

# Solutions of the Klein-Gordon Equation for the Harmonic Oscillator Potential Plus NAD Potential

H. Goudarzi, A. Jafari, S. Bakkeshizadeh <sup>1</sup> and V. Vahidi

Department of Physics, Faculty of Science  
Urmia University, Urmia, P.O. Box: 165, Iran

## Abstract

In this paper, the solutions of the Klein-Gordon equation for a diatomic molecule in a non-central potential are investigated analytically. The potential consist of the Harmonic oscillator potential plus a novel angle-dependent (NAD) potential. The Klein-Gordon equation is separated into radial and angular parts, and energy eigenvalues and eigenfunctions are derived by using Nikiforov-Uvarov (NU) method.

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## 1. Introduction

It is well known that when a particle is in a strong electromagnetic field, relativistic effects must be considered [1], this gives a correction to non-relativistic quantum mechanics. If we consider the case where the interaction potential isn't strong enough to create particle-antiparticle pairs, we can apply the Klein-Gordon equation to the treatment of a zero-spin particle and apply the Dirac equation to that of a 1/2-spin particle [2]. Fishbane et al. [3] have shown that the confining potential in the Dirac equation involving the interaction of fermions dose not lead to Klein paradoxes if the strength of the vector potential is appropriately limited as compared to the scalar potential. Su and Zhang [4] have demonstrated that, if we want to obtain a confining solution for the Dirac equation, a scalarlike potential must be introduced, which is

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<sup>1</sup>e-mail: somayehbakkeshizadeh@ymail.com

equivalent to a dependence of the rest mass upon position. In fact, the problem of exact solutions of the Klein-Gordon equation and Dirac equation for a number of special potentials has also been a line of great interest in recent years [5-11]. Some authors, by using different methods, studied the bound states of the Klein-Gordon equation and the Dirac equation with mixed typical potentials under the condition that each of the scalar potentials is equal to its vector potential. These investigations include the Hulthen potential [12-14], Morse potential [15], Poschl-Teller potential [16, 17], Kratzer potential [18,19], Rosen-Morse-type potentials [20], the Coulombic ring-shaped potential [21-23] and the oscillatory ring-shaped potential [24-27]. The methods include the standard method, supersymmetry and the shape invariance potential [6, 11, 13], and the Nikiforov-Uvarov method [28].

The concept of the Harmonic oscillator gives us a very good first approximation for understanding the spectroscopy and the structure of diatomic molecules in their ground electronic states. Recently, Berkdemir [29] proposed a novel angle-dependent (NAD) potential and obtained the exact solutions of the Schrodinger equation for the Coulomb and harmonic oscillator potentials add NAD potential. An important aspect of the use of the NAD potential is to study the rotational-vibrational dynamics of a diatomic molecule in non-central potentials. Moreover, rotational-vibrating energy states of a diatomic molecule can be exactly calculated by means of a radial potential connected by the NAD potential.

The purposes of this paper is to investigate the contribution of the parameters come from NAD potential into the energy spectrum of a diatomic molecule in the Harmonic oscillator. To make this analysis, the NAD potential is added to the radial parts of the Harmonic oscillator as an angle dependent part. The Harmonic oscillator plus the NAD potential is given in the following form,

$$V(r) = Kr^2 + \frac{\hbar^2}{2\mu r^2} \left( \frac{\gamma + \beta \sin^2\theta + \eta \sin^4\theta}{\sin^2\theta \cos^2\theta} \right). \quad (1)$$

where  $r$  represents spherical coordinates  $r$ ,  $\theta$  and  $\varphi$ , also  $\gamma, \beta, \eta$  and  $K$  arbitrary constant values and  $\mu$  denote the mass particle. The solution of the Klein-Gordon equation for this combined potential is exactly obtained by using a systematical solution method which is introduced by Nikiforov-Uvarov (NU). The NU method is used to solve Schrodinger, Dirac, Klein-Gordon and Duffin-Kemmer-Petiau wave equations for certain kind of potentials [30-34]. This work is organized as follows: in section 2, the NU method is given briefly. In section 3 we consider the separation of variables for the Klein-Gordon equation. Section 4, 5 devoted to the exact solutions of the radial and angular Klein-Gordon equation by the NU method. Finally, we present a brief discussion of the results achieved.

