

Analytical Solutions of the D-dimensional Klein-Gordon equation with Hua Potential via N-U Method

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Abstract. In this article, the D-dimensional Klein-Gordon equation within the framework of Greene-Aldrich approximations scheme for Hua potential is solved for s-wave and arbitrary angular momenta. The energy eigenvalues and corresponding wave functions are obtained in an exact analytical manner via the Nikiforov-Uvarov (N-U) method. Further, it is shown that in the non-relativistic limit, the energy eigenvalues reduces to that of Schrödinger equation for the potential. Our results are in excellent agreement with other related works.

KEY WORDS: Hua potential, Greene-Aldrich approximation, Nikiforov-Uvarov (N-U) method.

1 Introduction

The solutions of the relativistic and non-relativistic quantum mechanical wave equations with various physical potentials play an important role to dictate quantum-mechanical phenomena and related dynamics of a quantum system. The eigenvalues and their corresponding wave functions give significant information in describing various quantum systems [1–3]. The problem of finding analytical solutions of D-dimensional Klein-Gordon equation for a number of special potentials has been a line of great interest in recent years [4–11].

It is important to create a model which contain potential concepts i.e. to describe the behaviour and interaction between atoms and particles. Potentials play important role to describe the interaction between nuclei, nuclear particle and the structures of the diatomic molecules. Various potentials are used to analyze the nature of vibration of Quantum System such as pseudo-harmonic [12], modified Eckart plus Hylleraas [13], morse type [14], Wood-Saxon [15], Rosen-Morse [16], harmonic oscillator [17] specially on lower dimensions. The solutions are also crucial in quantum soluble systems. Methods involve in literature

are Nikiforov-Uvarov method [18, 19], asymptotic iteration method [20], Point-Canonical transformation [21], Lie algebraic method [22], super symmetry approach [23], Laplace transform approach [24, 25], factorization method [26] etc. In this article, the approximate solutions of Klein-Gordon equation in D-dimensions is obtained for Hua potential. The Hua potential [27], is an intermolecular potential and widely applied to molecular physics and quantum chemistry. The expression of Hua potential is:

$$V(r) = V_0 \left(\frac{1 - e^{-2\alpha r}}{1 - qe^{-2\alpha r}} \right)^2. \quad (1)$$

Bearing in mind the deeper physical insight that analytical methodologies provide into the physics of problem, the most economic and powerful Nikiforov-Uvarov (N-U) method is applied in my calculations on the D-dimensions.

To investigate the behaviour of Hua potential within the frame work of Klein-Gordon equation I use Greene-Aldrich approximation [28] and applying some simple constraints such that the equation can be solved by N-U method.

My work is organized as follows: To make it self-contained a brief review of N-U method is given in Section 2. In Section 3, the D-dimensional Klein-Gordon equation is presented considering the Hua potential as well as Greene-Aldrich approximation. In Section 4, the energy eigenvalues and corresponding wave functions are obtained for the D-dimensional Klein-Gordon equation by using N-U method. The non-relativistic limit of the energy eigenvalues and corresponding wave functions are obtained in Section 5. Section 6 contains the concluding remark.

2 Nikiforov-Uvarov Method

The N-U method is based on solving a second order linear differential equation by reducing it to a generalized hypergeometric type. In both relativistic and non-relativistic quantum mechanics, the wave equation with a given potential can be solved by this method by reducing the one dimensional K-G equation to an equation of the form

$$\Psi''(x) + \frac{\tilde{\tau}(x)}{\sigma(x)}\Psi'(x) + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}\Psi(x) = 0, \quad (2)$$

where $\sigma(x)$ and $\tilde{\sigma}(x)$ are polynomials of degree atmost 2 and $\tilde{\tau}(x)$ is a polynomial of degree atmost 1. In order to find a particular solution to Eq. (2), we set the following wave function as a multiple of two independent parts

$$\Psi(x) = \Phi(x)y(x). \quad (3)$$

Thus equation (2) reduces to a hyper-geometric type equation of the form

$$\sigma(x)y''(x) + \tau(x)y'(x) + \lambda y(x) = 0,$$

where $\tau(x) = \tilde{\tau}(x) + 2\pi(x)$ satisfies the condition $\tau'(x) < 0$ and $\pi(x)$ is defined as

$$\pi(x) = \frac{\sigma'(x) - \tilde{\tau}(x)}{2} \pm \sqrt{\left(\frac{\sigma'(x) - \tilde{\tau}(x)}{2}\right)^2 - \tilde{\sigma}(x) + K\sigma(x)}, \quad (4)$$

