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A novel angle-dependent potential and its exact solution

Cüneyt Berkdemir

Abstract   The quantum mechanics of a diatomic molecule in a noncentral potential of the type $V(\mathbf{r}) = V_\theta(\theta)/r^2 + V_r(r)$ are investigated analytically. The θ-dependent part of the relevant potential is suggested for the first time as a novel angle-dependent (NAD) potential $V_\theta(\theta) = \frac{\hbar^2}{2\mu} \left(\frac{\gamma + \beta \sin^2 \theta + \alpha \sin^4 \theta}{\sin^2 \theta \cos^2 \theta} \right)$ and the radial part is selected as the Coulomb potential or the harmonic oscillator potential, i.e., $V_r(r) = -H/r$ or $V_r(r) = K r^2$, respectively. Exact solutions are obtained in the Schrödinger picture by means of a mathematical method named the Nikiforov–Uvarov (NU). The effect of the angle-dependent part on the solution of the radial part is discussed in several values of the NAD potential's parameters as well as different values of usual quantum numbers.

Keywords   Diatomic molecule · Novel angle-dependent (NAD) potential · Coulomb potential and harmonic oscillator · Nikiforov–Uvarov method · Exact solution

1 Introduction

The exact solutions of the Schrödinger equation play an important role in extracting the quantum treatments in various physical and chemical applications including those in molecular physics. For example, the exact solutions of the Schrödinger equation for a particle in the Coulomb potential or the harmonic oscillator are an important milestone in quantum chemistry [1,2]. The problem of a particle in the three-dimensional ring-shaped potential has been transformed into the problem of a coupled pair of Schrödinger equations for two-dimensional harmonic oscillators with inverse

C. Berkdemir (✉)
Department of Physics, Erciyes University, 38039 Kayseri, Turkey
e-mail: berkdemir@erciyes.edu.tr

quadratic and square potentials. Numerous articles have been deal with a nonrelativistic quantum mechanical study of a dynamical system which generalizes the Kepler–Coulomb, the Hartmann and the isotropic harmonic oscillator systems in three dimensions [3]. The concepts of the Coulomb potential or the harmonic oscillator give us a very good first approximation for understanding the spectroscopy and the structure of diatomic molecules in their ground electronic states. Although most of these potentials are central, there are some noncentral separable (in spherical coordinates) potentials [4]. The study of exact solutions of the Schrödinger equation with noncentral potentials is of considerable interest. The Hartmann potential introduced in 1972 by Hartmann [5] is one of the noncentral potentials, which can be realized by adding a potential proportional to the Coulomb potential. This potential was suggested to describe the energy spectrums of ring-shaped molecules like benzene and cyclic polyenes. The exact motion of a diatomic molecule in a new class of noncentral potentials was studied by Hautot [6] to compute classical and quantum trajectories. The accidental degeneracy occurring in the quantum mechanical treatment of the ring-shaped potential was explained by constructing an SU(2) dynamical invariance algebra. Moreover, the classical trajectories were calculated for two Hamiltonian systems with ring shaped potentials [7–10]. A new ring-shaped potential obtained by replacing the Coulomb part of the Hartmann potential with a harmonic oscillator term was investigated by Quesne [11] to find discrete spectrums and integrals of motion. The motion of a particle in a Coulomb potential and a harmonic oscillator plus Aharonov–Bohm potential was investigated from a classical and a quantum mechanical viewpoint [12–15]. A new exactly solvable noncentral ring-shaped potential was proposed by Dong et al. [16] and they were studied its quantum characteristics of bound and scattering states. The zero-energy quantum states for a class of noncentral potentials have been obtained in the parabolic potential barrier [17]. These states are used in a growing number of physical applications. Numerous examples, especially in an analysis of vortices, can be found in the literature [18]. In addition, some other interesting investigations related to the noncentral potentials have been carried out [19,20].

In the present study, a novel angle-dependent (NAD) potential is suggested for the fist time as an alternative of the Hartmann-type potential. As one of exactly solvable problems in quantum mechanics, this potential is defined as follows

$$\frac{V_\theta(\theta)}{r^2} = \frac{\hbar^2}{2\mu r^2} \left(\frac{\gamma + \beta \sin^2 \theta + \alpha \sin^4 \theta}{\sin^2 \theta \cos^2 \theta} \right), \tag{1}$$

where α, β and γ are arbitrary constant values. The factor $\hbar^2/2\mu$ is introduced in view of the future favourableness. An important aspect of the use of the NAD potential is to study the rotational-vibrational dynamics of a diatomic molecule in noncentral potentials. Moreover, ro-vibrating energy states of a diatomic molecule can be exactly calculated by means of a radial potential connected by the NAD potential. Hence, a close connection between both the Coulomb potential plus the NAD potential and the harmonic oscillator plus the NAD potential can be established to compare the energy states of diatomic molecules. Such a connection does not give a surprising result because many relations between the Coulomb potential and the harmonic

