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Exact solution of Schrödinger equation with deformed ring-shaped potential

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Exact solution of the Schrödinger equation with deformed ring-shaped potential is obtained in the parabolic and spherical coordinates. The Nikiforov–Uvarov method is used in the solution. Eigenfunctions and corresponding energy eigenvalues are calculated analytically. The agreement of our results is good.

KEY WORDS: deformed ring-shaped potential, the Nikiforov–Uvarov method

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1. Introduction

The exact solutions of the Schrödinger equation with some well-known central and noncentral potentials is an important subject in quantum mechanical problems. Such solutions are helpful for checking and improving models and numerical methods besides of understanding about the characteristics of a quantum system. The exact solutions of this equation are possible only for certain potentials such as Coulomb, Morse, Pöschl-Teller and harmonic oscillator, etc. [1]. The other exactly solvable one is the deformed ring-shaped potential introduced by Hartmann [2]. This potential involves an attractive Coulomb potential with a repulsive inverse square potential one. In spherical coordinates it can be defined as

$$V(r,\theta) = \left[\frac{2}{r} - \ q\delta\frac{a_0}{r^2 sin^2\theta}\right]\delta\sigma^2 a_0\epsilon_0, \tag{1}$$

where a_0 and ϵ_0 denote the Bohr radius and the ground state energy of the hydrogen atom, respectively. δ and σ are positive real parameters as well. Their range varies from 1 upto 10. This potential can be used in quantum chemistry and nuclear physics to describe ring-shaped molecules like benzene and interactions between deformed pair of nuclei. We point out that the potential takes

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Table 1
Energy levels for a hydrogen-like atom with $\delta\sigma^2 = Z$ and $q = 0$.

m	$n + n'$	$E_{n,\,n'}$ (our work)	E [18]	$\bar{n}$
0	0	−13.605820	−13.60582	1
1	0			
0	1	−3.401455	−3.40145	2
2	0			
1	1	−1.511757	−1.51176	3
0	2			
3	0			
2	1			
1	2	−0.850363	−0.85036	4
0	2			
4	0			
3	1			
2	2	−0.544232	−0.54423	5
1	3			
0	4			
5	0			
4	1			
3	2			
2	3	−0.377939		6
1	4			
0	5			

the form of the Coulomb potential in the limiting case $\delta\sigma^2 = Z$ and $q = 0$ for hydrogen-like atoms (Table 1). The energy eigenvalues of the potential has been calculated before by using some useful methods. For example, these are a non-objective canonical transformation, namely, Kustaanheimo–Stiefel (KS) transformation, dynamical group method, path integral and SUSYQM method, etc. [2–17]. Moreover, this potential can be defined as a Coulomb plus Aharonov–Bohm potential by defining the parameters as $-ee' = 2a_0\epsilon_0\delta\sigma^2$, $-A/2\mu = q\epsilon_0 a_0^2\delta^2\sigma^2$ and $B = 0$. [18–20].

In the present work, we have obtained an exact solution of the Schrödinger equation with the q-deformed ring-shaped potential by using the Nikiforov–Uvarov (NU) method in both parabolic and spherical coordinates. The method is based on the solution of differential equation transformed into the hypergeometric type [21,22].

The paper is organized as follows: In section 2 we introduce the Nikiforov–Uvarov method. In section 3 we apply the method to solve the Schrödinger equation in both parabolic and spherical coordinates, respectively. In section 4 we present numerical results for $Z = 1$ and $q = 0$ with the conclusion.

2. The Nikiforov–Uvarov Method

The Nikiforov–Uvarov method first reduces the second order differential equations (ODEs) to the hypergeometric type with an appropriate coordinate transformation $x = x(s)$ as

$$\frac{\mathrm{d}^2\Psi(s)}{\mathrm{d}s^2} + \frac{\tilde{\tau}(s)}{\sigma(s)}\frac{\mathrm{d}\Psi(s)}{\mathrm{d}s} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0, \tag{2}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials with at most second degree, and $\tilde{\tau}(s)$ is a polynomial with at most first degree [21,22]. If we take the following factorization

$$\Psi(s) = \phi(s)\ y(s), \tag{3}$$

the equation (2) takes the form [22]

$$\sigma(s)\frac{\mathrm{d}^2 y(s)}{\mathrm{d}s^2} + \tau(s)\frac{\mathrm{d}y(s)}{\mathrm{d}s} + \lambda y(s) = 0, \tag{4}$$

where

$$\sigma(s) = \pi(s)\frac{\mathrm{d}}{\mathrm{d}s}(\ln\phi(s)), \tag{5}$$

and

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{6}$$

Also, λ is given

$$\lambda_n + n\tau' + \frac{[n(n-1)\sigma'']}{2} = 0, \quad n = 0, 1, 2, \ldots \tag{7}$$