## 2. Nikiforov-Uvarov Method

The second-order differential equations whose solutions are the special functions can be solved by using the NU method. This method was purposed to solve the second-order differential equation of hypergeometric-type and in this method the differential equations can be written in the following form,

$$\frac{d^2\psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)} \frac{d\psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \quad (2)$$

where  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are polynomials, at most second degree, and  $\tilde{\tau}(s)$  is a first degree polynomial. By writing the general solution as  $\psi(s) = \phi(s)y(s)$ , we obtain a hypergeometric type equation,

$$\frac{d^2y(s)}{ds^2} + \frac{\tau(s)}{\sigma(s)} \frac{dy(s)}{ds} + \frac{\lambda}{\sigma(s)}y(s) = 0. \quad (3)$$

The function  $\phi(s)$  is defined as a logarithmic derivative,

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \quad (4)$$

where  $y(s)$  is the hypergeometric type function whose polynomial solutions are given by Rodrigues relation,

$$y_n(s) = \frac{a_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)], \quad (5)$$

where  $a_n$  is a normalization constant, and  $\rho(s)$  is the weight function satisfying the following equation,

$$(\rho\sigma)' = \tau\rho. \quad (6)$$

The function  $\pi(s)$  and the parameter  $\Lambda$  required for this method are defined as

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \quad (7)$$

$$\Lambda = k + \pi'(s). \quad (8)$$

In the NU method,  $\pi(s)$  is a polynomial with the parameter  $s$  and the determination of  $k$  is the essential point in the calculation of  $\pi(s)$ . For finding the value of  $k$ , the expression under the square root must be square of a polynomial, so we have a new eigenvalue equation,

$$\Lambda = \lambda_n = -\tau' - \frac{n(n-1)}{2} \frac{d^2\sigma(s)}{ds^2}, \quad (9)$$

where the derivation of the function  $\tau(s) = \tilde{\tau}(s) + 2\pi(s)$  should be negative, and by comparing Eqs. (8) and (9), we obtain the energy eigenvalues.

### 3. Klein-Gordon equation and separation in spherical coordinates

The Klein-Gordon equation with scalar and vector potentials, [35]

$$\{P^2 + [\mu + S(r, \theta)]^2 - [E - V(r, \theta)]^2\} \psi(r, \theta, \varphi) = 0. \quad (10)$$

With equal scalar and vector potentials we obtain

$$\{P^2 + (\mu^2 - E^2) + 2(\mu + E)V(r, \theta)\} \psi(r, \theta, \varphi) = 0, \quad (11)$$

where  $P$  is the momentum operator. In spherical coordinate the wave function is written as follows

$$\psi(r) = \frac{U(r)}{r} H(\theta) e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \dots \quad (12)$$

By substituting Eq. (12) into Eq. (11) and using the separation of variables, for  $H(\theta)$  and  $U(r)$  we have the following equations

$$\frac{d^2 H(\theta)}{d\theta^2} + \frac{\cos\theta}{\sin\theta} \frac{dH(\theta)}{d\theta} - \left[ \frac{m^2}{\sin^2\theta} + 2a \left( \frac{\gamma + \beta \sin^2\theta + \eta \sin^4\theta}{\sin^2\theta \cos^2\theta} \right) - L \right] H(\theta) = 0, \quad (13)$$

$$\frac{d^2 U}{dr^2} - 2\mu \left[ 2aKr^2 + A + \frac{L}{2\mu r^2} \right] U(r) = 0. \quad (14)$$

where  $L$  is the separation constant,  $a, A$  are defined as

$$a = E + \mu, \quad (15)$$

$$A = \mu^2 - E^2. \quad (16)$$

### 4. Eigenvalues and eigenfunctions of the polar angle equation

By introducing a new variable  $x = \sin^2\theta$ , Eq. (13) becomes

$$\frac{d^2 H}{dx^2} + \frac{(2-3x)}{2x(1-x)} \frac{dH}{dx} - \frac{1}{4x^2(1-x)^2} \times \left[ -x^2(L+2a\eta) + x(m^2 - 2a\beta + L) - (m^2 + 2a\gamma) \right] H(x) = 0. \quad (17)$$