in which K is a parameter. Determining K is the essential point in calculation of $\pi(x)$. Since $\pi(x)$ has to be a polynomial of degree at most one, the expression under the square root sign in Eq. (4) can be put into order to be the square of a polynomial of first degree [18], which is possible only if its discriminant is zero. So, we obtain K by setting the discriminant of the square root equal to zero. Therefore, one gets a general quadratic equation for K . By using

$$\lambda = K + \pi'(x) = -n\tau'(x) - \frac{n(n-1)}{2}\sigma''(x), \quad (5)$$

the values of K can be used for the calculation of energy eigenvalues. Polynomial solutions $y_n(x)$ are given by the Rodrigues relation

$$y_n(x) = \frac{B_n}{\rho(x)} \left(\frac{d}{dx}\right)^n [\sigma^n(x)\rho(x)], \quad (6)$$

in which B_n is a normalization constant and $\rho(x)$ is the weight function satisfying

$$\rho(x) = \frac{1}{\sigma(x)} \exp \int \frac{\tau(x)}{\sigma(x)} dx. \quad (7)$$

On the other hand, the second part of the wave function $\phi(x)$ in relation (3) is given by

$$\phi(x) = \exp \int \frac{\pi(x)}{\sigma(x)} dx. \quad (8)$$

3 The Klein-Gordon Equation in D-Dimensions

The time independent D-dimensional Klein-Gordon equation in the atomic units $\hbar = c = \mu = 1$, may be written as [29]

$$\nabla_D^2 \Psi(r, \Omega_D) + \left[(E - V(r))^2 - (M + S(r))^2 \right] \Psi(r, \Omega_D) = 0, \quad (9)$$

where M denotes the particle mass, E is the energy, $V(r)$ and $S(r)$ are vector and scalar potentials respectively. The D-dimensional Laplacian operator ∇_D^2 is given by [30]

$$\nabla_D^2 = r^{1-D} \frac{\partial}{\partial r} \left(r^{D-1} \frac{\partial}{\partial r} \right) + \frac{L_D^2(\Omega_D)}{r^2}, \quad (10)$$

where $L_D^2(\Omega_D)$ is the ground angular momentum [31]. In addition, we know that $L_D^2(\Omega_D)/r^2$ is a generalization of the centrifugal barrier for the D-dimensional space and involves angular coordinates Ω_D and the eigenvalues of $L_D^2(\Omega_D)$ [30]. $L_D^2(\Omega_D)$ is a partial differential operator on the unit space S^{D-1} define analogously to a three-dimensional angular momentum [31] as $L_D^2(\Omega_D) = -\sum_{i \geq j}^D (L_{ij}^2)$, where $L_{ij}^2 = x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i}$ for all Cartesian component x_i of the D-dimensional vector (x_1, x_2, \dots, x_D) .

To eliminate the first order derivative, the total wave function may be defined as

$$\Psi(r, \Omega_D) = r^{\frac{(D+1)}{2}} R_{nl}(r) Y_{lm}(\Omega_D), \quad (11)$$

where $Y_{lm}(\Omega_D)$ is the generalized spherical harmonic function. The eigenvalues equation for the generalized angular momentum operator is given by $L_D^2 Y_{lm}(\Omega_D) = l(l + D - 2) Y_{lm}(\Omega_D)$. With this, we can write the radial part of the D-dimensional Klein-Gordon equation as follows:

$$\begin{aligned} \frac{d^2 R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2(MS(r) + EV(r)) \right. \\ \left. + V^2(r) - S^2(r) - \frac{(2l + D - 3)(2l + D - 1)}{4r^2} \right] R_{nl}(r) = 0. \quad (12) \end{aligned}$$

Assuming $V(r) = S(r)$, equation (12) becomes

$$\begin{aligned} \frac{d^2 R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2V(r)(M + E) \right. \\ \left. - \frac{(2l + D - 3)(2l + D - 1)}{4r^2} \right] R_{nl}(r) = 0. \quad (13) \end{aligned}$$

The solution for the above equation with $l \neq 0$ is mainly depending on replacing the orbital centrifugal term of singularity with the help of a suitable approximation scheme. The approximation scheme used in this article to deal with the centrifugal term is Greene-Aldrich approximation scheme given by:

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1 - qe^{-2\alpha r})^2}. \quad (14)$$

Inserting the potential function and the modified centrifugal term as given in Eq (1) and Eq (14) respectively, Eq (13) reduces to

