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Scattering States of the Schrödinger Equation with a Position-Dependent-Mass and a Non-Central Potential

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In this paper, we study the time-independent Schrödinger equation within the formalism of a position-dependent effective mass. By using a generalized decomposition of a non-central effective potential, The deformed Schrödinger equation can be easily solved analytically through separation of variables. The energy eigenvalues and the normalization constant of the radial wave functions, as well as the scattering phase shifts are obtained.

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I. INTRODUCTION

Conceptual meanings of the dependence of the exact solutions and the wave equations have been considered in [1–4]. The derived physical quantities, such as the eigenfunctions and the eigenvalues of these equations, can be compared to either experimental results or results obtained from other methods. The exact solutions of the wave equations can be used as criteria in other numerical and theoretical methods. The evolutions of non-relativistic quantum particles are usually described by using the Schrödinger equation while for relativistic quantum particles, one has to deal with the correct equations of motion, such as the Klein-Gordon or the Dirac Equation, depending on the particle's spin. These equations have been investigated via different methods. Usually, the mass parameter in the above-mentioned wave equations has been considered to be a constant. Recently, increasing interest has been drawn to solving the quantum wave equations with a position-dependent mass. The Schrödinger equation with a position-dependent-mass distribution was initially proposed by Von Roos [5]. In certain physical systems, the effective mass parameter should be position-dependent to be consistent with the experimental data [6]. In this context, the Schrödinger equation with different phenomenological potentials and appropriate mass distributions has been investigated using various methods [7–10]. For some molecular Hamiltonians, the energy spectra and the eigenfunctions of particles with a position-dependent-mass have been derived [11]. According to [11], particles with a position-dependent mass are more likely to tunnel than ordinary ones. The use of this effective mass formalism has been considered for the dynamics of electrons in inhomogeneous crystals for many years [12, 13]. It has been also applied in many different fields of physics, such as helium clusters [14], semiconductors [15–17], quantum dot [18], quantum liquids [19] and atomic nuclei [20–22].

In this work, we are going to consider the three-dimensional time-independent Schrödinger equation within the effective mass formalism. This paper is organized as follows: In Sec. II., after some preliminaries, the separation of variables is carried out for the deformed Schrödinger equation with a non-central potential in spherical coordinates. In Sec. III., we introduce a new non-central potential, and we investigate the scattering-states solutions, as well as the phase shifts,

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under this effective potential . Finally, Sec. IV., is devoted to the conclusion.

II. VARIABLE SEPARATION OF THE HAMILTONIAN CONSIDERING A NON-CENTRAL POTENTIAL IN THE POSITION-DEPENDENT-MASS FORMALIS

The theoretical background of the position-dependent effective-mass formalism (PDEMF) has recently been considered [23,24]. In the PDEMF, for the Schrödinger equation, the mass operator $m(x)$ and the momentum operator $\vec{p} = -i\hbar\vec{\nabla}$ no longer commute. Therefore, several methods can be used to generalize the usual form of the kinetic energy operator $\vec{p}^2/2m_0$ and, consequently, the Hamiltonian, in order to obtain a Hermitian operator to describe the quantum state of a physical system that is not trivial in this case. In order to avert any specific choices, one can use the general form of the Hamiltonian originally proposed by Von Roos [25]. In [26], by choosing the position-dependent mass $m(\vec{r}) = \frac{m_0}{f(\vec{r})^2}$, where m_0 is a constant mass and $f(r)$ represents a deforming function,the authors obtain a new form of the Hamiltonian, and in a special case, that Hamiltonian reduce to the most common BenDaniel-Duke form [27].