oscillator have already known. However, the addition of a noncentral potential of the type $\left(\frac{\gamma+\beta\sin^2\theta+\alpha\sin^4\theta}{r^2\sin^2\theta\cos^2\theta}\right)$ makes this connection still deeper by smoothing out many discrepancies between the Coulomb potential and the harmonic oscillator [11]. The Coulomb potential plus the NAD potential or the harmonic oscillator plus the NAD potential are given in the following forms, respectively,

$$V(\mathbf{r}) = -\frac{H}{r} + \frac{\hbar^2}{2\mu r^2}\left(\frac{\gamma + \beta\sin^2\theta + \alpha\sin^4\theta}{\sin^2\theta\cos^2\theta}\right), \quad \text{for Coulomb + NAD} \quad (2)$$

$$V(\mathbf{r}) = Kr^2 + \frac{\hbar^2}{2\mu r^2}\left(\frac{\gamma + \beta\sin^2\theta + \alpha\sin^4\theta}{\sin^2\theta\cos^2\theta}\right), \quad \text{for Harmonic oscillator+NAD,}$$
$$(3)$$

where H and K are real parameters with respect to the relevant potentials and $\mathbf{r}$ represents spherical coordinates r, θ and ϕ. The solution of the Schrödinger equation for the Coulomb potential plus the NAD potential or the harmonic oscillator plus the NAD potential gives the energy states of a diatomic molecule. An alternative method introduced to find a solution of the Schrödinger equation was presented by Nikiforov and Uvarov [21]. The proposed method is advantageously applied for finding the energy states of a diatomic molecule. In addition to this valuable method, other methods used to obtain the solution of the Schrödinger equation are given as the path integral approach [22], hypergeometric series method [23], the SUSY quantum mechanics and shape invariance method [24], L^2-series solutions for a large class of noncentral potentials [25], a group-theoretical study on the Coulomb potential plus an angle-dependent potential [26] and other algebraic approaches [27–39]. In most of these studies, the eigenvalues and eigenfunctions are obtained via separation of variables in spherical coordinates.

One of the purposes of this paper is to investigate the contribution of the parameters come from a novel angle-dependent (NAD) potential into the energy spectrum of a particle (or diatomic molecule) in the Coulomb potential or the harmonic oscillator. To make this analysis, the NAD potential is added to the radial parts of the Coulomb potential and the harmonic oscillator as an angle-dependent part. The solution of the Schrödinger equation for these combined potentials is exactly obtained by using a systematical solution method which is introduced by Nikiforov–Uvarov (NU) [21]. The concept of the Nikiforov–Uvarov (NU) method is that it can be used to obtain exact solutions of such noncentral but separable potentials in an algebraic viewpoint. In this method, the angle-dependent part as well as the radial part of the Schrödinger equation can be separately investigated by using the idea of exactly solvability. The details of the NU method and the solutions of the Schrödinger equation for the Coulomb potential plus the NAD potential and the harmonic oscillator plus the NAD potential are given in the next sections. Moreover, the importance of the NAD potential is indicated in quantum chemistry to describe ring-shaped molecules like benzene because its mathematical form likes to the angle-dependent part of the Hartmann potential or a generalized Ahanorov–Bohm oscillator system. The relevant remarks on the NAD

potential are made in the next sections where the dependence of the parameters and the various angles of the potential on the energy spectrum is also discussed.

2 The details of the Nikiforov–Uvarov method

The Nikiforov–Uvarov (NU) method is based on solving the hypergeometric type second-order differential equations by means of the special orthogonal functions [40]. For a given potential, the Schrödinger or the Schrödinger-like equations in spherical coordinates are reduced to a generalized equation of hypergeometric type with an appropriate coordinate transformation $r \rightarrow s$ or $\theta \rightarrow s$ and then they are solved systematically to find the exact or particular solutions. The main equation which is closely associated with the method is given in the following form [21]

$$\psi''(s) + \frac{\widetilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \tag{4}$$

where $\sigma(s)$ and $\widetilde{\sigma}(s)$ are polynomials at most second-degree, $\widetilde{\tau}(s)$ is a first-degree polynomial and $\psi(s)$ is a function of the hypergeometric type.

By taking $\psi(s) = \phi(s)y(s)$ and choosing an appropriate function $\phi(s)$, Eq. 4 is reduced to a comprehensible form;

$$y''(s) + \left(2\frac{\phi'(s)}{\phi(s)} + \frac{\widetilde{\tau}(s)}{\sigma(s)}\right)y'(s) + \left(\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)}\frac{\widetilde{\tau}(s)}{\sigma(s)} + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\right)y(s) = 0. \tag{5}$$

