EXACT WAVE FUNCTIONS AND DYNAMICAL SYMMETRY GROUP FOR THE MODIFIED NONRELATIVISTIC RING-SHAPED KRATZER POTENTIAL

**SHAKIR M. NAGIYEV, KÖNÜL SH. JAFAROVA,
SHOVQIYYA A. AMIROVA, VEFA A. TARVERDIYEVA**
Institute of Physics, Ministry of Science and Education,
Javid Ave. 131, AZ 1143, Baku, Azerbaijan
shakir.m.nagiyev@gmail.com, konule2016@gmail.com, shovqiyya@mail.ru,
vefa.tarverdiyeva@mail.ru

We propose a new exactly solvable potential which consists of the modified Kratzer potential plus a new ring-shaped potential $(\beta + \gamma\cos\theta + \nu\cos^2\theta)/r^2\sin^2\theta$. The exact solutions of the bound states of the Schrödinger equation for this potential are presented analytically by using the functional method. The wavefunctions of the radial and angular parts are taken on the form of the Laguerre polynomials and the Jacobi polynomials, respectivly. Total energy of the system is different from the modified Kratzer potential because of the contribution of the angular part. We also build a dynamical symmetry group for the radial part of the equation of motion, which allows us to find the energy spectrum purely algebraically.

Keywords: Schrödinger equation; ring-shaped modified Kratzer potential; dynamical symmetry group; Laguerre and Jacobi polynomials.
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1. Introduction

When describing the physical properties of quantum dynamical systems, such as molecules and atoms, atomic nuclei and hadrons, relativistic or non-relativistic potential models play an important role [1-5]. Due to the fact that almost all interactions occurring in nature do not have an obvious type of potential, a model or phenomenological potential is proposed for the study of a quantum system, in which its most essential properties are highlighted and non-existent ones are discarded. Potential models are widely used to study the laws of motion of quantum microparticles in external potential fields (see, for example, [5, 6] and references there)).

The state of a system in quantum mechanics is completely described by the wave function. These states can generally be either bound or scattered states. By solving the corresponding equations of motion (the Schrödinger equation, the Klein-Gordon equation, the Dirac equation or the equation of finite-difference quantum mechanics (see [7] and references there)) within the framework of the potential model, we find an explicit form of the wave function and energy spectrum for these states.

Among quantum mechanical problems, exactly solvable problems occupy a special place. It is well known that the number of potentials allowing an exact solution of relativistic and non-relativistic wave equations is small. These include, for example, Coulomb, harmonic oscillator, Kratzer [4, 8], Hartmann [9], Quesne [10] and Hautot [6] potentials. Some classes of exactly-solvable Klein–Gordon equations are considered in [11].

Note that Hartmann, Quesne and Hautot [6] potentials are non-central potentials. The class of noncentral potentials [6, 7, 9, 10, 12–19] plays a particularly important role in quantum mechanics, nuclear physics, and theoretical chemistry. Non-central or ring-shaped potentials usually consist of two terms

$$V(r,\theta) = V(r) + \frac{f(\theta)}{r^2}, \quad (1)$$

where is the first term $V(r)$ describes the central field, and the second term $\frac{f(\theta)}{r^2}$ characterizes the ring-shaped potential.

The purpose of this work is to find exact solutions of the Schrödinger equation using functional methods and to construct a dynamic symmetry group for the new ring-shaped modified Kratzer potential of the form

$$V(r,\theta) = D\left(1 - \frac{a}{r}\right)^2 + \frac{\beta + \gamma\cos\theta + \nu\cos^2\theta}{r^2\sin^2\theta}. \quad (2)$$

Here D is the dissociation energy, a is the equilibrium internuclear separation, and $\beta,\ \gamma,\ \nu$ are the parameters. The first term in (2) involves an attractive Coulomb potential and a repulsive inverse square potential. The second term of (2) describes the annularity of the interaction between the atoms. When $\beta = \gamma = \nu = 0$, the ring-shaped Kratzer potential reduces to a Kratzer potential for which the analytical solutions of the Schrödinger equation are known [4, 12]. The Kratzer potential [4, 12] is widely used in atomic and molecular physics and quantum chemistry. Other varieties of the ring-shaped Kratzer potential were studied in [13, 17].