In spherical coordinates $\vec{r} = \{r = ||\vec{r}||, \theta, \varphi\}$ with $f(\vec{r}) = f(r)$, separation of variables is customary used to obtain the wave function as $\psi(r,\theta,\varphi) = \frac{1}{r}\frac{U(r)}{f(r)}Y_{(\ell)}^{(\Lambda)}(\theta,\varphi)$, with $Y_{(\ell)}^{(\Lambda)}(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$, and with a potential of the form [26]

$$V(r,\theta,\varphi) = V_1(r) + \frac{f(r)^2}{r^2}V_2(\theta) + \frac{f(r)^2}{r^2\sin^2(\theta)}V_3(\varphi), \quad (1)$$

where $V_1(r)$, $V_2(\theta)$ and $V_3(\varphi)$ are arbitrary functions depending on specific arguments.

Then, the position-dependent-mass Schrödinger equation with the non-central potential defined in Eq. (1) can be transformed into a separate system in all three coordinates as shown in [26]:

$$\left[\frac{d^2}{dr^2} + \frac{2m_0}{\hbar^2}\left(\frac{E - V_1(r)}{f(r)^2}\right) - \frac{L^2}{r^2} - \bar{F}(r,\lambda,\delta)\right]U(r) = 0, r \in [0,\infty], \quad (2)$$

where $\bar{F}(r,\lambda,\delta) = \frac{(2-\delta-\lambda)}{f(r)}\left(\frac{f''(r)}{2} + \frac{f'(r)}{r}\right) \times \left(\left(\frac{1}{2}-\delta\right)\left(\frac{1}{2}-\lambda\right) - \frac{1}{4}\right)\left(\frac{f'(r)}{f(r)}\right)^2$,

$$\left[\frac{d^2}{d\theta^2} + \cot(\theta)\frac{d}{d\theta} + L^2 - \frac{\Lambda^2}{\sin^2(\theta)} - \frac{2m_0}{\hbar^2}V_2(\theta)\right]\Theta(\theta) = 0, \theta \in [0,\pi], \quad (3)$$

$$\left[\frac{d^2}{d\varphi^2} - \frac{2m_0}{\hbar^2}V_3(\varphi) + \Lambda^2\right]\Phi(\varphi) = 0,\ \varphi \in [0,2\pi], \quad (4)$$

with Λ^2 and $L^2 = \ell(\ell+1)$ being real and dimensionless separation constants. The components of the wavefunction are also constrained to satisfy the boundary conditions, $U(0) = U(\infty) = 0$ for the bound states, or $U(0) = 0$ for the continuous states; $\Phi(\varphi) = \Phi(\varphi + 2\pi)$, while $\Theta(0)$ and $\Theta(\pi)$ are finite.

III. SCATTERING STATE SOLUTIONS AND PHASE SHIFTS

In this section, we consider a particle influenced by a new non-central potential, dubbed the double-ring-shaped polynomial field potential, which is obtained from Eq. (1) with

$$V_1(r) = a + b\cdot r + c\cdot r^2,, \quad (5)$$

$$V_2(\theta) = \left(\frac{B}{\sin^2(\theta)} + \frac{A(A-1)}{\cos^2(\theta)}\right), \quad (6)$$

$$V_3(\varphi) = \left(\frac{\alpha^2 D(D-1)}{\sin^2(\alpha\varphi)} + \frac{\alpha^2 C(C-1)}{\cos^2(\alpha\varphi)}\right), \quad (7)$$

where the parameters are chosen as $A, C, D > 1; a, b, B \geq 0; c = \frac{1}{2}m_0\omega^2$, $\alpha = 1, 2, 3, \cdots$. When $a = b = 0$ and $D = C = 1$, the potentia reduces to a double-ring-shaped oscillator potential. Also, when $a = b = B = 0$ and $A = C = D = 1$, it reduces to a spherical oscillator potential, which is considered as one of the most important models in classical and quantum physics. In the subsequent subsections, we are going to study the scattering states of the Schrödinger equation with the double-ring-shaped polynomial field potential in spherical coordinates.