The coefficient of $y'(s)$ is taken in the form $\tau(s)/\sigma(s)$, where $\tau(s)$ is a polynomial of degree at most one, i.e.,

$$2\frac{\phi'(s)}{\phi(s)} + \frac{\widetilde{\tau}(s)}{\sigma(s)} = \frac{\tau(s)}{\sigma(s)}, \tag{6}$$

and hence the most regular form is obtained as follows,

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \tag{7}$$

where

$$\pi(s) = \frac{1}{2}[\tau(s) - \widetilde{\tau}(s)]. \tag{8}$$

The most useful demonstration of Eq. 8 is

$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s). \tag{9}$$

The new parameter $\pi(s)$ is a polynomial of degree at most one. In addition, the term $\phi''(s)/\phi(s)$ which appears in the coefficient of $y(s)$ in Eq. 5 is arranged as follows

$$\frac{\phi''(s)}{\phi(s)} = \left(\frac{\phi'(s)}{\phi(s)}\right)' + \left(\frac{\phi'(s)}{\phi(s)}\right)^2 = \left(\frac{\pi(s)}{\sigma(s)}\right)' + \left(\frac{\pi(s)}{\sigma(s)}\right)^2. \tag{10}$$

In this case, the coefficient of $y(s)$ is transformed into a more suitable arrangement by taking the form in Eq. 7;

$$\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)}\frac{\widetilde{\tau}(s)}{\sigma(s)} + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)} = \frac{\bar{\sigma}(s)}{\sigma^2(s)}, \tag{11}$$

where

$$\bar{\sigma}(s) = \widetilde{\sigma}(s) + \pi^2(s) + \pi(s)[\widetilde{\tau}(s) - \sigma'(s)] + \pi'(s)\sigma(s). \tag{12}$$

Substituting the right-hand sides of Eqs. 6 and 11 into Eq. 5, an equation of the same type as Eq. 4 is obtained as

$$y''(s) + \frac{\tau(s)}{\sigma(s)}y'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}y(s) = 0. \tag{13}$$

As a consequence of the above algebraic transformations, the functional form of Eq. 4 is protected by following a systematic way. Therefore, the transformations allow us to replace the function of the hypergeometric type $\psi(s)$ by the substitution $\phi(s)y(s)$, where $\phi(s)$ satisfies Eq. 7 whit an arbitrary linear polynomial $\pi(s)$. If the polynomial $\bar{\sigma}(s)$ in Eq. 13 is divisible by $\sigma(s)$, i.e.,

$$\bar{\sigma}(s) = \lambda\sigma(s), \tag{14}$$

where λ is a constant, Eq. 13 is reduced to an equation of hypergeometric type

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \tag{15}$$

and also its solution is given as a function of hypergeometric type. To determine the polynomial $\pi(s)$, Eq. 12 is compared with Eq. 14 and then a quadratic equation for $\pi(s)$ is obtained as follows,

$$\pi^2(s) + \pi(s)[\widetilde{\tau}(s) - \sigma'(s)] + \widetilde{\sigma}(s) - k\sigma(s), \tag{16}$$

where

$$k = \lambda - \pi'(s). \tag{17}$$

The solution of this quadratic equation for $\pi(s)$ yields the following equality

$$\pi(s) = \frac{\sigma'(s) - \widetilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \widetilde{\tau}(s)}{2}\right)^2 - \widetilde{\sigma}(s) + k\sigma(s)}. \qquad (18)$$

In order to obtain the possible solutions according to the plus and minus signs of Eq. 18, the parameter k within the square root sign must be known explicitly. To provide this requirement, the expression under the square root sign has to be the square of a polynomial, since $\pi(s)$ is a polynomial of degree at most 1. In this case, an equation of the quadratic form is available for the constant k. Setting the discriminant of this quadratic equal to zero, the constant k is determined clearly. After determining k, the polynomial $\pi(s)$ is obtained from Eq. 18, and then $\tau(s)$ and λ are also obtained by using Eqs. 8 and 17, respectively.

A common trend which is followed to generalize the solutions of Eq. 15 is to show that all the derivatives of functions of hypergeometric type are also of hypergeometric type. For this purpose, Eq. 15 is differentiated by using the representation $v_1(s) = y'(s)$

$$\sigma(s)v_1''(s) + \tau_1(s)v_1'(s) + \mu_1 v_1(s) = 0, \qquad (19)$$

where $\tau_1(s) = \tau(s) + \sigma'(s)$ and $\mu_1 = \lambda + \tau'(s)$. $\tau_1(s)$ is a polynomial of degree at most 1 and μ_1 is independent of the variable s. It is clear that Eq. 19 is an equation of hypergeometric type again. By taking $v_2(s) = y''(s)$ as a new representation, the second derivation of Eq. 15 becomes

$$\sigma(s)v_2''(s) + \tau_2(s)v_2'(s) + \mu_2 v_2(s) = 0, \qquad (20)$$

where

$$\tau_2(s) = \tau_1(s) + \sigma'(s) = \tau(s) + 2\sigma'(s), \qquad (21)$$

$$\mu_2 = \mu_1 + \tau_1'(s) = \lambda + 2\tau'(s) + \sigma''(s). \qquad (22)$$

In a similar way, an equation of hypergeometric type for $v_n(s) = y^{(n)}(s)$ is constructed as a family of particular solutions of Eq. 15 corresponding to a given λ;

$$\sigma(s)v_n''(s) + \tau_n(s)v_n'(s) + \mu_n v_n(s) = 0, \qquad (23)$$

and here the general recurrence relations for $\tau_n(s)$ and μ_n are found as follows, respectively,

$$\tau_n(s) = \tau(s) + n\sigma'(s), \qquad (24)$$

$$\mu_n = \lambda + n\tau'(s) + \frac{n(n-1)}{2}\sigma''(s). \qquad (25)$$

When $\mu_n = 0$, Eq. 25 becomes as follows

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad (n = 0, 1, 2, \ldots) \tag{26}$$

and then Eq. 23 has a particular solution of the form $y(s) = y_n(s)$ which is a polynomial of degree n. To obtain an eigenvalue solution through the NU method, the relationship between λ and λ_n must be set up by means of Eqs. 17 and 26.