2. Exact solution of the Schrödinger equation with the ring-shaped modified Kratzer potential

2.1. Separation of variables.

Let us write the Schrödinger equation with potential (2) in a spherical coordinate system

131, H.Javid ave, AZ-1143, Baku
Institute of Physics
E-mail: jophphysics@gmail.com

$$\left\{\frac{1}{r^2}\partial_r(r^2\partial_r)+\frac{\Delta_{\theta,\varphi}}{r^2}+\frac{2m_0}{\hbar^2}\left[E-D\left(1-\frac{a}{r}\right)^2-\frac{f(\theta)}{r^2}\right]\right\}\psi(\mathbf{r})=0, \tag{3}$$

where

$$\Delta_{\theta,\varphi}=\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta)+\frac{1}{\sin^2\theta}\partial_\varphi^2. \tag{4}$$

equation (3) allows separation of variables. To do this, let's put

$$\psi(\mathbf{r})=R(r)F(\theta,\varphi). \tag{5}$$

After substituting (5) into (3) we obtain two equations:

a) radial Schrödinger equation

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left(\frac{2m_0}{\hbar^2}\left[E-D\left(1-\frac{a}{r}\right)^2\right]-\frac{\Lambda}{r^2}\right)R=0, \tag{6}$$

b) the angular part of the Schrödinger equation

$$\left[\Delta_{\theta,\varphi}-\frac{2m_0}{\hbar^2}f(\theta)+\Lambda\right]F(\theta,\varphi)=0, \tag{7}$$

Here Λ there is a splitting parameter.

2.2. Exact solution of the radial equation.

In equation (6) we move on to the dimensionless variable $\rho=\frac{r}{a}$. In terms ρ equation (6) will take the form

$$R''+\frac{2}{\rho}R'+\left(\frac{2m_0a^2}{\hbar^2}\left[E-D\left(1-\frac{1}{\rho}\right)^2\right]-\frac{\Lambda}{\rho^2}\right)R=0. \tag{8}$$

Here the primes mean differentiation by ρ.

Let us now note that since the limits of potential (2) at $r\to\infty$ and at $r\to 0$ equal

$$\lim_{r\to\infty}V(r,\theta)=V_\infty=D,\qquad \lim_{r\to 0}V(r,\theta)=\infty, \tag{9}$$

then we can say that the energy spectrum at $E<D$ will be discrete, and when $E>D$ will be continuous.

Introducing dimensionless quantities

$$\varepsilon=\frac{2m_0a^2}{\hbar^2}(D-E),\ \ \alpha=\frac{2m_0a^2D}{\hbar^2}, \tag{10}$$

we rewrite equation (8) in the form

$$R''+\frac{2}{\rho}R'+\left(\frac{2\alpha}{\rho}-\frac{\Lambda_1}{\rho^2}-\varepsilon\right)R=0. \tag{11}$$

where $\Lambda_1=\Lambda+\alpha$.

To study equation (11), as usual, we put

$$R(\rho)=\frac{\chi(\rho)}{\rho}. \tag{12}$$

In this case, equation (11) is reduced to the form

$$\chi''+\left(\frac{2\alpha}{\rho}-\frac{\Lambda_1}{\rho^2}-\varepsilon\right)\chi=0. \tag{13}$$

Let us consider separately the cases $\varepsilon>0$ and $\varepsilon<0$.

1) $\varepsilon > 0$ case. Wherein the radial wave function satisfies the boundary conditions

$$\chi(0) = \chi(\infty) = 0. \tag{14}$$

Therefore, at small ρ the solution is proportional ρ^s. At large ρ we get the equation

$$\chi'' - \varepsilon\chi = 0, \tag{15}$$

whence, taking into account (14), we have $\chi = e^{-\sqrt{\varepsilon}\rho}$.

Therefore, in (13) it is natural to make the substitution

$$\chi = \rho^s e^{-\sqrt{\varepsilon}\rho}\Omega(\rho) \equiv g(\rho)\Omega(\rho), \tag{16}$$

where $s = \frac{1}{2} + \sqrt{\frac{1}{4} + \Lambda_1}$. If the coefficients of equation (13) are denoted by $a_2 = 1$, $a_1 = 0$, $a_0 = \frac{2\alpha}{\rho} - \frac{\Lambda_1}{\rho^2} - \varepsilon$, then the function Ω will satisfy the equation

$$b_2\Omega'' + b_1\Omega' + b_0\Omega = 0, \tag{17}$$

where

$$b_2 = a_2, b_1 = a_1 + 2a_2\frac{g'}{g}, b_0 = a_0 + a_1\frac{g'}{g} + a_2\frac{g''}{g}. \tag{18}$$

Now equation (17) takes the form

$$\rho\Omega'' + \left(2\mathrm{s} - 2\sqrt{\varepsilon}\rho\right)\Omega' + \left(2\alpha - 2\mathrm{s}\sqrt{\varepsilon}\right)\Omega = 0 \tag{19}$$