1. Exact Solutions of the First Angular Equation

We start our investigation with the angular, φ, part of the Schrödinger equation. After introducing the shape form of the potential shown in Eq. (7) into Eq. (4), we get

$$\left[\frac{d^2}{d\varphi^2}+\Lambda^2 - \frac{2m_0}{\hbar^2}\left(\frac{\alpha^2 D(D-1)}{\sin^2(\alpha\varphi)} + \frac{\alpha^2 C(C-1)}{\cos^2(\alpha\varphi)}\right)\right]\Phi(\varphi)=0. \quad (8)$$

With a new variable $x=\sin(\alpha\varphi)^2$, this equation transforms into

$$\frac{d^2\Phi(x)}{dx^2}+\frac{\frac{1}{2}-x}{x(1-x)}\frac{d\Phi(x)}{dx}+\frac{(-\xi_1^2x^2+\xi_2^2x-\xi_3^2)}{x^2(1-x)^2}\Phi(x)=0, \quad (9)$$

with

$$\xi_1^2=\frac{\Lambda^2}{4\alpha^2}, \quad (10)$$

$$\xi_2^2=\frac{m_0}{2\hbar^2}\left(D(D-1)-C(C-1)\right)+\frac{\Lambda^2}{4\alpha^2}, \quad (11)$$

$$\xi_3^2=\frac{m_0}{2\hbar^2}D(D-1). \quad (12)$$

According to the Nikiforov-Uvarov procedure, the resulting energy eigenvalues are

$$n_\varphi^2+(2n_\varphi+1)\left(\left(\frac{1}{16}+\left(\xi_1^2+\xi_3^2-\xi_2^2\right)\right)^{\frac{1}{2}}+\left(\frac{1}{16}+\xi_3^2\right)^{\frac{1}{2}}+\frac{1}{2}\right)+2\left(\frac{1}{16}+\left(\xi_1^2+\xi_3^2-\xi_2^2\right)\right)^{\frac{1}{2}}\left(\frac{1}{16}+\xi_3^2\right)^{\frac{1}{2}} + \left(2\xi_3^2-\xi_2^2-\frac{1}{8}\right)=0. \quad (13)$$

Replacing ξ_1, ξ_2 and ξ_3 by their expressions given in Eq. (10), Eq. (11) and Eq. (12) respectively, we finally derive the exact formula for Λ:

$$\Lambda=\pm\alpha\left(\frac{\sqrt{1+\frac{8m_0C(C-1)}{\hbar^2}}}{2}+\frac{\sqrt{1+\frac{8m_0D(D-1)}{\hbar^2}}}{2}+2n_\varphi+1\right),\ n_\varphi=0,1,2,\cdots, \quad (14)$$

which exactly reproduce the result reported in [26]. The corresponding eigenfunctions of Eq. (9) read as

$$\Phi(x)=x^{\frac{1}{2}+\left(\frac{1}{16}+\xi_3^2\right)^{\frac{1}{2}}}(1-x)^{\frac{1}{4}+\left(\frac{1}{16}+\xi_1^2+\xi_3^2-\xi_2^2\right)^{\frac{1}{2}}}P_{n_\varphi}^{\left(\left(\frac{1}{4}+4\xi_3^2\right)^{\frac{1}{2}},\left(\frac{1}{4}+4\left(\xi_1^2+\xi_2^2-\xi_3^2\right)\right)^{\frac{1}{2}}\right)}(1-2x), \quad (15)$$

where $P_n^{(a,b)}(z)$ is the generalized Jacobi functions.

2. Exact Solutions of the Second Angular Equation

The substitution of the potential in Eq. (5) into Eq. (2) leads to the following differential equation:

$$\left[\frac{d^2}{d\theta^2}+\cot(\theta)\frac{d}{d\theta}+L^2-\frac{\Lambda^2}{\sin^2(\theta)} - \frac{2m_0}{\hbar^2}\left\{\frac{B}{\sin^2(\theta)}+\frac{A(A-1)}{\cos^2(\theta)}\right\}\right]\Theta(\theta)=0. \quad (16)$$