3 The separation in spherical coordinates

In spherical coordinates, the Schrödinger equation for a diatomic molecule moving within the Coulomb or harmonic oscillator plus NAD potentials given in Eq. 2 or 3, respectively, can be explicitly turned into the more useful one;

$$\left\{ \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[4x(1-x)\frac{\partial^2}{\partial x^2} + 2(2-3x)\frac{\partial}{\partial x} + \frac{1}{x}\frac{\partial^2}{\partial\varphi^2}\right] + \frac{2\mu}{\hbar^2}(E - V(\mathbf{r})) \right\}\Psi(\mathbf{r}) = 0. \tag{27}$$

Introducing a new variable $x = \sin^2\theta$. The energy E in Eq. 27 is real and it is either discrete for bound states ($E < 0$) or continuous for scattering states ($E > 0$). This equation is separable for potentials of the following form,

$$V(\mathbf{r}) \equiv V(r, \theta, \varphi) = V_r(r) + \frac{1}{r^2}\left[V_\theta(x) + \frac{1}{x}V_\varphi(\varphi)\right]. \tag{28}$$

If the wave function is written as $\Psi(\mathbf{r}) \equiv \Psi(r, \theta, \varphi) = r^{-1}R(r)\Theta(\theta)\Phi(\varphi)$, the wave equation in Eq. 27 for the potential given in Eq. 2 or 3 can be separated to a set of second-order differential equations in all three coordinates as follows:

$$\left(\frac{d^2}{dr^2} - \frac{L}{r^2} + \frac{2\mu}{\hbar^2}(E - V_r(r))\right)R(r) = 0, \tag{29}$$

$$\left(4x(1-x)\frac{d^2}{dx^2} + 2(2-3x)\frac{d}{dx} - \frac{m^2}{x} + L - \frac{2\mu}{\hbar^2}V_\theta(x)\right)\Theta(x) = 0, \tag{30}$$

$$\left(\frac{d^2}{d\varphi^2} - \frac{2\mu}{\hbar^2}V_\varphi(\varphi) + m^2\right)\Phi(\varphi) = 0, \tag{31}$$

where m^2 and L are separation constants. A noteworthy explanation interested in these constants is that m is the usual magnetic quantum number and L represents

the usual centrifugal kinetic energy term, i.e., $L = \ell(\ell + 1)$, where ℓ is the angular momentum quantum number, when the angular dependence of the potentials vanish. Since the wave function $\Psi(\mathbf{r})$ must be finite in all space for the bound states, the boundary conditions for Eq. 29 require $R(0) = 0$ and the square-integrability of $R(r)$ on $(0, \infty)$, which implies that $R(\infty) = 0$. The finite solutions for $\Theta(\theta)$ in the range of $0 \leq \theta \leq \pi$ are able to map into a differential equation of hypergeometric type. Moreover, the boundary conditions for Eq. 31 must be $\Phi(\varphi + 2\pi) = \Phi(\varphi)$. If we specialize to the case where $V_\varphi(\varphi) = 0$, then the normalized solution of Eq. 31 that satisfies the boundary conditions becomes

$$\Phi(\varphi) \equiv \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \qquad m = 0, \pm 1, \pm 2, \ldots \tag{32}$$

3.1 The solution of the angle-dependent part

Equation 30 is the θ-dependent wave equation for the NAD potential. To solve this equation, the angle-dependent part of the Schrödinger equation must be well-defined in spherical coordinates. The NAD potential is given as follows

$$V_\theta(\theta) = \frac{\hbar^2}{2\mu} \left(\frac{\gamma + \beta \sin^2 \theta + \alpha \sin^4 \theta}{\sin^2 \theta \cos^2 \theta} \right). \tag{33}$$

Substituting Eq. 33 into Eq. 30, keeping in mind the variable $x = \sin^2 \theta$, the θ-dependent wave equation can be rearranged in the following form

$$\left(4x(1-x) \frac{d^2}{dx^2} + 2(2-3x) \frac{d}{dx} - \frac{m^2}{x} + L - \left(\frac{\gamma + \beta x + \alpha x^2}{x(1-x)} \right) \right)$$
$$\Theta(x) = 0. \tag{34}$$

Having perform some basic arrangements on Eq. 34, a form which is comparable with Eq. 4 given by the NU method is obtained

$$\frac{d^2\Theta(x)}{dx^2} + \frac{(2-3x)}{2x(1-x)} \frac{d\Theta(x)}{dx} + \frac{1}{[2x(1-x)]^2}$$
$$\times (-x^2(\alpha + L) + x(m^2 + L - \beta) - m^2 - \gamma)\Theta(x) = 0. \tag{35}$$

