIGEN VALUE

Using equation (3), the energy eigen-value become

$$\begin{aligned} 2n + \frac{1}{2} + (2n+1) \left[\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right] \\ + n(n-1) - \\ \frac{1}{4\alpha^2} \left[\begin{array}{l} 2m^2 - 2E^2 + 2v_0 E \\ + 4A\alpha E - 8\alpha^2 EB \\ + 4EC + 4A\alpha m - 8\alpha^2 Bm \\ + 4Cm - 4\alpha^2 \lambda + 2v_0 m - 2m^2 \\ + 2E^2 - 4EC - 4Cm \end{array} \right] + \frac{1}{2\alpha} \sqrt{[m^2 - E^2 + 2EC + 2Cm](1 + 8EB + 8Bm + 4\lambda)} = 0 \end{aligned} \quad (16)$$

Equation (16) can further be reduced

$$E = \frac{-(2v_0 m + 4A\alpha m)}{[2v_0 + 4A\alpha - 8\alpha^2 B]} \quad (17)$$

Let's define non-relativistic limit transformation equation as

$$m + E \rightarrow \frac{2\mu}{\hbar}, m - E \rightarrow -E_{nl} \quad (18)$$

Applying equation (18) to (17) gives

$$E_{nl} = \frac{4\alpha^2 \left\{ (n^2 - 3n + 1) + (2n + 1) \left(\sqrt{1 + \frac{16\mu B}{\hbar^2} + 4\lambda} + \frac{1}{\alpha} \sqrt{\frac{4\mu C}{\hbar^2} - \frac{2\mu E_{nl}}{\hbar^2}} \right) \right\} - (2v_0 m + 4A\alpha m)}{[2v_0 + 4A\alpha - 8\alpha^2 B]} \quad (19)$$

Equation (19) is the energy equation for the combined potential.

(b) CALCULATION OF THE WAVE FUNCTION

Using equation (4), the wave function is given as

$$\Psi_{n,l}(r) = N_n e^{-2\alpha r \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]}} \left(1 - e^{-2\alpha r} \right)^{-\frac{1}{2} \left[\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right]} \times P_n^{\left\{ 1+2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]}, 2+\sqrt{1+8EB+8Bm+4\lambda}+\frac{1}{\alpha}\sqrt{m^2-E^2+2EC+2Cm} \right\}} \left(1 - 2e^{-2\alpha r} \right) \quad (20)$$

4.0 Normalised Wave Function Using Confluent Hypergeometric Functions

The wave function is given in equation in S-dimension is given as

$$\Psi_{n,l}(s) = N_n s^{\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]}} \left(1 - s \right)^{-\frac{1}{2} \left[\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right]} \times P_n^{\left\{ 1+2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]}, 2+2\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + 2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right\}} \left(1 - 2s \right) \quad (21)$$

Let

$$\xi_1 = \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \text{ and } \wedge = \sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} \quad (22)$$

Then, the wave function become

$$\Psi_{n,l}(s) = N_n s^{\xi_1} \left(1 - s \right)^{-\frac{1}{2} - [\wedge + \xi_1]} \times P_n^{\{(1+2\xi_1), (2+2\wedge+2\xi_1)\}} \left(1 - 2s \right) \quad (23)$$

However, to normalized a wave function we, introduced the normalization integral

$$\int_0^\infty \Psi(r) \Psi^*(r) dr = 1 \quad (24)$$

In a situation where $\Psi(r)$ and its complex conjugate are real function, then equation (24) can be expressed as

$$\int_0^\infty |\Psi(r)|^2 dr = 1 \quad (25)$$

Considering the fact that $s = e^{-2\alpha r}$ then when $r = 0, s = 1$ and when $r = \infty, s = 0$,

Hence the wave function will be physically valid for $s \in [0, 1]$ and $r \in (0, \infty)$

Applying equation (25) the wave function become

$$-\frac{N_n^2}{2\alpha} \int_0^{2\xi_1-1} s^{2\xi_1-1} (1-s)^{-1-[2\wedge+2\xi_1]} \times \left[P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) \right]^2 ds = 1 \quad (26)$$