The energy eigenvalues can be calculated from the above equation. We first have to determine $\pi(s)$ and λ by defining

$$k = \lambda - \pi'(s). \tag{8}$$

Solving the quadratic equation for $\pi(s)$ with equation (8), we get

$$\pi(s) = \left(\frac{\sigma' - \tilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}. \tag{9}$$

Here, $\pi(s)$ is a polynomial with the parameter s and prime factors denote the differentials at first degree. The determination of k is the essential point in the calculation of $\pi(s)$. It is obtained by setting the discriminant of the square root to zero [22]. Therefore, we obtain a general quadratic equation for k.

The determination of the wave function is now in order. We consider the equation (5) and the Rodriguez relation

$$y_n(s) = \frac{C_n}{\rho(s)} \frac{\mathrm{d}^n}{\mathrm{d}s^n} \left[\sigma^n(s)\ \rho(s)\right], \tag{10}$$

where C_n is normalization constant and the weight function $\rho(s)$ satisfy the following relation

$$\frac{\mathrm{d}}{\mathrm{d}s} \left[\sigma(s)\ \rho(s)\right] = \tau(s)\ \rho(s). \tag{11}$$

Equation (10) refers to the classical orthogonal polynomials that have many important properties especially orthogonality relation can be defined as

$$\int_a^b y_n(s)\ y_m(s)\rho(s)\, ds = 0, \quad m \neq n. \tag{12}$$

3. Calculations

The Schrödinger equation in spherical coordinates becomes

$$\nabla^2 \Psi + \frac{2m}{\hbar^2} \left[E - V(r, \theta)\right] \Psi = 0. \tag{13}$$

We are first going to study for solution of the problem using parabolic coordinates.

3.1. Parabolic coordinates

One can write the second type parabolic coordinates as [3,4,23]

$$x = \xi\eta \cos\varphi, \quad y = \xi\eta \sin\varphi, \quad \text{and} \quad z = \frac{1}{2}\left(\eta^2 - \xi^2\right), \tag{14}$$

and

$$\xi\ \eta = r \sin\theta \quad \text{and} \quad r = \frac{1}{2}\left(\eta^2 + \xi^2\right). \tag{15}$$

If we write trial wave function in the following form [4]

$$\Psi(\xi, \eta, \varphi) = \frac{1}{\sqrt{\xi\eta}}\, u(\xi)\, v(\eta)\, \mathrm{e}^{im'\varphi}, \tag{16}$$

one can get two-coupled differential equations

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - \frac{(\Upsilon^2 - \frac{1}{4})}{\xi^2} u + \left(\frac{2mE}{\hbar^2}\right) \xi^2 u - \left(\frac{2m}{\hbar^2}\right) \mu_1 u = 0, \tag{17}$$

and

$$\frac{\mathrm{d}^2 v}{\mathrm{d}\eta^2} - \frac{(\Upsilon^2 - \frac{1}{4})}{\eta^2} v + \left(\frac{2mE}{\hbar^2}\right)\eta^2 v - \left(\frac{2m}{\hbar^2}\right)\mu_2 v = 0, \tag{18}$$

where $\Upsilon = \sqrt{m'^2 + q\delta^2\sigma^2}$ and $\mu_1 = \mu_2 = 2\sigma^2\ \delta\ a_0\ \epsilon_0$. We will first solve equation (17) and then easily get the other one.

By using the transformation $s = \xi^2$, equation (17) is therefore transformed into the equation of hypergeometric type. Hence, we have

$$u''(s) + \frac{1}{2s}u'(s) + \frac{1}{4s^2}\left[-\varepsilon^2 s^2 - \alpha_1^2 s - \beta^2\right]u(s) = 0, \tag{19}$$

where $\varepsilon^2 = \dfrac{2mE}{\hbar^2}$, $\alpha_1^2 = \dfrac{2m}{\hbar^2}\mu_1$ and $\beta^2 = \left(\Upsilon^2 - \dfrac{1}{4}\right)$.