To solve this equation, we also introduce the transformation $z=\cos(\theta)^2$, and obtain

$$\frac{d^2\Theta(z)}{dz^2}+\frac{1-\frac{3}{2}z}{z(1-z)}\frac{d\Theta(z)}{dz}+\frac{\left(-\chi_1^2z^2+\chi_2^2z-\chi_3^2\right)}{z^2(1-z)^2}\Theta(z)=0, \quad (17)$$

with

$$\chi_1^2=\frac{L^2}{4}=\frac{\ell(\ell+1)}{4}, \quad (18)$$

$$\chi_2^2=\frac{m_0}{2\hbar^2}\left(B-A\left(A-1\right)\right)+\frac{1}{4}\left(L^2+\Lambda^2\right), \quad (19)$$

$$\chi_3^2=\frac{m_0}{2\hbar^2}B+\frac{\Lambda^2}{4}. \quad (20)$$

Like Eq. (9), the eigenfunctions of Eq. (17) are the generalized Jacobi functions:

$$\Theta(z) = z^{\chi_3}(1-z)^{\frac{1}{4}+\left(\frac{1}{16}+\chi_1^2+\chi_3^2-\chi_2^2\right)^{\frac{1}{2}}} P_{n_\theta}^{\left(2\chi_3,\left(\frac{1}{4}+4\left(\chi_1^2+\chi_2^2-\chi_3^2\right)\right)^{\frac{1}{2}}\right)}(1-2z), \tag{21}$$

and the corresponding eigenvalues are solutions of the equation

$$\frac{1}{2}n_\theta + n_\theta^2 + (2n_\theta+1)\left(\left(\frac{1}{16}+\chi_1^2+\chi_3^2-\chi_2^2\right)^{\frac{1}{2}} + \chi_3 + \frac{1}{4}\right) + 2\chi_3\left(\frac{1}{16}+\chi_1^2+\chi_3^2-\chi_2^2\right)^{\frac{1}{2}} + 2\chi_3^2 - \chi_2^2 = 0. \tag{22}$$

Replacing χ_1, χ_2 and χ_2 by their expressions shown in Eq. (18), Eq. (19) and Eq. (20), respectively, we finally obtain the full expression for ℓ:

$$\ell = \frac{1+\sqrt{1+\frac{8m_0A(A-1)}{\hbar^2}}}{2} + \sqrt{\Lambda^2+\frac{2m_0B}{\hbar^2}} + 2n_\theta,$$
$$n_\theta = 0, 1, 2, \cdots, \tag{23}$$

which again coincides with the formula derived in [26] by using the asymptotic iteration method.

3. SCATTERING PHASE SHIFTS

In order to study the scattering states and the phase shifts in the problem of a position-dependent-mass Schrödinger equation with a double-ring-shaped polynomial field potential given by Eq.(1), we must define the deformation function $f(r)$. Thus, in this section, we use a simple linear representation [26]

$$f(r) = 1 + f_0 r. \tag{24}$$

By substituting $f(r)$ into Eq. (2) and by using the potential in Eq. (5), the confluent form of Heun's differential equation show up:

$$\left[\frac{d^2}{dr^2} + \frac{2m_0}{\hbar^2(1+f_0r)^2}\left(E-a-cr^2-br - \frac{\hbar^2}{2m_0}P\right) - \frac{Q}{r(1+f_0r)} - \frac{L^2}{r^2}\right]U(r) = 0, \tag{25}$$

with

$$P = \left[\left(\frac{1}{2}-\lambda\right)\left(\frac{1}{2}-\delta\right)-\frac{1}{4}\right]f_0,$$
$$Q = [2-\delta-\lambda]\,f_0. \tag{26}$$

This equation is not easy to solve; however because we are dealing with scattering states, we can safely neglect the in front of the term f_0r; in Eq. (25) with $f_0 > 0$. Consequently, the above Heun's equation simplifies to the following differential equation:

$$\left[\frac{d^2}{dr^2} + \left(-\frac{\ell'(\ell'+1)}{r^2} + \bar{K}^2 + \frac{2\bar{\Lambda}}{r}\right)\right]U_{n,\ell'}(r) = 0, \tag{27}$$