Jacobi polynomial can be expressed in two ways as hypergeometric partial sum series as

$$P_n^{(\rho,\nu)}(\xi_1) = 2^{-n} \sum_{p=0}^n (-1)^{n-p} \binom{n+\rho}{p} \binom{n+\nu}{p} (1-\xi_1)^{n-p} (1+\xi_1)^p \quad (27)$$

$$P_n^{(\rho,\nu)}(\xi_1) = \frac{\Gamma(n+\rho+1)}{n! \Gamma(n+\rho+\nu+1)} \sum_{r=0}^n \binom{n}{r} \frac{\Gamma(n+\rho+\nu+r+1)}{\Gamma(r+\rho+1)} \left(\frac{\xi_1-1}{2} \right)^r \quad (28)$$

Where

$$\binom{n}{r} = {}^n c_r = \frac{n!}{(n-r)! r!} = \frac{\Gamma(n+1)}{\Gamma(n-r+1) \Gamma(r+1)} \quad (29)$$

Making use of equation (27)

$$P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) = 2^{-n} (2s)^{n-p} 2^p (1-s)^p \sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1+1}{p} \binom{n+2\wedge+2\xi_1+2}{n-p} \quad (30)$$

$$\text{Where } \xi_1 = (1-2s), \rho = 1+2\xi_1 \text{ and } \nu = 2+2\wedge+2\xi_1 \quad (31)$$

Evaluating the term under the summation sign of equation (30) as a partial sum.

For p=0,

$$\sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1+1}{p} \binom{n+2\wedge+2\xi_1+2}{n-p} = (-1)^n \binom{n+2\xi_1+1}{0} \binom{n+2\wedge+2\xi_1+2}{n} = (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1) \Gamma(2\wedge+2\xi_1+3)} \quad (32)$$

For p=0, n

$$\sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1+1}{p} \binom{n+2\wedge+2\xi_1+2}{n-p} = \sum_{p=0}^n \frac{(-1)^p \Gamma(n+2\xi_1+2) \Gamma(n+2\xi_1+2\wedge+3)}{p! (n-p)! \Gamma(n+2\xi_1-p+2) \Gamma(2\xi_1+2\wedge+p+3)} \quad (33)$$

Substituting equation (33) and (32) into (30) gives

$$P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) = 2^{-n} (2s)^{n-p} 2^p (1-s)^p (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1) \Gamma(2\wedge+2\xi_1+3)} \times \sum_{p=0}^n \frac{(-1)^p \Gamma(n+2\xi_1+2) \Gamma(n+2\xi_1+2\wedge+3)}{p! (n-p)! \Gamma(n+2\xi_1-p+2) \Gamma(2\xi_1+2\wedge+p+3)} \quad (34)$$

Using equation (28)

$$P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) = \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \sum_{r=0}^n \frac{\Gamma(n+4+4\xi_1+2\wedge+r) (-1)^r s^r}{r! (n-r)! \Gamma(r+2\xi_1+2)} \quad (35)$$

Then

$$\left[P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) \right]^2 = \text{Equation (34) multiplied by (35)}$$

Then

$$\begin{aligned} \left[P_n^{\{(1+2\xi_1),(2+2\wedge+2\xi_1)\}} (1-2s) \right]^2 &= \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \sum_{r=0}^n \frac{\Gamma(n+4+4\xi_1+2\wedge+r) (-1)^r s^r}{r! (n-r)! \Gamma(r+2\xi_1+2)} \times \\ 2^{-n} (2s)^{n-p} 2^p (1-s)^p (-1)^n &\frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1) \Gamma(2\wedge+2\xi_1+3)} \times \\ \sum_{p=0}^n \frac{(-1)^p \Gamma(n+2\xi_1+2) \Gamma(n+2\xi_1+2\wedge+3)}{p! (n-p)! \Gamma(n+2\xi_1-p+2) \Gamma(2\xi_1+2\wedge+p+3)} \end{aligned} \quad (36)$$