Comparing with Eq. (2) the following expressions are obtained

$$\tilde{\tau} = 2-3x, \quad \sigma = 2x(1-x), \quad \tilde{\sigma} = -x^2(L+2a\eta) + x(m^2 - 2a\beta + L) - (m^2 + 2a\gamma). \quad (18)$$

Putting them in Eq. (7) the function  $\pi$  is

$$\pi = -\frac{x}{2} \pm \frac{1}{2} \sqrt{x^2(1+4(2a\eta+L)-8k) + x(8k-4(m^2+L-2a\beta)) + 4(m^2+2a\gamma)}, \quad (19)$$

According to the NU method, the expression in the square root must be the square of the polynomial. So, one can find new possible functions for each  $k$  as

$$\pi = -\frac{x}{2} \pm \frac{1}{2} \times \left\{ \begin{array}{l} \text{for } k_1 = -\frac{[(\sqrt{1+8a(\eta+\beta+\gamma)}-2\sqrt{m^2+2a\gamma})x+\sqrt{m^2+2a\gamma}],}{(m^2+2a(\beta+2\gamma)-L)} + \frac{1}{2}\sqrt{(m^2+2a\gamma)[1+8a(\eta+\beta+\gamma)]}, \\ \text{for } k_2 = -\frac{[(\sqrt{1+8a(\eta+\beta+\gamma)}+2\sqrt{m^2+2a\gamma})x-\sqrt{m^2+2a\gamma}],}{(m^2+2a(\beta+2\gamma)-L)} - \frac{1}{2}\sqrt{(m^2+2a\gamma)[1+8a(\eta+\beta+\gamma)]}. \end{array} \right. \quad (20)$$

In Eq. (20), one of the four possible forms of  $\pi$  is finding the negative derivation of  $\tau$  given by equation  $\tau = \tilde{\tau} + 2\pi$ . Other forms are not suitable physically. Therefore, the most suitable form of  $\pi$  is selected as

$$\pi = -\frac{x}{2} - \frac{1}{2} \left[ \left( \sqrt{1+8a(\eta+\beta+\gamma)} + 2\sqrt{m^2+2a\gamma} \right) x - \sqrt{m^2+2a\gamma} \right], \quad (21)$$

For  $k_2 = -\frac{(m^2+2a(\beta+2\gamma)-L)}{2} - \frac{1}{2}\sqrt{(m^2+2a\gamma)[1+8a(\eta+\beta+\gamma)]}$ . Hence,  $\tau(x)$  is obtained as follows

$$\tau(x) = \left( 2 + \sqrt{m^2+2a\gamma} \right) - x \left( 4 + \sqrt{1+8a(\eta+\beta+\gamma)} + 2\sqrt{m^2+2a\gamma} \right). \quad (22)$$

The key rule of the derivative of  $\tau$  appears in Eq. (9) which is a polynomial of degree  $\Lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma''$ , where  $\Lambda$  denotes  $k_2 + \pi'$  from Eq. (8). Consequently,  $\Lambda$  and  $\lambda_n$  are obtained, respectively,

$$\Lambda = -\frac{(m^2+2a(\beta+2\gamma)-L)}{2} - \frac{1}{2} \times \left( (1 + \sqrt{8a(\eta+\beta+\gamma)})(1 + \sqrt{m^2+2a\gamma}) + \sqrt{m^2+2a\gamma} \right), \quad (23)$$

$$\lambda_n = 2n^2 + 2n + 2n\sqrt{m^2+2a\gamma} + n\sqrt{1+8a(\eta+\beta+\gamma)}, \quad (n = 0, 1, \dots) \quad (24)$$

Taking  $\sigma'' = -4$ . In order to find an expression which is relating to  $L$ , the right-hand sides of Eqs. (23) and (24) must be compared with each other. In this case the result obtained will depend on the NAD potential constants as well as the usual quantum numbers;

$$L = \sqrt{1+8a(\eta+\beta+\gamma)} \left( 1 + 2n + \sqrt{m^2+2a\gamma} \right) + \left( 1 + 2n + \sqrt{m^2+2a\gamma} \right)^2 + 2a(\beta+\gamma). \quad (25)$$