When the main equation given in Eq. 4 is compared by Eq. 35, the following polynomials are obtained

$$\tilde{\tau}(s \to x) = 2 - 3x, \tag{36}$$

$$\sigma(s \to x) = 2x(1-x), \tag{37}$$

$$\tilde{\sigma}(s \to x) = -x^2(\alpha + L) + x(m^2 + L - \beta) - m^2 - \gamma. \tag{38}$$

The polynomials given by Eqs. 36–38 are inserted into Eq. 18 and hence the equality for the polynomial $\pi(s \to x)$ is obtained

$$
\pi(x) = -\frac{x}{2} \pm \frac{1}{2}
$$
$$
\times \sqrt{x^2(1+4(\alpha+L) - 8k)+x(8k - 4(m^2 + L - \beta))+4(m^2 + \gamma)}, \quad (39)
$$

or

$$
\pi(x) = -\frac{x}{2} \pm \frac{1}{2}\sqrt{ax^2 + bx + c}, \quad (40)
$$

where $a = 1+4(\alpha+L) - 8k$, $b = 8k - 4(m^2+L-\beta)$ and $c = 4(m^2+\gamma)$. According to the NU method, the polynomial $\pi(x)$ must be a polynomial of degree at most 1. To provide this condition, the equation of quadratic form under the square root sign of Eq. 40 is converted to the square of a polynomial. The constant k embedded within a and b is therefore determined by setting the discriminant of this quadratic equal to zero: $\Delta = b^2 - 4ac = 0$,

$$
(8k - 4(m^2 + L - \beta))^2 - 16(1 + 4(\alpha + L) - 8k)(m^2 + \gamma) = 0. \quad (41)
$$

After preparing a more suitable arrangement of Eq. 41, a new quadratic equation according to the constant k is obtained

$$
4k^2 + 4k(m^2 + \beta + 2\gamma - L) + (m^2 + L - \beta)^2
$$
$$
- (m^2 + \gamma)(1 + 4(\alpha + L)) = 0. \quad (42)
$$

The solution of Eq. 42 gives two roots of k individually;

$$
k_{1,2} = -\frac{(m^2 + \beta + 2\gamma - L)}{2} \pm \frac{1}{2}\sqrt{(m^2 + \gamma)[1 + 4(\alpha + \beta + \gamma)]}, \quad (43)
$$

where the signs of plus and minus represent the roots of k_1 and k_2, respectively. When the individual values of k given in Eq. 43 are substituted into Eq. 18, the four possible forms of $\pi(x)$ are written as follows

$$
\pi(x) = -\frac{x}{2} \pm \frac{1}{2}
$$
$$
\times
\begin{cases}
\left[\left(\sqrt{1 + 4(\alpha + \beta + \gamma)} - 2\sqrt{m^2 + \gamma}\right)x + \sqrt{m^2 + \gamma}\right], \\
\text{for} \quad k_1 = -\frac{(m^2+\beta+2\gamma-L)}{2} + \frac{1}{2}\sqrt{(m^2 + \gamma)[1 + 4(\alpha + \beta + \gamma)]}. \\[2mm]
\left[\left(\sqrt{1 + 4(\alpha + \beta + \gamma)} + 2\sqrt{m^2 + \gamma}\right)x - \sqrt{m^2 + \gamma}\right], \\
\text{for} \quad k_2 = -\frac{(m^2+\beta+2\gamma-L)}{2} - \frac{1}{2}\sqrt{(m^2 + \gamma)[1 + 4(\alpha + \beta + \gamma)]}
\end{cases}
$$
$$
(44)
$$

In Eq. 44, one of the four possible forms of $\pi(x)$ is used in finding the negative derivative of $\tau(x)$ given by Eq. 9. Other forms are not suitable physically. Therefore, the most suitable form of $\pi(x)$ is selected as

$$\pi(x) = -\frac{x}{2} - \frac{1}{2}\left[\left(\sqrt{1 + 4(\alpha + \beta + \gamma)} + 2\sqrt{m^2 + \gamma}\right)x - \sqrt{m^2 + \gamma}\right], \quad (45)$$

for $k_2 = -\frac{(m^2 + \beta + 2\gamma - L)}{2} - \frac{1}{2}\sqrt{(m^2 + \gamma)[1 + 4(\alpha + \beta + \gamma)]}$. Hence, $\tau(x)$ and $\tau'(x)$ are obtained as follows

$$\tau(x) = 2\left(1 + \sqrt{m^2 + \gamma}\right) - x\left(4 + \sqrt{1 + 4(\alpha + \beta + \gamma)} + 2\sqrt{m^2 + \gamma}\right),$$

$$\tau'(x) = -\left(4 + \sqrt{1 + 4(\alpha + \beta + \gamma)} + 2\sqrt{m^2 + \gamma}\right) < 0. \quad (46)$$