Equation (36) can be further simplified to

$$\left[P_n^{\{(1+2\xi_1), (2+2\wedge+2\xi_1)\}} (1-2s) \right]^2 = \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \sum_{r=0}^n \frac{\Gamma(n+4+4\xi_1+2\wedge+r)}{r!(n-r)!\Gamma(r+2\xi_1+2)} \times \\ (s)^{n-p+r} (1-s)^p (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1)\Gamma(2\wedge+2\xi_1+3)} \times$$
(37)

$$\sum_{p=0}^n \frac{(-1)^{p+r} \Gamma(n+2\xi_1+2)\Gamma(n+2\xi_1+2\wedge+3)}{p!(n-p)!\Gamma(n+2\xi_1-p+2)\Gamma(2\xi_1+2\wedge+p+3)}$$

Substituting equation (37) into (26)

$$\begin{aligned} & -\frac{N_n^2}{2\alpha} \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \\ & \sum_{p,r=0}^n \frac{(-1)^{p+r} \Gamma(n+2\xi_1+2)\Gamma(n+2\xi_1+2\wedge+3)}{p!(n-p)!\Gamma(n+2\xi_1-p+2)\Gamma(2\xi_1+2\wedge+p+3)} \frac{\Gamma(n+4+4\xi_1+2\wedge+r)}{r!(n-r)!\Gamma(r+2\xi_1+2)} \times \\ & (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1)\Gamma(2\wedge+2\xi_1+3)} \times \int_0^{2\xi_1-1+n-p+r} (1-s)^{-1-2\wedge-2\xi_1+p} ds = 1 \end{aligned} \quad (38)$$

Let's defined confluent hypergeometric function expressed in terms of gamma function as

$${}_2F_1(\alpha_0, \beta_0 : \alpha_0 + 1; 1) = \alpha_0 \int_0^1 (s)^{\alpha_0-1} [1-s]^{-\beta_0} ds = 1 \quad (39)$$

Assuming that

$$\gamma_0 = \alpha_0 + 1, \text{ then } {}_2F_1(\alpha_0, \beta_0 : \gamma_0; 1) = \alpha_0 \int_0^1 (s)^{\alpha_0-1} [1-s]^{-\beta_0} ds = 1 \quad (40)$$

However,

$${}_2F_1(\alpha_0, \beta_0 : \gamma_0; 1) = \frac{\Gamma(\gamma_0)\Gamma(\gamma_0 - \alpha_0 - \beta_0)}{\Gamma(\gamma_0 - \alpha_0)\Gamma(\gamma_0 - \beta_0)} \quad (41)$$

Hence, the integral expression in equation (38) can be evaluated as

$$\int_0^{2\xi_1-1+n-p+r} (1-s)^{-1-2\wedge-2\xi_1+p} ds = \frac{\Gamma(\alpha_0+1)\Gamma(p-2\wedge-2\xi_1)}{\alpha_0\Gamma(\alpha_0-2\wedge-2\xi_1+p)} \quad (42)$$

Substituting equation (42) into (38) gives

$$\begin{aligned} & -\frac{N_n^2}{2\alpha} \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \\ & \sum_{p,r=0}^n \frac{(-1)^{p+r} \Gamma(n+2\xi_1+2)\Gamma(n+2\xi_1+2\wedge+3)}{p!(n-p)!\Gamma(n+2\xi_1-p+2)\Gamma(2\xi_1+2\wedge+p+3)} \frac{\Gamma(n+4+4\xi_1+2\wedge+r)}{r!(n-r)!\Gamma(r+2\xi_1+2)} \times \\ & (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1)\Gamma(2\wedge+2\xi_1+3)} \times \frac{\Gamma(\alpha_0+1)\Gamma(p-2\wedge-2\xi_1)}{\alpha_0\Gamma(\alpha_0-2\wedge-2\xi_1+p)} = 1 \end{aligned} \quad (43)$$