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$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[(E^2 - M^2) - 2(M + E)V_0 \left(\frac{1 - e^{-2\alpha r}}{1 - qe^{-2\alpha r}} \right)^2 - \frac{(2l + D - 3)(2l + D - 1)\alpha^2 e^{-2\alpha r}}{(1 - qe^{-2\alpha r})^2} \right] R_{nl}(r) = 0. \quad (15)$$

4 Solutions of the D-Dimensional Klein-Gordon Equation

In order to solve Eq (15) by the N-U method, we need to recast it into a solvable form. To do so, I introduce a new variable $s = e^{-2\alpha r}$ and Eq (15) takes the form

$$\frac{d^2 R(s)}{ds^2} + \frac{(1 - qs)}{s(1 - qs)} \frac{d}{ds} - \frac{1}{s^2(1 - qs)^2} \left[(q^2 \epsilon^2 + \beta^2) s^2 - 2(q\epsilon^2 + \beta^2 - \gamma^2) s + (\epsilon^2 + \beta^2) \right] R(s) = 0, \quad (16)$$

where I have used the notations

$$\epsilon^2 = \frac{E^2 - M^2}{4\alpha^2}, \quad \beta^2 = \frac{2(M + E)V_0}{4\alpha^2}, \quad \gamma^2 = \frac{1}{2}(2l + D - 1)(2l + D - 3).$$

Comparing Eq (16) with Eq (2),

$$\begin{aligned} \tilde{\tau}(s) &= (1 - qs), & \sigma(s) &= s(1 - qs) \\ \tilde{\sigma}(s) &= -[(q^2 \epsilon^2 + \beta^2) s^2 - 2(q\epsilon^2 + \beta^2 - \gamma^2) s + (\epsilon^2 + \beta^2)]. \end{aligned} \quad (17)$$

Substituting them into relation (4) leads to

$$\pi(s) = -\frac{qs}{2} \pm \left[(q^2 \epsilon^2 + \beta^2 + \frac{q^2}{4} - qK) s^2 - [2(q\epsilon^2 + \beta^2 - \gamma^2) - K] s + (\epsilon^2 + \beta^2) \right]^{1/2}. \quad (18)$$

Further, the discriminant of the upper expression under the square root has to be set equal to zero. So, one can easily obtain

$$\begin{aligned} \Delta &= [2(q\epsilon^2 + \beta^2 - \gamma^2) - K]^2 \\ &\quad - 4(\epsilon^2 + \beta^2)(q^2 \epsilon^2 + \beta^2 + \frac{q^2}{4} - qK) = 0. \end{aligned} \quad (19)$$

Solving Eq (19) for the constant K , the double roots are obtained as

$$K_{1,2} = 2(1 - q)\beta^2 - 2\gamma^2 \pm 2ab,$$

where $a = \sqrt{\epsilon^2 + \beta^2}$ and $b = \sqrt{(1-q)^2\beta^2 + 2q\gamma + \frac{q^2}{4}}$. Thus substituting these values for each K into equation (18), one can easily obtains

$$\pi(s) = -\frac{qs}{2} \pm \begin{cases} (b - qa)s - a; & \text{for } K_1 = 2(1-q)\beta^2 - 2\gamma^2 + 2ab \\ (b + qa)s - a; & \text{for } K_2 = 2(1-q)\beta^2 - 2\gamma^2 - 2ab \end{cases} \quad (20)$$

By choosing an appropriate value for K in $\pi(s)$ which satisfies the condition $\tau'(s) < 0$, one gets $\pi(s) = -(aq + b + q/2)s + a$ for $K_2 = 2(1-q)\beta^2 - 2\gamma^2 - 2ab$; giving the function

$$\tau(s) = -2(aq + b + q)s + 1 + 2a. \quad (21)$$

As per Eq (5), the constant λ is defined as

$$\lambda = 2(1-q)\beta^2 - 2\gamma^2 - 2ab - \left(\frac{q}{2} + aq + b\right). \quad (22)$$

Also by Eq (5):

$$\lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s). \quad (23)$$

Here,

$$\tau'(x) = -2(aq + b + q) \quad \text{and} \quad \sigma''(s) = -2q. \quad (24)$$

Carrying out some simple algebraic calculation with the eq (22), eq (23) and eq (24), we have

$$a = \frac{1}{2} \left[\frac{\beta^2 \left(\frac{1}{q^2} - 1\right) - \left(n + \frac{1}{2} + \frac{b}{q}\right)^2}{n + \frac{1}{2} + \frac{b}{q}} \right]. \quad (25)$$