Comparing equation (19) with equation (2), we get

$$\sigma(s) = 2s, \quad \tilde{\tau}(s) = 1, \quad \text{and} \quad \tilde{\sigma}(s) = \left(-\varepsilon^2 s^2 - \alpha_1^2 s - \beta^2\right). \tag{20}$$

Substituting these into equation (9), we write

$$\pi(s) = \frac{1}{2} \pm \frac{1}{2}\sqrt{4\varepsilon^2 s^2 + (8k + 4\alpha_1^2)s + 4\beta^2}. \tag{21}$$

The constant k can be determined from the condition that the discriminant of the square root must be zero, so that

$$k_{1,2} = -\frac{1}{2}\alpha_1^2 \pm \varepsilon\beta. \tag{22}$$

Hence the final result for equation (21) can be written as

$$\pi(s) = \frac{1}{2} \pm \begin{cases} (\varepsilon s - \beta), & \text{for} \quad k = -\frac{1}{2}\alpha_1^2 - \varepsilon\beta \\ (\varepsilon s + \beta), & \text{for} \quad k = -\frac{1}{2}\alpha_1^2 + \varepsilon\beta. \end{cases} \tag{23}$$

A proper value for $\pi(s)$ is chosen, so that the function

$$\tau(s) = 2(1 + \beta) - 2\varepsilon s, \tag{24}$$

must have a negative derivative [22]. From equation (7) we can obtain

$$\begin{aligned} \lambda_n &= -\frac{1}{2}\alpha_1^2 - \varepsilon - \beta\varepsilon \\ &= 2n\varepsilon. \end{aligned} \tag{25}$$

Following the same procedure again one gets for equation (18) as

$$\begin{aligned} \lambda_{n'} &= -\frac{1}{2}\alpha_2^2 - \varepsilon - \beta\varepsilon \\ &= 2n'\varepsilon. \end{aligned} \tag{26}$$

By combining each side of the equations (25) and (26) we obtain energy eigenvalues

$$E_{n,n'} = -\left[\frac{\delta^2\ \sigma^4}{(n+n'+1+\beta)^2}\right]\epsilon_0. \quad n, n' = 0, 1, 2\ldots \tag{27}$$

This solution is identical for $\beta \simeq \Upsilon^2$ with the ones obtained before [3,4,6–9,13].

Now, we are going to determine the wave function. Considering equation (3) and using equation (5) we get

$$\phi(s) = s^{\nu/4}\ e^{-\frac{\varepsilon}{2}s}, \tag{28}$$

where $\nu = 1 + 2\beta$.
From the equations (11) and (10), we obtain

$$y_n(s) = \frac{C_n}{\rho(s)}\frac{\mathrm{d}^n}{\mathrm{d}s^n}\left[s^n\ \rho(s)\right], \tag{29}$$

with $\rho(s) = s^{(\nu-1)/2}\ \mathrm{e}^{-\varepsilon s}$. Equation (33) stands for the associated Laguerre polynomials. That is

$$y_n(s) \equiv L_n^{\beta}(s), \tag{30}$$

Hence we have found the wave function that belongs to the equation (17) as

$$u_n(\xi) = C_n\ s^{\nu/4}\ \mathrm{e}^{-\frac{\varepsilon}{2}s}\ L_n^{\beta}(s), \tag{31}$$

with $s = \xi^2$. Similarly, we can also write the wave function for equation (18)

$$v_n(\eta) = C_{n'}\ s^{\nu/4}\ \mathrm{e}^{-\frac{\varepsilon}{2}s}\ L_{n'}^{\beta}(s), \tag{32}$$

with $s = \eta^2$. Therefore, the total wave function takes

$$\Psi_{n,n',m'}(\xi, \eta, \varphi) = \frac{1}{\sqrt{\xi\ \eta}}\ C_{n,n'}\ s^{\nu/2}\ \mathrm{e}^{-\varepsilon s}\ L_n^{\beta}(s)\ L_{n'}^{\beta}(s)\ \mathrm{e}^{im'\varphi}, \tag{33}$$

where the normalization constant $C_{n,n'}$ can be found from the equation (12) as

$$C_{n,n'} = \sqrt{\frac{4(n!)(n')!}{(n+\beta)!\ (n'+\beta)!}}, \quad n,\ n' = 0, 1, 2\ldots \tag{34}$$

One can easily see that in the case of $r\sin\theta = \xi\eta$, the problem reduces to harmonic oscillator plus inverse square potential case. The latter, we have studied that this problem also reduces to that of molecular Kratzer potential like (Coulomb plus inverse square).