After changing the variable $\rho = t/2\sqrt{\varepsilon}$ we get

$$t\Omega''(\mathrm{t}) + (2\mathrm{s} - \mathrm{t})\Omega'(\mathrm{t}) + \left(\frac{\alpha}{\sqrt{\varepsilon}} - \mathrm{s}\right)\Omega(\mathrm{t}) = 0 \tag{20}$$

Comparing this equation with the equation for Laguerre polynomials [20] $y = L_n^\lambda(x)$:

$$xy'' + (\lambda + 1 - x)y' + ny = 0, \tag{21}$$

we find that

$$\lambda = 2s - 1,\ n = \frac{\alpha}{\sqrt{\varepsilon}} - s,\ n = 0,1,2, \ldots$$

The last condition leads to energy quantization equation

$$E_n = D - \frac{2m_0a^2D^2}{\hbar^2}\left[n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2m_0a^2D}{\hbar^2} + \Lambda}\right]^{-2}, \tag{22}$$

and the function $\Omega(\mathrm{t})$ coincides with the Laguerre polynomial

$$\Omega(\mathrm{t}) = L_n^{2\mathrm{s}-1}(t) = L_n^{2\mathrm{s}-1}\left(\frac{2\alpha\rho}{n+s}\right). \tag{23}$$

Therefore the radial wave function

$$R_{n\Lambda}(r) = C_{n\Lambda}\rho^{s-1}e^{-\sqrt{\varepsilon_n}\rho}L_n^{2\mathrm{s}-1}\left(\frac{2\alpha\rho}{n+s}\right). \tag{24}$$

Note that the parameter Λ we find from the solution of the angular part of the Schrödinger equation (7).

2.3. Dynamical symmetry group SU(1, 1)

Let us now consider the radial equation (11) by the help of SU(1,1) Lie algebra. The generators of SU(1,1) algebra may be realized as [21]

$$K_0 \equiv \Gamma_0 = \frac{1}{2}\left(-\rho\partial_\rho^2 - 2\partial_\rho + \frac{\Lambda_1}{\rho} + \rho\right),$$
$$K_1 \equiv \Gamma_4 = \frac{1}{2}\left(-\rho\partial_\rho^2 - 2\partial_\rho + \frac{\Lambda_1}{\rho} - \rho\right), \quad (25)$$
$$K_2 \equiv T = -i\left(\rho\partial_\rho + 1\right),$$

By a direct check, one can verify that these operators satisfy the commutation relations

$$[\Gamma_0, \Gamma_4] = iT, [T, \Gamma_0,] = i\Gamma_4, [\Gamma_4, T] = -i\Gamma_0. \quad (26)$$

The casimir operator is $C_2 = \Gamma_0^2 - \Gamma_4^2 - T^2 = \mu(\mu - 1)$, where $\mu > 0$ is an eigenvalue of the operator C_2.

We denote that states of a positive discrete series as $|n,\mu>$, $n = 0,1,2, \ldots$, such that

$$\Gamma_0|n,\mu> = (n+\mu)|n,\mu>,$$
$$C_2|n,\mu> = \mu(\mu-1)|n,\mu>. \quad (27)$$

It should be noted that in our case from equation (25), we obtain $C_2 = \Lambda_1 = s(s-1)$, so $\mu = s$. Equation (11) can be written with the help of generators (25) as

$$[(1+\varepsilon)\Gamma_0 + (1-\varepsilon)\Gamma_4 - 2\alpha]R = 0. \quad (28)$$

Let us introduce a new parameter λ and perform a tilting transformation

$$\tilde{R} = e^{-i\lambda T}R. \quad (29)$$

To solve this equation algebraically, we use the formulas

$$e^{-i\lambda T}\Gamma_0 e^{i\lambda T} = \Gamma_0 \mathrm{ch}\lambda + \Gamma_4 \mathrm{sh}\lambda,$$
$$e^{-i\lambda T}\Gamma_4 e^{i\lambda T} = \Gamma_4 \mathrm{ch}\lambda + \Gamma_0 \mathrm{sh}\lambda. \quad (30)$$

As a result, for the function $\tilde{R}$ (29) we get the equation

$$(b\Gamma_0 + c\Gamma_4 - 2\alpha)\tilde{R} = 0, \quad (31)$$

where

$$b = (1+\varepsilon)\mathrm{ch}\lambda + (1-\varepsilon)\mathrm{sh}\lambda,$$
$$c = (1+\varepsilon)\mathrm{sh}\lambda + (1-\varepsilon)\mathrm{ch}\lambda.$$

We consider separately the cases when $E < D$ and $E > D$.