The separation constant  $L$  in Eq. (25) contains the contributions that come from the angle-dependent part of the NAD potential. Let us now find the corresponding eigenfunctions for the angel part. According Eqs. (4) and (6),  $\phi$  and as follows

$$\phi(x) = x^{B/4}(1-x)^{(1+A+B)/4}, \quad (26)$$

$$\rho(x) = \frac{1}{2}x^{B/2}(1-x)^{(A+B)/2}, \quad (27)$$

where  $A = \sqrt{1 + 8a(\eta + \beta + \gamma)}$  and  $B = \sqrt{m^2 + 2a\gamma}$ . Substituting Eq. (27) into Eq. (5),  $y_n(x)$  can be found to be

$$y_n(x) = B_n 2^n x^{-B/2} (1-x)^{-(A+B)/2} \frac{d^n}{dx^n} \left( \frac{1}{2} x^{n+B/2} (1-x)^{n+(A+B)/2} \right). \quad (28)$$

The polynomial solution of  $y_n$  is expressed in terms of a Jacobi polynomial which is one of the orthogonal polynomials, giving  $\approx P_n^{(B/2, (A+B)/2)}(1-2x)$ . By using  $H_n(x) = \phi(x)y(x)$  the solution of Eq. (17) can be written as

$$H_n(x) = C_n x^{B/4} (1-x)^{(1+A+B)/4} P_n^{(B/2, (A+B)/2)}(1-2x). \quad (29)$$

where  $C_n$  is a normalized constant. The useful projection of Eq. (29) can also be given in terms of the confluent hypergeometric function  $F(\alpha_1, \beta_1, \gamma_1, z)$  with parameters  $\alpha_1, \beta_1, \gamma_1$ . The representation of this function in terms of Jacobi polynomials is

$$P_n^{(B/2, (A+B)/2)}(z) = \frac{\Gamma(n + B/2 + 1)}{n! \Gamma(B/2 + 1)} F(\alpha_1, \beta_1, \gamma_1, \frac{1-z}{2}), \quad (30)$$

$$P_n^{(B/2, (A+B)/2)}(1-2x) = \frac{\Gamma(n + B/2 + 1)}{n! \Gamma(B/2 + 1)} F(\alpha_1, \beta_1, \gamma_1, x), \quad (z = 1 - 2x) \quad (31)$$

$$P_n^{(B/2, (A+B)/2)}(1-2x) = \frac{\Gamma(n + B/2 + 1)}{n! \Gamma(B/2 + 1)} \times F(-n, n + B/2 + (A+B)/2 + 1, B/2 + 1, x), \quad (32)$$

where  $\alpha_1 = -n, \beta_1 = n + B/2 + (A+B)/2 + 1$  and  $\gamma_1 = B/2 + 1$ . The  $\theta$ -dependent wave equation in Eq. (29) becomes

$$H_n(x) = G_n x^{B/4} (1-x)^{(1+A+B)/4} F(-n, n + B/2 + (A+B)/2 + 1, B/2 + 1, x). \quad (33)$$

where  $G_n$  is a new normalized constant.

## 5. Eigenvalues and eigenfunctions of the radial equation

Now we return to study Eq. (14), with change variable  $z = r^2$  we have

$$\frac{d^2 U}{dz^2} + \frac{1}{2z} \frac{dU}{dz} - \frac{1}{4z^2} (Cz^2 + Dz + L) U(z) = 0, \quad (34)$$

in which  $C = 4\mu Ka, D = 2\mu A$ . To apply the NU method, Eq. (34) is compared with Eq. (2) and the following expressions are obtained

$$\tilde{\tau} = 1, \quad \sigma = 2z, \quad \tilde{\sigma} = -Cz^2 - Dz - L. \quad (35)$$

The function  $\pi$  is obtained by putting the above expressing in Eq. (7);

$$\pi = \frac{1}{2} \pm \sqrt{Cz^2 + (2K + D)z + \left(L + \frac{1}{4}\right)}. \quad (36)$$

According to the NU method, the expression in the square root must be the square of the polynomial, so

$$k_{1,2} = -\frac{1}{2}D \pm \frac{1}{2}\sqrt{C(4L + 1)}. \quad (37)$$

We can find four possible functions  $\pi$  for each  $k$  as

$$\pi = \left\{ \begin{array}{l} \frac{1}{2} \pm \sqrt{C} \left( z + \sqrt{\frac{4L+1}{4C}} \right), \text{ for } k_1 = -\frac{1}{2}D + \frac{1}{2}\sqrt{C(4L+1)}, \\ \frac{1}{2} \pm \sqrt{C} \left( z - \sqrt{\frac{4L+1}{4C}} \right), \text{ for } k_2 = -\frac{1}{2}D - \frac{1}{2}\sqrt{C(4L+1)}, \end{array} \right\}. \quad (38)$$

