

Exact S-Wave Solution of the Klein-Gordon Equation with the Deng-Fan Molecular Potential using the Nikiforov-Uvarov (NU) Method

O. J. Oluwadare*, K. J. Oyewumi and O. A. Babalola,

Theoretical Physics Section, Physics Department, University of Ilorin, Ilorin, Kwara State, Nigeria

In this work, we solve the Klein-Gordon equation with equal scalar and vector Deng-Fan molecular potentials. The exact s-wave ($\kappa = 0$) solutions of the Klein-Gordon equation with equally mixed scalar and vector Deng-Fan molecular potentials, the normalized wave function and the corresponding energy equations are obtained by using the Nikiforov-Uvarov method.

1. Introduction

It is generally known in quantum mechanics that when a particle is restricted within a potential well, the particle can not only take on certain discrete values of energy E_n but can also tunnel from the potential well even if the spectrum of eigenvalues E_n is less than the potential energy. In this case, the bound state solution must be considered, leading to quantum mechanical description of such a particle.

The presence of a particle in a strong potential field necessitates a relativistic description of such a particle [1-3]. By considering the 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 [1,2,4,5,6-8].

Also, by assuming equal scalar and vector potential and by using different methods such as supersymmetry, asymptotic iteration method, Nikiforov-Uvarov method, and other related methods, the analytical solutions of the Klein-Gordon equation and the Dirac equation with various physical potentials have been studied by various researchers [1-8,10,11,13-32]. In this work, our focus is to obtain the exact s-wave solutions of the Klein-Gordon equation with equally mixed scalar and vector Deng-Fan molecular potentials using the Nikiforov-Uvarov approach.

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 [33] in an attempt to find a more suitable diatomic potential to describe the vibrational spectrum [34]. Although, this potential is qualitatively similar to the Morse potential but it has correct asymptotic behaviour as the inter-nuclear distance approaches to zero [32-40].

The Deng-Fan potential model can be used to describe the motion of nucleons in the mean field produced by the interactions between nuclei [32-40]. Approximate κ -state solutions of the Dirac equation for this potential under spin and pseudospin symmetry conditions have been obtained by using the Nikiforov-Uvarov method [32]. This potential has been used to describe diatomic molecular energy spectra and electromagnetic transitions, and it is an ideal inter-nuclear potential in diatomic molecules with the same behaviour for $r \rightarrow 0$ [36]. Rong et al. [35] used this potential model to obtain the X-H stretching motion in small molecules. Approximate solutions of the Schrödinger equation with this potential model have been obtained via the standard method [37], and the supersymmetric shape invariance formalism [38].

Furthermore, by using a proper approximation scheme for the centrifugal term, Wei and Chen have studied l -wave continuum states of the Schrödinger equation for the modified Morse potential [39]. Relativistic treatment of spinless particles subject to a rotating Deng-Fan oscillator has been investigated by using the standard method [2]. In this study, exact s-wave solutions of the Klein-Gordon equation with equally mixed scalar and vector Deng-Fan molecular potentials, the normalized wave function and the corresponding energy equations are obtained by 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 equally mixed scalar and vector Deng-Fan molecular potentials is solved by using the Nikiforov-Uvarov method. The relativistic energy equations and the corresponding normalized wave

*mjphysics@yahoo.com

functions are obtained and finally, the conclusion is given in Section 4.

2. Overview of Nikiforov-Uvarov (NU) Method

The Nikiforov-Uvarov method has been successfully applied to relativistic and non-relativistic quantum mechanical problems and other field of studies as well [6-8,21,23,40-51]. The method reduces the second order linear differential equation to generalized equation of hypergeometric type. With an appropriate coordinate transformation, $s = s(r)$, the equation takes the form

$$\Psi''(s) + \frac{\bar{\tau}(s)}{\sigma(s)} \Psi'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)} \Psi(s) = 0 \quad (1)$$

Where, $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials of at most second degree and $\bar{\tau}(s)$ is a first degree polynomial.

By taking the following factorization

$$\Psi(s) = \phi(s)y(s) \quad (2)$$

Eqn. (1) reduces to the hypergeometric type equation of the form [48]

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0 \quad (3)$$

Where,

$$\tau(s) = \bar{\tau}(s) + 2\pi(s) \quad (4)$$

satisfies the condition $\tau'(s) < 0$, which will have a negative derivative and is related to the function $\phi(s)$ by [35]

$$\pi(s) = \sigma(s) \frac{d}{ds} [\ln \phi(s)] \quad (5)$$

The parameter λ is defined by

$$\lambda = \lambda_n = -n\tau'(s) - \left[\frac{n(n-1)}{2} \sigma'' \right]; \quad (n = 0, 1, 2, \dots) \quad (6)$$

The energy eigenvalues can be calculated from Eqn. (6). In order to calculate the energy eigenvalues, we need first to determine λ by using the first derivative of $\pi(s)$ and defining

$$K = \lambda - \pi'(s) \quad (7)$$

By solving the resulting quadratic equation for $\pi(s)$, we obtain the following expression

$$\pi(s) = \left(\frac{\sigma' - \bar{\tau}}{2} \right) \pm \sqrt{\left(\frac{\sigma' - \bar{\tau}}{2} \right)^2 - \bar{\sigma} + k\sigma} \quad (8)$$