3.2. Spherical coordinates

Considering equation (13) we write the total wave function as

$$\Psi(r,\theta,\varphi) = \frac{U(r)}{r}\ \Theta(\theta)\ \Phi(\varphi), \tag{35}$$

with the well-known azimuthal angle solution

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}}\ \mathrm{e}^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \ldots \tag{36}$$

Thus we get as

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \left(\kappa - \frac{(m^2 + b')}{\sin^2\theta}\right)\Theta = 0, \tag{37}$$

and

$$\frac{\mathrm{d}^2U}{\mathrm{d}r^2} + \frac{2}{\gamma}\left(-E' - \frac{a'}{r} - \frac{\kappa}{r^2}\right)U = 0, \tag{38}$$

where $E' = \dfrac{2mE}{\hbar^2}$, $a' = \dfrac{2ma}{\hbar^2}$ and $b' = \dfrac{2mb}{\hbar^2}$, κ and m^2 are also separation constants.

Using the NU-method, we are going to solve them. By defining $m' = \sqrt{m^2 + b}$ in equation (37) and taking $x = \cos\theta$, it will have a form of hypergeometric type

$$\frac{\mathrm{d}^2\Theta}{\mathrm{d}x^2} - \frac{2x}{(1-x^2)}\frac{\mathrm{d}\Theta}{\mathrm{d}x} + \frac{1}{(1-x^2)^2}\left[\kappa(1-x^2) - m'^2\right]\Theta(x) = 0. \tag{39}$$

Comparing it with equation (2), we get

$$\sigma(x) = x, \quad \tilde{\tau}(x) = -2x, \quad \text{and} \quad \tilde{\sigma}(x) = \kappa(1-x^2) - m'^2. \tag{40}$$

Substituting these into equation (9), we get

$$\pi(x) = \pm\sqrt{-(k+\kappa)(1-x^2) + m'^2}. \tag{41}$$

The constant k is determined from the condition that the discriminant of the square root must be zero. Thus, we find

$$\pi(x) = \begin{cases} \pm\ m', & \text{for} \quad k = \kappa \\ \pm\ m'\ x, & \text{for} \quad k = \kappa - m'^2. \end{cases} \tag{42}$$

A proper value for $\pi(x)$ can be chosen, so that the function

$$\tau(x) = -2(m' + 1)\ x, \tag{43}$$

has a negative derivative. From equation (7) we can obtain

$$\begin{aligned}\lambda_n &= \kappa - m'(m'+1) \\ &= 2n\ (m'+1) + n\ (n-1).\end{aligned} \tag{44}$$

Solving for κ, we have

$$\kappa = \kappa_n = \ell'(\ell'+1), \tag{45}$$

where $\ell' = n + m'$.

Now we are going to determine the wave function. From the equations (11) and (10), we can write

$$y_n(x) = \frac{B_n}{\rho(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left[(1-x^2)^{n+m'}\right] \tag{46}$$

with $\rho(x) = (1-x^2)^{m'}$. Therefore, equation (46) stands for Jacobi polynomial as

$$y_n \equiv\ P_n^{(m',m')}(x), \tag{47}$$

where $n = l' - m'$. The wave function becomes

$$\begin{aligned}\Theta(x) &= \Theta_{l',m'} \\ &= C_{l',m'}\ (1-x^2)^{m'/2}\ P_{l'-m'}^{(m',m')}(x)\end{aligned} \tag{48}$$

with $x = \cos\theta\ \ (x \in [-1, 1])$. Using equation (12), we get

$$C_{\ell',m'} = \frac{1}{2^{m'}(\ell'+1)} \sqrt{\frac{2\ell'+1}{2}(\ell'-m')!(\ell'+m')!}. \tag{49}$$

Let us now consider equation (38)

$$u''(r) + \frac{1}{r^2}\left[-E'r^2 - a'r - \kappa\right] u(r) = 0, \tag{50}$$

Comparing this equation with equation (2), we obtain

$$\sigma(r) = r, \quad \tilde{\tau}(r) = 0, \quad \text{and} \quad \tilde{\sigma}(r) = -E'r^2 - a'r - \kappa. \tag{51}$$