The key rule of the derivative of $\tau(x)$ appears in Eq. 26 which is a polynomial of degree ν; $\lambda = \lambda_\nu = -\nu\tau' - \frac{\nu(\nu-1)}{2}\sigma''$, where λ denotes $k_2 + \pi'$ from Eq. 17. Consequently, λ and λ_ν are obtained, respectively,

$$\lambda = -\left(\frac{m^2 + \beta + 2\gamma - L}{2}\right)$$
$$-\frac{1}{2}\left[\left(1 + \sqrt{1 + 4(\alpha + \beta + \gamma)}\right)\left(1 + \sqrt{m^2 + \gamma}\right) + \sqrt{m^2 + \gamma}\right], \quad (47)$$

$$\lambda_\nu = 2\nu^2 + 2\nu + 2\nu\sqrt{m^2 + \gamma} + \nu\sqrt{1 + 4(\alpha + \beta + \gamma)}, \quad (\nu = 0, 1, 2, \ldots) \ (48)$$

taking $\sigma'' = -4$. In order to find an expression which is relating to L, the right-hand sides of Eqs. 47 and 48 must be compared with each other. In this case the result obtained will depend on the NAD potential's constants as well as the usual quantum numbers:

$$L = \left(1 + 2\nu + \sqrt{m^2 + \gamma}\right)^2 + \sqrt{1 + 4(\alpha + \beta + \gamma)}$$
$$\times \left(1 + 2\nu + \sqrt{m^2 + \gamma}\right) + \beta + \gamma, \quad (49)$$

or

$$L = \left(1 + 2\nu + \sqrt{m^2 + \gamma} + \sqrt{1/4 + \alpha + \beta + \gamma}\right)^2 - \left(\sqrt{\alpha + 1/4}\right)^2. \quad (50)$$

The separation constant L in Eq. 50 contains the contributions that come from the angle-dependent part of the NAD potential. Of course, when the angle dependence of

the NAD potential is disappeared by setting the parameters of the potential to zero, i.e., $V_\theta(\theta) = 0$, L equals to $\ell(\ell + 1)$, where $\ell = 1 + 2v + |m|$. It is also pointed out that the NAD potential has singularities at angles $\theta = p\pi/2$ in laboratory coordinates ($p = 0, 1, 2, 3, \ldots$), as well as at very large and/or very small r. As a result, θ and r do not take these values once the solution of the Schrödinger equation for the combined potentials is obtained exactly.

Let us now find the corresponding eigenfunctions for the NAD potential. To find a solution of Eq. 30, the θ-dependent wave function $\Theta(x)$ can be separated $\phi(x)y(x)$, i.e., $\Theta(x) = \phi(x)y(x)$, where $\phi(x)$ satisfies $\phi'(x)/\phi(x) = \pi(s)/\sigma(s)$ given in Eq. 7. By substituting $\pi(x)$ and $\sigma(x)$ given in Eqs. 45 and eq36, respectively, into the expression $\phi(x)'/\phi(x) = \pi(x)/\sigma(x)$, $\phi(x)$ is found

$$\phi(x) = x^{B/4}(1 - x)^{(1+A+B)/4}, \tag{51}$$

where $A = \sqrt{1 + 4(\alpha + \beta + \gamma)}$ and $B = \sqrt{m^2 + \gamma}$. $y(x)$ represents a second order differential equation of hypergeometric type given in Eq. 15:

$$x(1 - x)y''(x) + \frac{1}{2}\left[2 + B - (A + 2B + 4)x\right]y'(x)$$
$$-\frac{1}{4}\left[\beta + \gamma - L + B^2 + B + (1 + A)(1 + B)\right]y(x) = 0. \tag{52}$$

The polynomial solutions of this differential equation of hypergeometric type are uniquely determined by the Rodrigues formula:

$$y_v(x) = \frac{B_v}{\rho(x)}\frac{d^v}{dx^v}\left[\sigma^v(x)\rho(x)\right], \tag{53}$$

where B_v is a normalized constant and $\rho(x)$ is the weight function satisfying a Pearson equation. In the continuous case it has the form

$$\frac{d}{dx}[\sigma(x)\rho(x)] = \tau(x)\rho(x). \tag{54}$$

From Eqs. 37 and 46, the weight function $\rho(x)$ is obtained

$$\rho(x) = x^{B/2}(1 - x)^{(A+B)/2}. \tag{55}$$

Substituting Eq. 55 into the Rodrigues formula given in Eq. 53, $y_v(x)$ becomes as follows

$$y_v(x) = B_v 2^v x^{-B/2}(1 - x)^{-(A+B)/2}\frac{d^v}{dx^v}\left[x^{(v+B/2)}(1 - x)^{v+(A+B)/2}\right]. \tag{56}$$

On the other hand, the solution of Eq. 15 can be expressed in terms of the Jacobi polynomials $P_v^{(a_1, b_1)}(z)$, where $a_1 > -1$ and $b_1 > -1$:

$$(1 - z^2)y''(z) + [b_1 - a_1 - (a_1 + b_1 + 2)z]y'(z)$$
$$+ \nu(\nu + a_1 + b_1 + 1)y(z) = 0. \tag{57}$$