Here, $\pi(s)$ is a polynomial with the parameter s and the prime denote the first derivative of the functions $\sigma(s)$ and $\tau(s)$, respectively. The determination of k is the essential point in the calculation of $\pi(s)$ and it can be obtained by setting the discriminant of the square root to zero [48]. The wave function in relation (2) satisfies the condition

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \quad (9)$$

and can be determined by using the Rodrigues' relation. The polynomial solutions $y_n(s)$ are given by

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)] \quad (10)$$

Where, B_n is a normalization constant and the weight function $\rho(s)$ satisfies the following relation

$$\frac{d}{ds} [\sigma(s)\rho(s)] = \tau(s)\rho(s) \quad (11)$$

3. Exact S-Wave Solutions of the Klein-Gordon Equation

The time-independent relativistic radial Klein-Gordon equation with the equally mixed scalar $S(r)$ and vector $V(r)$ potentials is written for a spin-zero particle in the natural units, $\hbar = c = 1$, as [1-3,8-10,13,15,18,31]

$$\frac{d^2 R_n(r)}{dr^2} + [(E - V(r))^2 - (M + S(r))^2] R_n(r) = 0 \quad (12)$$

Where, E and M are the relativistic energy and the rest mass of the spin-zero particle, respectively, and $\psi_n(r) = R_n(r)/r$ is the radial wave function.

The equal scalar and vector Deng-Fan molecular potentials ($S(r) = V(r)$) for a diatomic molecules was proposed by Deng and Fan in 1957 as [33]

$$V(r) = D_e \left[1 - \frac{b}{e^{ar} - 1} \right]^2, \quad b = e^{ar_e} - 1, \quad r \in [0, \infty] \quad (13)$$

where D_e , r_e and a are three parameters denoting the dissociation energy, the equilibrium inter-nuclear distance and the range of the potential well,

$$\frac{d^2 R_n(r)}{dr^2} + \left[(E^2 - M^2) - 2(E + M)D_e \left(1 - \frac{be^{-ar}}{1 - e^{-ar}} \right)^2 \right] R_n(r) = 0 \quad (14)$$

Taking a transformation equation of the form $s = e^{-ar}$, then Eqn. (14) reduces to

$$\frac{d^2 R_n(s)}{ds^2} + \frac{1-s}{s(1-s)} \frac{dR_n(s)}{ds} + \frac{1}{s^2(1-s)^2} [-(\epsilon_n^2 + (2+b)\beta^2 b)s^2 + (2(\beta^2 b + \epsilon_n^2) - \gamma)s - \epsilon_n^2] R_n(s) = 0 \quad (15)$$

Where, we have used the following dimensional parameters

$$\epsilon^2 = \frac{E^2 - M^2}{a^2}, \quad \beta^2 = \frac{2(E + M)D_e}{a^2}, \quad \text{and} \quad -\epsilon_n^2 = \epsilon^2 - \beta^2 \quad (16)$$

In order to solve Eqn. (16) by using the Nikiforov-Uvarov (NU) method, we compare it with Eqn. (1) and obtain the following polynomials:

$$\bar{\tau}(s) = 1 - s, \quad \sigma(s) = s(1 - s), \quad \sigma^2(s) = s^2(1 - s)^2 \quad (17)$$

$$\bar{\sigma}(s) = -(\epsilon_n^2 + (2 + b)\beta^2 b)s^2 + 2(\beta^2 b + \epsilon_n^2)s - \epsilon_n^2$$

Using the following substitutions:

$$A = \epsilon_n^2 + (2 + b)\beta^2 b, \quad B = 2(\beta^2 b + \epsilon_n^2), \quad C = \epsilon_n^2 \quad (18)$$

Then, we have

$$\bar{\sigma}(s) = -As^2 + Bs - C \quad (19)$$

Substituting these polynomials into Eqn. (8), we obtain the following

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2} \left[\left(\sqrt{1 + 4\beta^2 b^2} + 2\epsilon_n \right) s - 2\epsilon_n \right] \quad (20)$$

respectively, and b is the position of minimum r_e . It is worth noting that this molecular potential has the correct physical boundary conditions at $r = 0$ and $r = \infty$.