Substituting the values of a and b in Eq (25) and simplifying, we have

$$\epsilon_n^2 = -\beta^2 + \frac{1}{4} \left[\frac{\beta^2 \left(\frac{1}{q^2} - 1\right) - \left(n + \frac{1}{2} + \sqrt{\left(\frac{1}{q} - 1\right)^2 \beta^2 + \frac{2\gamma^2}{q} + \frac{1}{4}}\right)^2}{n + \frac{1}{2} + \sqrt{\left(\frac{1}{q} - 1\right)^2 \beta^2 + \frac{2\gamma^2}{q} + \frac{1}{4}}} \right]^2 \quad (26)$$

This constitutes the energy eigenvalue equation for Hua potential and the approximate energy eigenvalue (by putting the values of notationals ϵ, β, γ) is of the form

$$E_{nl} \approx V_0 - \frac{\alpha^2}{M} \left[\frac{\frac{MV_0}{4\alpha^2} \left(\frac{1}{q^2} - 1 \right) - \chi^2}{\chi} \right]^2, \quad (27)$$

where,

$$\chi = n + \frac{1}{2} + \sqrt{\frac{MV_0}{4\alpha^2} \left(\frac{1}{q} - 1 \right)^2 + \frac{(2l + D - 1)(2l + D - 3)}{q}} + \frac{1}{4}.$$

From Eq (7) it can be shown that the weight function $\rho(s)$ is $\rho(s) = s^{2a}(1-qs)^{2b}$ and by substituting $\rho(s)$ into the Rodrigues relation (6), one gets

$$\begin{aligned} y_n(s) &= \frac{B_n}{s^{2a}(1-qs)^{2b}} \left(\frac{d}{ds} \right)^n [s^n (1-qs)^n s^{2a}(1-qs)^{2b}] \\ &= \frac{B_n}{s^{2a}(1-qs)^{2b}} P_n^{(2a,2b)}(1-2qs), \end{aligned} \quad (28)$$

where $P_n^{(2a,2b)}(1-2qs)$ stands for Jacobi polynomial [32, 33] and B_n is the normalizing constant. The other part of the wave function is simply found from Eq (8) as

$$\phi(s) = s^a (1-qs)^{\left(\frac{1}{2}+b\right)}. \quad (29)$$

Finally, the wave function is obtained as follows:

$$R(s) = B_n s^a (1-qs)^{\left(b+\frac{1}{2}\right)} P_n^{(2a,2b)}(1-2qs). \quad (30)$$

5 Non-Relativistic Limit

It is well-known that the Schrodinger equation represents the non-relativistic spinless particle while the Klein-Gordon equation represents particle with spin-zero. This suggests that a relationship may exists between the solutions of these two important equations. Actually, the non-relativistic limit may be derived from the relativistic one when the energies of the potentials $S(r)$ and $V(r)$ are small compared to the rest mass, the non-relativistic energies can be determined by taking the non-relativistic limit values of the relativistic eigenenergies with the transformation $E + \mu c^2 \rightarrow 2\mu c^2$ and $E - \mu c^2 \rightarrow E$. With this, the relativistic energy in Eq (26) reduces to

$$E = -2V_0 - \frac{\alpha^2}{2\mu c^2} \left[\frac{\frac{\mu c^2 V_0}{\alpha^2} \left(\frac{1}{q^2} - 1 \right) - \zeta^2}{\zeta} \right], \quad (31)$$

where

$$\zeta = n + \frac{1}{2} + \sqrt{\frac{\mu c^2 V_0}{\alpha^2} \left(\frac{1}{q} - 1\right)^2 + \frac{(2l + D - 1)(2l + D - 3)}{q}} + \frac{1}{4}.$$

And the corresponding wave function is obtained as follows:

$$R(s) = B_n s^A (1 - qs)^{(B+\frac{1}{2})} P_n^{(2A, 2B)}(1 - 2qs), \quad (32)$$

where

$$A = \frac{1}{\alpha} \sqrt{\left(E + \frac{V_0}{2}\right) \mu c^2} \quad \text{and}$$

$$B = \frac{1}{\alpha} \sqrt{(1 - q)^2 \mu c^2 V_0 + \alpha^2 q (2l + D - 1)(2l + D - 3) + \frac{q^2 \alpha^2}{4}}.$$

6 Conclusions

In this article, the solutions of the D-dimensional Klein-Gordon equation with equal scalar and vector potentials for the Hua potential using N-U method upon application of Greene-Aldrich approximation to the centrifugal term. Relativistic and non-relativistic energy eigenvalues are obtained and the corresponding wave functions in terms of the Jacobi polynomials are presented.

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