with

$$\ell'(\ell'+1) = \ell(\ell+1) - \frac{2m_0}{\hbar^2}\left(\frac{E-a}{f_0^2}\right) + \left(\frac{1}{2}-\delta\right)\left(\frac{1}{2}-\lambda\right) - (\lambda+\delta) + \frac{7}{4}, \tag{28}$$

$$\bar{\Lambda} = -\frac{m_0}{\hbar^2}\frac{b}{f_0^2}, \tag{29}$$

$$\bar{K}^2 = -\frac{m_0}{\hbar^2}\frac{2c}{f_0^2}. \tag{30}$$

Notice here that the ℓ' parameter plays the role of the orbital angular momentum in problems with spherical central potentials. Having in mind the boundary conditions of the scattering states, *i.e.*, $U_{n,\ell'}(r=0) = 0$, we use the following ansatz for the asymptotic behavior of the wave function at the origin [28]:

$$U_{n,\ell'}(r) = A\cdot(\bar{K}r)^{\ell'+1}e^{i\bar{K}r}\xi_{n,\ell'}(r). \tag{31}$$

Insertion of Eq. (31) into Eq. (27) results in

$$\left[r\frac{d^2}{dr^2} + \left(2\ell'+2i\bar{K}r+2\right)\frac{d}{dr} + \left(2\bar{\Lambda}+2i\bar{K}(\ell'+1)\right)\right]\xi_{n,\ell'}(r) = 0. \tag{32}$$

If, in addition, we introduce a new variable $s = -2i\bar{K}r$, then Eq. (32) can be alternatively written as

$$\left[s\frac{d^2}{ds^2} + (2\ell'+2-s)\frac{d}{ds} + \left(\ell'+1-i\frac{\bar{\Lambda}}{\bar{K}}\right)\right]\xi_{n,\ell'}(s) = 0, \tag{33}$$

with $s = |s|e^{-i\frac{\pi}{2}}$. Eq. (33) is just the confluent Hypergeometric equation. The general form of confluent hypergeometric can be written as

$$z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0.$$

where a and b are constant, the solution to the above equation can be written with the aid of Kummer's functions as

$$M(a,b,z) = \sum_{n=0}^{\infty}\left(\frac{a^{(n)}z^n}{b^{(n)}n!}\right) = {}_1F_1(a,b,z),$$

Comparing (33) with the general form of the confluent hypergeometric differential equation results in, as $r \to 0$,

$$\xi_{n,\ell'}(s) = {}_1F_1\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}, 2\ell' + 2, -2i\bar{K}r\right). \quad (34)$$

Therefore, our analytical expression for the radial wave function for the scattering states that are obtained by substituting Eq. (34) into Eq. (31), as follows:

$$\begin{aligned} U_{n,\ell'}(r) &= A \cdot (\bar{K}r)^{\ell'+1} e^{i\bar{K}r} {}_1F_1 \\ & \left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}, 2\ell' + 2, -2i\bar{K}r\right). \end{aligned} \quad (35)$$

Now, we want to obtain the asymptotic behavior of the wave function for $r \to 0$, and then calculate the normalization constant and the phase shifts. To this end, we use the transformation formulae for the confluent hypergeometric function when $s \to \infty$:

$${}_1F_1(\alpha, \gamma, s) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^s s^{\alpha-\gamma} + \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} e^{\pm i\pi\alpha} s^{-\alpha}, \quad (36)$$

where "+" and "−" correspond to $arg(s) \in -\pi/2, 3\pi/2$ and $arg(s) \in -3\pi/2, \pi/2$, respectively. By with the substitution $s = |s|e^{-i\frac{\pi}{2}}$, Eq. (36) can be re-expressed as

$$\begin{aligned} {}_1F_1(\alpha, \gamma, s) &= \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^s |s|^{\alpha-\gamma} e^{-i(\alpha-\gamma)\pi/2} \\ &+ \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} e^{i\pi\alpha/2} |s|^{-\alpha}, \end{aligned} \quad (37)$$