1) When $E < D$(discrete spectrum) in (31), a compact generator Γ_0 can be diagonalized [20]. Setting $c = 0$, we obtain $\mathrm{th}\lambda = (1+\varepsilon)(1-\varepsilon)$. As a result, we have $b = 2\sqrt{\varepsilon}$ and

$$\left(2\sqrt{\varepsilon}\Gamma_0 - 2\alpha\right)\tilde{R} = 0. \quad (32)$$

It follows from (32) the energy equation (22).

2) When $E > D$, noncompact generator Γ_4 is diagonalized, having a continuous real spectrum $\delta \in R$. In this case $b = 0$ and we have $\mathrm{th}\lambda = -(1+\varepsilon)/(1-\varepsilon)$. As a result we have $c = 2\sqrt{\varepsilon}$ and

$$\left(2\sqrt{-\varepsilon}\Gamma_4 - 2\alpha\right)\tilde{R}_1 = 0. \quad (33)$$

Consequently, $\frac{\alpha}{\sqrt{-\varepsilon}} = \delta$ or

$$E_\delta = D + \frac{2m_0 a^2 D^2}{\hbar^2 \delta^2}. \quad (34)$$

3. The solutions of the angular equation

We now find the solutions the angle-dependent equation (7). The variables in (7) can be separated in the usual way

$$F(\theta,\varphi) = \Theta(\theta)\frac{e^{im\varphi}}{\sqrt{2\pi}}. \quad (35)$$

Here, m is the usual magnetic quantum number and is integer. Equation for $\Theta(\theta)$ now looks like

$$\left(\partial_\theta^2 + \text{ctg}\theta\partial_\theta - \frac{m\prime^2+\gamma_0\cos\theta+\nu_0\cos^2\theta}{\sin^2\theta} + \Lambda\right)\Theta(\theta) = 0. \tag{36}$$

The orthonormalized solutions of this equation were found in [7]. We give here their explicit form

$$\Theta_{km}(\theta) = \text{c}_{km}\left(\sin^2\frac{\theta}{2}\right)^{A_1}\left(\cos^2\frac{\theta}{2}\right)^{A_2} P_k^{(2A_1,2A_2)}(\cos\theta), \tag{37}$$

where $k = 0,1,2,...$, the functions $P_k^{(\alpha,\beta)}(x)$ are the Jacobi polynomials [21] and the positive parameters $A_{1,2}$ are

$$A_{1,2} = \frac{1}{2}\sqrt{m^2 + \nu_0 + \beta_0 \pm \gamma_0}. \tag{38}$$

Normalization coefficients

$$c_{km} = \sqrt{\frac{(k+A_1+A_2+1/2)k!\Gamma(k+2A_1+2A_2+1)}{\Gamma(k-2A_1+1)\Gamma(k-2A_2+1)}} \tag{39}$$

are determined from the normalizing condition for the angular wave functions (37)

$$\int_0^\pi \Theta_{km}(\theta)\,\Theta_{k'm}(\theta)\sin\theta d\theta = \delta_{kk'}\ . \tag{40}$$

As shown in [7], the separation constant *Λ* depends on *k* and *m*

$$\Lambda \equiv \Lambda_{\text{km}} = \text{k}\left[\text{k} + 1 + \sqrt{\text{m}^2 + \nu_0 + \beta_0 + \gamma_0} + \sqrt{\text{m}^2 + \nu_0 + \beta_0 - \gamma_0}\right] +$$
$$+ \frac{1}{2}\left[\sqrt{\text{m}^2 + \nu_0 + \beta_0 + \gamma_0} + \sqrt{\text{m}^2 + \nu_0 + \beta_0 - \gamma_0}\right] +$$
$$+ \frac{1}{2}\sqrt{(\text{m}^2 + \nu_0 + \beta_0 + \gamma_0)(\text{m}^2 + \nu_0 + \beta_0 - \gamma_0)} + \frac{1}{2}(\text{m}^2 + \beta_0 - \nu_0) \tag{41}$$

Thus, the exact discrete energy eigenvalues of the Schrödinger equation for our quantum system are (see, (22) and (41))

$$E_{nkm} = D - \frac{2m_0a^2D^2}{\hbar^2}\left[n + \frac{1}{2} + \sqrt{\frac{1}{4} + \Lambda_{\text{km}} + \frac{2m_0a^2D}{\hbar^2}}\right]^{-2}, \tag{42}$$

where $n = 0,1,2,\dots, k = 0,1,2,\dots, m = 0, \pm1, \pm2, \dots$

We consider a special case of the formula (42). For $f(\theta) = 0$ will have a results of the paper [12].

4. Conclusion

In this paper, we considered an exactly solvable model, namely a non-relativistic ring-shaped modified Kratzer potential model.

The main results of this paper are the explicit and exact expressions for the energy spectrum and corresponding wave functions. We have also find the dynamical symmetry group $SU(1,1)$.

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