If we insert these into equation (9), one gets

$$\pi(r) = \frac{1}{2} \pm \sqrt{4E'r^2 + 4(k+a')r + (1+4\kappa)}. \tag{52}$$

We can determine the constant k by using the condition that discriminant of the square root is zero, that is

$$k_{1,2} = -a' \pm \sqrt{E'\ (1+4\kappa)}. \tag{53}$$

Hence, the final form of the equation (52) for each value of k becomes

$$\pi(r) = \frac{1}{2} \pm \frac{1}{2} \begin{cases} [2\sqrt{E'}r + \sqrt{1+4\kappa}], & \text{for } k = -a' + \sqrt{E'(1+4\kappa)} \\ [2\sqrt{E'}r - \sqrt{1+4\kappa}], & \text{for } k = -a' - \sqrt{E'(1+4\kappa)}. \end{cases} \tag{54}$$

A proper value for $\pi(r)$ is taken, so that the function

$$\tau(r) = (1 + \sqrt{1+4\kappa}) - 2\sqrt{E'}r, \tag{55}$$

has a negative derivative. From equation (7), we can write

$$\begin{aligned} \lambda_n &= -a' - \sqrt{E'(1+4\kappa)} - \sqrt{E'} \\ &= 2n\ \sqrt{E'}. \end{aligned} \tag{56}$$

Therefore, it gives us the energy eigenvalues of the radial equation with the deformed ring-shaped potential

$$E = \left[-\left(\frac{\delta^2\ \sigma^4}{n_r + \ell' + 1} \right)^2 \epsilon_0 \right], \quad n_r = 0, 1, 2, \ldots \tag{57}$$

where n_r denotes the radial quantum number which belongs to the equation (38).

To determine the wave function, we consider the equations (3) and (5) for obtaining

$$\phi(r) = \ \mathrm{e}^{-\sqrt{E'}\ r}\ r^{(\nu-1)/2}, \tag{58}$$

where $\nu = 1 + 2\sqrt{1+4\kappa}$. Thus from the equations (11) and (10) we have

$$y_n(r) = \frac{B_n}{\rho(r)} \frac{\mathrm{d}^n}{\mathrm{d}r^n} \left[\sigma^{n(r)}\ \rho(r) \right] \tag{59}$$

with $\rho(r) = \mathrm{e}^{-\sqrt{E'}r}\ r^{(1-\nu)/2}$. Equation (59) stands for associated Laguerre polynomials, that is

$$y_n(r) = L_n^{\bar{k}}(r), \tag{60}$$

where $\bar{k} = (\nu - 1)/2$. The radial part wave function is written as

$$U_n(r) = C_n\ \mathrm{e}^{-\sqrt{E'}r}\ r^{\bar{k}}\ L_n^{\bar{k}}(r). \tag{61}$$

By using the orthogonality condition, we can determine the coefficient as

$$C_{n,\bar{k}} = \sqrt{\frac{n!}{2(n+\bar{k})(n+\bar{k})!}}, \tag{62}$$

with $\kappa = \ell'(\ell'+1)$. Hence, the total wave function takes the form

$$\Psi(r,\theta,\varphi) = \frac{1}{\sqrt{2\pi}}\; C_{n,\bar{k}}\; C_{\ell',m'}\left[\mathrm{e}^{-\sqrt{E'}r}\; r^{\bar{k}}\; (\sin\theta)^{m'} \times\; P_n^{(m',m')}(\cos\theta)\; L_n^{\bar{k}}(r)\; \mathrm{e}^{im\varphi}\right]. \tag{63}$$

4. Conclusion and remarks

We have obtained the exact eigenfunctions and corresponding energy eigenvalues of the Schrödinger equation with the deformed ring-shaped potential in both second type parabolic and also spherical coordinates by using the Nikiforov–Uvarov method. At first our problem reduces to the harmonic oscillator plus inverse square potential, it also reduces to the problem that molecular Kratzer (Coulomb plus inverse square) one in second case. Results obtained in two different coordinate systems are identical by following the conditions $\beta \simeq \Upsilon^2$ in equation (27) and $\ell' = n + m'$ in equation (57). Some numerical values of energy for a hydrogen-like atom due to the attractive Coulomb potential are presented in tabular form. The total wave functions, in both coordinates, are physical. They behaves asymptotically. The agreement of our analytic and numerical results is good.

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