For the polynomial of  $\tau = \tilde{\tau} + 2\pi$  which has a negative derivative we select  $k_2 = -\frac{1}{2}D - \frac{1}{2}\sqrt{C(4L + 1)}$  and  $\pi = \frac{1}{2} - \sqrt{C} \left( z - \sqrt{\frac{4L+1}{4C}} \right)$  with this selection and  $\Lambda = k + \pi'$ ,  $\tau$  and  $\Lambda$  can be written as, respectively,

$$\tau = 2 \left( 1 - \sqrt{C} \left( z - \sqrt{\frac{(4L + 1)}{4C}} \right) \right), \quad (39)$$

$$\Lambda = -\frac{D}{2} - \sqrt{C} \left( 1 + \frac{1}{2}\sqrt{4L + 1} \right). \quad (40)$$

Comparing the definition of  $\lambda_n$  in Eq. (9) with the Eq. (40), we obtain the energy equation

$$(E^2 - \mu^2) + \sqrt{4\mu Ka} \left[ \frac{2n + 1 + \sqrt{\frac{4L+1}{4}}}{\mu} \right] = 0. \quad (41)$$

where  $L = \sqrt{1 + 8a(\eta + \beta + \gamma)} (1 + 2n + \sqrt{m^2 + 2a\gamma}) + (1 + 2n + \sqrt{m^2 + 2a\gamma})^2 + 2a(\beta + \gamma)$ . Let us now find the radial wavefunctions for this potential. Using  $\sigma$  and  $\pi$  Eqs. (4) and (6), the following expressions are obtained

$$\rho = \frac{1}{2} z \sqrt{(4L+1)/4} e^{-\sqrt{4\mu Ka}z}, \quad (42)$$

$$\phi = z^{\frac{1}{4}(1+\sqrt{4L+1})} e^{-\sqrt{4\mu Ka}z}. \quad (43)$$

Then from Eq. (5) one has

$$y_n(z) = Q_n 2^n z^{\sqrt{(4L+1)/4}} e^{-\sqrt{4\mu Ka}z} \frac{d^n}{dz^n} \left( z^{n+\sqrt{(4L+1)/4}} e^{-\sqrt{4\mu Ka}z} \right). \quad (44)$$

Where  $Q_n$  is a normalized constant. Thus the wavefunctions  $U(z)$  can be obtained as

$$U(z) = Q_n 2^n z^{\frac{1}{4}(1+\sqrt{4L+1})} e^{-\sqrt{\mu K}az} \left[ z^{-\sqrt{(4L+1)/4}} e^{\sqrt{4\mu K}az} \frac{d^n}{dz^n} \left( z^{n+\sqrt{(4L+1)/4}} e^{-\sqrt{4\mu K}az} \right) \right]. \quad (45)$$

And it can be written as the generalized Laguerre polynomials

$$U(z) = N_n z^{\frac{1}{4}(1+\sqrt{4L+1})} e^{-\sqrt{\mu K}az} L_n^{\sqrt{(4L+1)/4}} \left( \sqrt{4\mu K}az \right), \quad (46)$$

where  $z = r^2$ . On the other hand

$$U(z) = N_n r^{\frac{1}{2}(1+\sqrt{4L+1})} e^{-\sqrt{\mu K}ar^2} L_n^{\sqrt{(4L+1)/4}} \left( \sqrt{4\mu K}ar^2 \right). \quad (47)$$

where  $N_n$  is a normalized constant and  $a = E + \mu$ .

## 6. Conclusions

In the paper, we have proposed a new exactly solvable potential which consists of the Harmonic oscillator plus a novel angle-dependent (NAD) potential and obtained the bound state solution of the Klein-Gordon equation by the NU method for a diatomic molecule. The angular and radial wavefunctions and energy equation are given by Eqs. (33), (47) and (41), respectively. We know that it is possible to study the Harmonic oscillator plus a novel angle-dependent potential and to solve exactly the Schrodinger, Dirac and Klein-Gordon equations for this system. Possible studies along this line are in progress.

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