In the case of equal scalar and vector Deng-Fan molecular potential, $V(r) = S(r)$, the relativistic radial Klein-Gordon equation becomes

$$k = 2\beta^2 b \pm \epsilon_n \sqrt{1 + 4\beta^2 b^2} \quad (21)$$

For polynomial $\tau(s) = \bar{\tau}(s) + 2\pi(s)$ with negative derivative, we select

$$\pi(s) = -\frac{s}{2} - \frac{1}{2} \left[\left(\sqrt{1 + 4\beta^2 b^2} + 2\epsilon_n \right) s - 2\epsilon_n \right]$$

$$\text{and} \quad k = 2\beta^2 b - \epsilon_n \sqrt{1 + 4\beta^2 b^2}$$

If combined this with $\lambda = k + \pi'$ defined in Eqn. (7), the above expression gives

$$\tau(s) = 1 + 2\epsilon_n - 2 \left(1 + \epsilon_n + \frac{1}{2} \sqrt{1 + 4\beta^2 b^2} \right) s \quad (22)$$

and

$$\lambda = 2\beta^2 b - \epsilon_n \sqrt{1 + 4\beta^2 b^2} - \frac{1}{2} - \frac{1}{2} \sqrt{1 + 4\beta^2 b^2} - \epsilon_n \quad (23)$$

With Eqn. (6), we have

$$\lambda = \lambda_n = 2n \left(1 + \epsilon_n + \frac{1}{2} \sqrt{1 + 4\beta^2 b^2} \right) + n^2 - n \quad (24)$$

By using the condition that $\lambda = \lambda_n$ in Eqns. (23) and (24), we obtain the eigenvalues ϵ_n as

$$\epsilon_n = \frac{(2 + b)\beta^2 b}{2n + 1 + \sqrt{1 + 4\beta^2 b^2}} - \frac{2n + 1 + \sqrt{1 + 4\beta^2 b^2}}{4} \tag{25}$$

From Eqns. (16) and (25), we obtain the energy eigenvalues as:

$$E^2 - M^2 = 2(E + M)D_e - a^2 \left[\frac{\frac{(2+b)(E+M)D_e b}{a^2}}{n + \eta} - \frac{n + \eta}{2} \right]^2 \tag{26}$$

$$y_n(s) \approx s^{-2\epsilon_n}(1 - s)^{-(2\eta-1)} \frac{d^n}{ds^n} [s^{n+2\epsilon_n}(1 - s)^{n+2\eta-1}] \tag{29}$$

Eqn. (29) may be expressed in terms of Jacobi polynomials [52] as

$$y_n(s) \equiv P_n^{(2\epsilon_n, 2\eta-1)}(s) \tag{30}$$

$$P_n^{(\alpha,\beta)}(s) = \frac{(\alpha+1)_n}{n!} {}_2F_1(-n, n + \alpha + \beta + 1; \alpha + 1; \frac{1-s}{2}) \tag{31}$$

Hence, Eqn. (30) may be expressed in form of hypergeometric representation of Jacobi polynomials as:

$$P_n^{(2\epsilon_n, 2\eta-1)}(s) = \frac{(2\epsilon_n+1)_n}{n!} {}_2F_1(-n, n + 2(\epsilon_n + \eta); 2\epsilon_n + 1; \frac{1-s}{2}) \tag{32}$$

Where, $(2\epsilon_n + 1)_n$ is the Pochhammer symbol [52].

Solving for $\phi(s)$ using $\pi(s)$ and $\sigma(s)$ in the expression given in Eqn. (9), we have

$$\phi(s) = s^{\epsilon_n}(1 - s)^\eta \tag{33}$$

Hence, using Eqns. (32) and (33) in Eqn. (2), we obtain the non-normalized radial wave functions as

$$R_n(s) = N_n \frac{(2\epsilon_n+1)_n}{n!} e^{-\epsilon_n ar} (1 - e^{-ar})^\eta {}_2F_1(-n, n + 2(\epsilon_n + \eta); 2\epsilon_n + 1; \frac{1-e^{-ar}}{2}) \tag{34}$$

Where, N_n is the normalization constant and which is obtained as

$$N_n = \frac{1}{\Gamma(2\epsilon_n + 1)} \left[\frac{a\epsilon_n(n + \epsilon_n + \eta)\Gamma(n + 2\epsilon_n + 1)\Gamma(n + 2\epsilon_n + 2\eta)}{2(n + \eta) n! \Gamma(n + 2\eta)} \right]^{1/2} \tag{35}$$

Where, n is the principal quantum number and

$$\eta = \frac{1}{2} \left[1 + \sqrt{1 + \frac{8(E + M)D_e b^2}{a^2}} \right] \tag{27}$$

Since the polynomial solutions of the hypergeometric function $y(s)$ depend on the determination of the weight function $\rho(s)$, which satisfies the differential equation, Eqn. (11). Thus, $\rho(s)$ is obtained as

$$\rho(s) = s^{2\epsilon_n}(1 - s)^{2\eta-1} \tag{28}$$

Substituting Eqn. (28) into the Rodrigue's relation given in Eqn. (10), we obtain

4. Conclusion

In this work, we have studied the exact s-wave analytical solutions of the Klein-Gordon equation with equally mixed scalar and vector Deng-Fan molecular potentials by using the Nikiforov-Uvarov (NU) method. The exact analytical bound state energy eigenvalues and the corresponding normalized wave functions have been obtained. By extension, the Schrödinger equation with the arbitrary angular momentum values for this potential can be solved by this method. The resulting solutions can be used to study the spectroscopy of some selected diatomic molecules.

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