The Jacobi polynomials are one of the orthogonal polynomials which are most used in the applications. One of the many equivalent definitions of $P_\nu^{(a_1, \, b_1)}(z)$ is

$$P_\nu^{(a_1, \, b_1)}(z) = \frac{(-1)^\nu}{2^\nu \nu!}(1 - z)^{-a_1}(1 + z)^{-b_1}\frac{d^\nu}{dz^\nu}\left[(1 - z)^{\nu + a_1}(1 + z)^{\nu + b_1}\right]. \tag{58}$$

After the substitution $z = 1 - 2x$ into Eqs. 57 and 58, these equations become, respectively,

$$x(1 - x)y''(x) + [a_1 + 1 - (a_1 + b_1 + 2)x]y'(x)$$
$$+ \nu(\nu + a_1 + b_1 + 1)y(x) = 0, \tag{59}$$

$$P_\nu^{(a_1, \, b_1)}(1 - 2x) = \frac{1}{\nu!}x^{-a_1}(1 - x)^{-b_1}\frac{d^\nu}{dx^\nu}\left[x^{\nu + a_1}(1 - x)^{\nu + b_1}\right]. \tag{60}$$

In the new case, Eq. 60 is comparable with Eq. 56;

$$a_1 = \frac{B}{2}; \quad b_1 = \frac{(A + B)}{2}; \quad B_\nu = \frac{1}{2^\nu \nu!}; \ P_\nu^{(B/2, \, (A+B)/2)}(1 - 2x) = y_\nu(x). \tag{61}$$

Hence, the θ-dependent wave function $\Theta(x)$ in terms of Jacobi polynomials is

$$\Theta(x) = C_\nu x^{B/4}(1 - x)^{(1+A+B)/4}P_\nu^{(B/2, \, (A+B)/2)}(1 - 2x), \tag{62}$$

where C_ν is a normalized constant. The useful projection of Eq. 62 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

$$P_\nu^{(B/2, \, (A+B)/2)}(z) = \frac{\Gamma(\nu + B/2 + 1)}{\nu! \Gamma(B/2 + 1)}F\left(\alpha_1, \beta_1, \gamma_1, \frac{1 - z}{2}\right),$$
$$P_\nu^{(B/2, \, (A+B)/2)}(1 - 2x) = \frac{\Gamma(\nu + B/2 + 1)}{\nu! \Gamma(B/2 + 1)}F(\alpha_1, \beta_1, \gamma_1, x), \ (z = 1 - 2x)$$
$$P_\nu^{(B/2, \, (A+B)/2)}(1 - 2x) = \frac{\Gamma(\nu + B/2 + 1)}{\nu! \Gamma(B/2 + 1)}$$
$$\times F(-\nu, \nu + B/2 + (A + B)/2 + 1, B/2 + 1, x), \tag{63}$$

where $\alpha_1 = -\nu$, $\beta_1 = \nu + B/2 + (A + B)/2 + 1$ and $\gamma_1 = B/2 + 1$. The θ-dependent wave equation in Eq. 62 becomes

$$\Theta(x) = C_\nu' x^{B/4}(1 - x)^{(1+A+B)/4}F$$
$$\times (-\nu, \nu + B/2 + (A + B)/2 + 1, B/2 + 1, x), \tag{64}$$

where C'_ν is a new normalized constant. After some simple manipulations, the L value given in Eq. 50 can also be obtained by comparing Eq. 52 with Eq. 59.

3.2 The solution of the radial part

Having separate the angle-dependent and radial parts of the Schrödinger equation for a diatomic molecule, the relevant differential equation for the radial motion is described by Eq. 29;

$$\left(\frac{d^2}{dr^2} - \frac{L}{r^2} + \frac{2\mu}{\hbar^2}(E - V_r(r)) \right) R(r) = 0,$$

where $V_r(r)$ is the Coulomb or harmonic oscillator potentials given by Eq. 2 or 3, respectively;

$$V_r(r) = -\frac{H}{r}, \quad \text{(for Coulomb potential)} \tag{65}$$

$$V_r(r) = Kr^2. \quad \text{(for Harmonic oscillator potential)} \tag{66}$$

3.2.1 The case of Coulomb potential plus the NAD potential

The Schrödinger equation for a diatomic molecule can be involved in the Coulomb potential $V_r(r) = -H/r$. Since this is a central potential (it has spherical symmetry) the Schrödinger equation can be separated in different independent equations when it is expressed in spherical coordinates. One of these independent equations is the radial part of the Schrödinger equation given in Eq. 29. In the presence of the Coulomb potential $V_r(r) = -H/r$, it can be written as follow,

$$\left(\frac{d^2}{dr^2} - \frac{L}{r^2} + \frac{2\mu}{\hbar^2}\left(E + \frac{H}{r}\right) \right) R(r) = 0. \tag{67}$$

Equation 67 is really just a small generalization of that for the hydrogen atom and it was solved by Fues [41]. Using the transformation $r \to s$ and letting the dimensionless notations

$$-\varepsilon_1^2 = \frac{2\mu E}{\hbar^2}, \quad \varepsilon_2 = \frac{2\mu H}{\hbar^2}, \quad \varepsilon_3 = L. \tag{68}$$