let

$$\begin{aligned} \chi_1 &= -\frac{1}{2\alpha} \frac{\Gamma(n+2+2\xi_1)}{\Gamma(n+4+4\xi_1+2\wedge)} \\ & \sum_{p,r=0}^n \frac{(-1)^{p+r} \Gamma(n+2\xi_1+2)\Gamma(n+2\xi_1+2\wedge+3)}{p!(n-p)!\Gamma(n+2\xi_1-p+2)\Gamma(2\xi_1+2\wedge+p+3)} \frac{\Gamma(n+4+4\xi_1+2\wedge+r)}{r!(n-r)!\Gamma(r+2\xi_1+2)} \times \\ & (-1)^n \frac{\Gamma(n+2\wedge+2\xi_1+3)}{\Gamma(n+1)\Gamma(2\wedge+2\xi_1+3)} \times \frac{\Gamma(\alpha_0+1)\Gamma(p-2\wedge-2\xi_1)}{\alpha_0\Gamma(\alpha_0-2\wedge-2\xi_1+p)} \end{aligned} \quad (44)$$

Then

$$N_n^2 \chi_1 = 1 \Rightarrow N_n = \frac{1}{\sqrt{\chi_1}} \quad (45)$$

Substituting for the normalization constant into equation (23) then, the total normalized wave function is given by

$$\Psi_{n,l}(s) = \frac{1}{\sqrt{\chi_1}} s^{\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]}} (1-s)^{-\frac{1}{2} [\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + \sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2Ec + 2cm]}]} \times \\ P_n^{\left[1+2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2EC + 2Cm]} \right], \left[2+2\sqrt{\frac{1}{4} + 2EB + 2Bm + \lambda} + 2\sqrt{\frac{1}{4\alpha^2} [m^2 - E^2 + 2Ec + 2cm]} \right]} (1-2s) \quad (46)$$

5.0 Numerical Computation of The Resulting Energy Equation as Applied to Oxygen Molecule

The combined potential is relevant in computing bound state energy for diatomic molecules. In this article, we implement Fortran programming to compute the bound state energy for oxygen molecule for the screening parameter $\alpha = 0.2$. The values for the real constant are: $A = -1, B = 2.0, C = 1.0$. The reduced mass of oxygen molecule expressed in atomic mass unit is 7.997457502amu. We use the following conversion: atomic unit: $au = amu \times 1822.8839$

Bound State Energy Of Oxygen Molecule With Thecombined Potential S In Klein-Gordon Equation Using NU For $\alpha = 0.2$

n	l	$E_n(\alpha=0.2) \times 10^7 eV$	n	l	$E_n(\alpha=0.2) \times 10^7 eV$	n	l	$E_n(\alpha=0.2) \times 10^7 eV$	n	l	$E_n(\alpha=0.2) \times 10^7 eV$
0	0	-0.22428226	0	1	-0.22428410	0	2	-0.22428776	0	3	-0.22429329
1	0	-0.22467084	1	1	-0.22467269	1	2	-0.22467634	1	3	-0.22468187
2	0	-0.22505969	2	1	-0.22506152	2	2	-0.22506520	2	3	-0.22507073
3	0	-0.22544879	3	1	-0.22545063	3	2	-0.22545430	3	3	-0.22545983
4	0	-0.22583814	4	1	-0.22583999	4	2	-0.22584367	4	3	-0.22584918
5	0	-0.22622772	5	1	-0.22622956	5	2	-0.22623327	5	3	-0.22623879
6	0	-0.22661759	6	1	-0.22661944	6	2	-0.22662312	6	3	-0.22662866
7	0	-0.22700770	7	1	-0.22700955	7	2	-0.22701323	7	3	-0.22701877
8	0	-0.22739807	8	1	-0.22739992	8	2	-0.22740360	8	3	-0.22740915

6.0 Conclusion

In this paper, we have studied the bound state solution of Klein-Gordon equation with combined potential using parametric Nikiforov-Uvarov method. We obtained the energy and normalized wave function using confluent hypergeometric function. The resulting energies are negative to ascertain bound state condition and decreases with an increase in quantum state for various quantum numbers which is conformity to experimental curve fitting data.

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8.0 References

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