from which we obtain

$$\begin{aligned} {}_1F_1\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}, 2\ell' + 2, -2i\bar{K}r\right) &= \frac{\Gamma(2\ell'+2)}{\Gamma(\ell'+1-i\frac{\bar{\Lambda}}{\bar{K}})} e^{-2i\bar{K}} \left(2\bar{K}r\right)^{-\left(\ell'+1+i\bar{\Lambda}/\bar{K}\right)} e^{i\left(\ell'+1+i\bar{\Lambda}/\bar{K}\right)\pi/2} \\ &+ \frac{\Gamma(2\ell'+2)}{\Gamma(\ell'+1+i\frac{\bar{\Lambda}}{\bar{K}})} \left(2\bar{K}r\right)^{-\left(\ell'+1-i\bar{\Lambda}/\bar{K}\right)} e^{-i\left(\ell'+1-i\bar{\Lambda}/\bar{K}\right)\pi/2}. \end{aligned} \quad (38)$$

Because

$$\Gamma\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}\right) = \left|\Gamma\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}\right)\right| e^{i\delta'}, \quad \delta'_\ell = arg\left(\Gamma\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}\right)\right) \quad (39)$$

and

$$\Gamma\left(\ell' + 1 + i\frac{\bar{\Lambda}}{\bar{K}}\right) = \left|\Gamma\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}\right)\right| e^{-i\delta'}, \quad (40)$$

where δ' is a real number, Eq. (38) becomes

$${}_1F_1\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}, 2\ell' + 2, -2i\bar{K}r\right) = \frac{\Gamma(2\ell'+2)}{\Gamma(\ell'+1-i\frac{\bar{\Lambda}}{\bar{K}})} \left(\frac{e^{-\frac{\bar{\Lambda}\pi}{2\bar{K}}} \cdot e^{-i\bar{K}r}}{\left(2\bar{K}r\right)^{\ell'+1}}\right) \times 2\sin\left(\bar{K}r + \bar{\Lambda}\ln(2\bar{K}r)/\bar{K} + \delta' - \ell'\pi/2 - \pi/2\right).$$

By putting Eq. (41) into Eq. (35), we get

$$U_{n,\ell'}(r \to \infty) = A \cdot \frac{\Gamma(2\ell'+2)}{\Gamma(\ell'+1-i\frac{\bar{\Lambda}}{\bar{K}})} \left(\frac{e^{-\frac{\bar{\Lambda}\pi}{2\bar{K}}}}{(2)^{\ell'+1}}\right) 2\sin\left(\bar{K}r + \bar{\Lambda}\ln(2\bar{K}r)/\bar{K} + \delta' - \ell'\pi/2\right). \quad (41)$$

On the other hand, by using the asymptotic behavior

$$U_{n,\ell}(r \to \infty) = 2\sin\left(\bar{K}r + \bar{\Lambda}\ln(2\bar{K}r)/\bar{K} + \delta_\ell - \ell\pi/2\right) \quad (42)$$

and by comparing the arguments of the sine terms in Eqs. (41) and (42), one can derive the phase shifts

$$\delta_\ell = \frac{\pi(\ell - \ell')}{2} + \delta'_\ell, \quad (43)$$

where ℓ' is given by Eq. (28). The normalization constant can also be evaluated by comparing the coefficients of the sine terms in Eqs. (41) and (42) as

$$A = \frac{\Gamma\left(\ell' + 1 - i\frac{\bar{\Lambda}}{\bar{K}}\right)}{\Gamma(2\ell'+2)} 2^{(\ell'+1)} e^{\frac{\pi\bar{\Lambda}}{2\bar{K}}}. \quad (44)$$

IV. CONCLUSION

In this paper, we have considered the time-independent Schrödinger equation with a position-dependent effective mass in a non-central potential. Using the potential form proposed in [26], we separated the deformed Schrödinger equation in all coordinates. Then the radial solution, as well as the exact analytical angular solution, is obtained. We have also studied the scattering states of the deformed Schrödinger equation under a non-central effective potential and derived the energy eigenvalues and the normalization constant of the radial wave functions, as well as the scattering phase shifts.

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