Equation 67 can be rewritten in a simple form as follows:

$$\frac{d^2 R(s)}{ds^2} + \frac{1}{s^2}(-\varepsilon_1^2 s^2 + \varepsilon_2 s - \varepsilon_3) R(s) = 0. \tag{69}$$

The complete solution of Eq. 69 by means of the NU method can be found in Ref. [42], having made of some notation setting. Hence, the energy spectrum with respect to the quantum numbers n, ν and m is obtained as

$$E_{n\nu m} = -\frac{\mu H^2}{2\hbar^2} \left(n + 1/2 + \sqrt{1/4 + L} \right)^{-2},$$ (70)

keeping in mind the value of L given in Eq. 50. The discrete energy eigenvalues are given

$$E_{n\nu m} = -\frac{\mu H^2}{2\hbar^2}$$

$$\left(n + 1/2 + \sqrt{1/4 + \left(1 + 2\nu + \sqrt{m^2 + \gamma} + \sqrt{1/4 + \alpha + \beta + \gamma} \right)^2 - \left(\sqrt{\alpha + 1/4} \right)^2} \right)^{-2},$$ (71)

where $n, \nu = 0, 1, 2, \ldots$.

3.2.2 The case of harmonic oscillator plus the NAD potential

The harmonic oscillator potential is important because not only does it demonstrate quantization of energy, but it also shows the phenomenon called quantum tunnelling, in which an electron can pass into a finite potential barrier, which is not permitted by classical mechanics.

Adopting the harmonic oscillator potential to Eq. 29, the radial Schrödinger equation turns into the following form [43],

$$\left(\frac{d^2}{dr^2} - \frac{L}{r^2} + \frac{2\mu}{\hbar^2} \left(E - Kr^2 \right) \right) R(r) = 0.$$ (72)

In order to obtain an analytical solution of Eq. 72 the radial part of the dimensionless Schrödinger equation of the harmonic oscillator potential is given by

$$\frac{d^2 R(y)}{dy^2} + \left[2\varepsilon_1 - \frac{L}{y^2} - y^2 \right] R(y) = 0,$$ (73)

where

$$r = y \left(\frac{\hbar}{\sqrt{2\mu K}} \right)^{1/2}; \quad \varepsilon_1 = \frac{E}{\hbar} \sqrt{\frac{\mu}{2K}}.$$ (74)

By using a transformation $y^2 \rightarrow s$ in Eq. 73, the translated equation turns into the following form

$$\frac{d^2R(s)}{ds^2} + \frac{1}{2s}\frac{dR(s)}{ds} + \frac{1}{4s^2}(-s^2 - \varepsilon_2^2 s - \varepsilon_3^2)R(s) = 0 \tag{75}$$

where

$$\varepsilon_2^2 = -2\varepsilon_1 \ (\varepsilon_1 < 0); \quad \varepsilon_3^2 = L. \tag{76}$$

By comparing Eq. 75 with Eq. 15 of Ref. [44] and following the solution steps of the NU method, the energy spectrum according to the quantum numbers n, ν and m is obtained as

$$E_{n\nu m} = \hbar\sqrt{\frac{8K}{\mu}}\left(n + \frac{1}{2} + \frac{1}{2}\sqrt{1/4 + L}\right), \tag{77}$$

keeping in mind the value of L given in Eq. 50. The discrete energy eigenvalues are given

$$E_{n\nu m} = \hbar\sqrt{\frac{8K}{\mu}}$$
$$\left(n + \frac{1}{2} + \frac{1}{2}\sqrt{1/4 + \left(1 + 2\nu + \sqrt{m^2 + \gamma} + \sqrt{1/4 + \alpha + \beta + \gamma}\right)^2 - \left(\sqrt{\alpha + 1/4}\right)^2}\right), \tag{78}$$

where $n, \nu = 0, 1, 2, \ldots$.

4 Conclusions

In this paper, we have solved the Schrödinger equation for a novel angle-dependent (NAD) potential. The energy eigenvalues and the corresponding eigenfunctions are obtained exactly by using the Nikiforov–Uvarov (NU) method. Eigenfunctions are expressed in terms of Jacobi polynomials for the θ-dependent part of the Schrödinger equation. The energy eigenvalues are obtained for the Coulomb potential plus NAD potential and the harmonic oscillator plus the NAD potential. It is seen that the NU method is an applicable tool for not only central potentials but also noncentral and combined potentials. The method of solving quantum mechanical problems may be useful in solving other complicated systems analytically. Results are in good agreement with the earlier works prepared on the Coulomb potential or the harmonic oscillator. It is point out that for the values of $\alpha, \beta, \gamma = 0$, the results are in good agreement with Refs. [42,44]. Moreover, it is also point out that these exact results obtained for the noncentral potentials may have some interesting applications in the study of different quantum mechanical systems and atomic physics. These applications can be accounted for some axial symmetric systems in quantum chemistry, such as some ring-shaped molecules, i.e., cyclic polyenes or benzene.

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