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Harmonic and anharmonic quantum-mechanical oscillators in noninteger dimensions

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ABSTRACT

We present new results for time-independent solutions for a Schrödinger equation with noninteger dimension by considering different, harmonic and anharmonic, forms for the potential energy. The solutions obtained for these potentials are exact and expressed in terms of the special functions such as Laguerre and Gegenbauer polynomials, associated Legendre functions, and hypergeometric functions. Graphical comparison of the probability density function with the ones for two-dimensional and three-dimensional case is given. We derive the mean values $\overline{r^\beta \sin^\delta\theta}$ for the harmonic oscillator in noninteger dimensions, which may be of interest in the perturbation theory for calculation of energy corrections. We consider anharmonic Kratzer potential energy function and we obtain bound and scattering states. Exact results in case of different forms of θ-dependent potentials are presented. In addition, they can be connected to rich variety of situations which enable us to model anisotropic interactions in real space.

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1. Introduction

The idea of fractional dimension introduced by Hausdorff has attracted the attention of several researchers and became widely used after the pioneers works of Mandelbrot [1] about the fractal nature of different phenomena in many fields of science. In this context, extensions of the evolution equations to noninteger (fractional) dimensional space have received special attention, in particular the Schrödinger equation [2–12] due to their successful applications in several contexts. For instance, optical spectra and excitonic properties of anisotropic systems, the excitonic states and absorption spectra in quantum wells [13–15], the study of donor and acceptor properties in semiconductor superlattices [16], quantum-confined semiconducting heterostructures [17], non-crystalline solids [18,19], the study of impurity levels in semiconducting heterostructures [20], polaron confined to a rectangular quantum well [21], are just a few examples of phenomena that could be adequately modeled by noninteger partial differential equations. These situations have been investigated by different approaches. One of them involves the presence of fractional derivatives [7] and the other uses the modified spatial operator [22]:

$$\tilde{\nabla}^2\psi(r,\theta) \equiv \frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left[r^{\alpha-1}\frac{\partial}{\partial r}\psi(r,\theta)\right] + \frac{1}{r^2\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left[\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\psi(r,\theta)\right], \qquad (1)$$

where α represents a noninteger dimension. Note that $\alpha = 2$ recovers the Laplacian in polar coordinates and $\alpha = 3$ leads us to the Laplacian in spherical coordinates, without the angular variable φ. The noninteger dimension present in Eq. (1) can be related to the degree of confinement of the system. In this sense, studies of He [13,14] enables, the originally anisotropic or confined interactions in three-dimensional space, to consider as isotropic and unconfined interactions in an environment of fractional dimension. Similarly, in [21], a noninteger-dimensional space approach was applied to the case of a polaron confined in a rectangular quantum well, where the real confined polaron plus quantum well system in real space is investigated as an unconfined polaron in noninteger-dimensional bulk. Spatial operator of form (1) was also used by Eid et al. in case of Coulomb potential energy function of form $\frac{1}{r^{\beta-2}}$ $(2 \leqslant \beta \leqslant 4)$ [2], and in case of a fractional-dimensional oscillator [3], as well as by Lucena et al. [5] and Martins et al. [6], to investigate the fractional diffusion equation and time fractional Schrödinger equation in noninteger dimensions, respectively. It is worth to mention that the generalization of Laplacian and the use of fractional operators for the modeling of diffusion on fractals have been studied in earlier works by

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O'Shaugnessy and Procaccia [23], Giona and Roman [24], and Metzler et al. [25].

In this paper, we present new results for the solutions, in the noninteger dimension scenario, of the time-independent Schrödinger equation with the following form:

$$-\frac{\hbar^2}{2M}\tilde{\nabla}^2\psi(r,\theta)+U(r)\psi(r,\theta)=E\psi(r,\theta), \tag{2}$$

where $U(r)$ is the potential energy function, $h=2\pi\hbar$ is the Planck's constant, M is the mass of oscillator, and E is the energy. Harmonic, as well as anharmonic potentials of the form proposed by Kratzer, and ring shape potentials are considered. The free case is recovered for $U(r)=0$. The wave functions are obtained analytically, and the eigenvalues are analyzed. The mean values $r^\beta\sin^\delta\theta$ for the harmonic oscillator in noninteger dimensions are derived. In addition, scattering states for the Schrödinger equation in noninteger dimensions in case of Kratzer potential energy function are obtained, and asymptotic behavior of the solution is analyzed. We give graphical presentation of the probability density function (PDF) and we compare with those in case of $\alpha=2$ and $\alpha=3$. We note that one may consider time-dependent equation with a power-law form for the diffusion coefficient. Such approach poses some interesting issues. For example, diffusion on fractals is ergodic in the sense that long time and ensemble averages are equivalent [26,27], and, in contrast, diffusion with space-dependent diffusion coefficients is weakly non-ergodic [28].

2. Schrödinger equation with noninteger dimensions

We start our analysis by substituting the spatial operator (1) in Eq. (2), which yields

$$\begin{aligned}&-\frac{\hbar^2}{2M}\left[\frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\right)\right.\\&\left.\quad+\frac{1}{r^2\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left(\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\right)\right]\psi(r,\theta)+U(r)\psi(r,\theta)\\&=E\psi(r,\theta).\end{aligned} \tag{3}$$

This equation can be solved by using the method of separation of variables, by representing function $\psi(r,\theta)$ in a form $\psi(r,\theta)=R(r)\Theta(\theta)$. Applying this procedure, one obtains

$$\begin{aligned}&\frac{r^{3-\alpha}}{R(r)}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^{\alpha-1}\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right]+\frac{2Mr^2}{\hbar^2}\left[E-U(r)\right]\\&=-\frac{1}{\Theta(\theta)\sin^{\alpha-2}\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left[\sin^{\alpha-2}\theta\frac{\mathrm{d}\Theta(\theta)}{\mathrm{d}\theta}\right]=m_\alpha^2,\end{aligned} \tag{4}$$

where $m_\alpha^2>0$ is a separation constant connected to the eigenvalue of the eigenfunction $\Theta(\theta)$. From Eq. (4) follows that

$$\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\frac{\alpha-1}{r}\frac{\mathrm{d}R(r)}{\mathrm{d}r}+\left[\frac{2ME}{\hbar^2}-\frac{m_\alpha^2}{r^2}-\frac{2M}{\hbar^2}U(r)\right]=0, \tag{5}$$

$$\frac{\mathrm{d}^2\Theta(\theta)}{\mathrm{d}\theta^2}+\frac{\alpha-2}{\tan\theta}\frac{\mathrm{d}\Theta(\theta)}{\mathrm{d}\theta}+m_\alpha^2\Theta(\theta)=0. \tag{6}$$

The solution of Eq. (5) depends on the potential energy function. Eq. (6) for the variable θ is the same, it does not depend on the potential energy function $U(r)$. Different situations, as we will see later, appear in case of θ-dependent potential energy function $U(r,\theta)$ which will be worked out in the next sections. In order to solve Eq. (6), we introduce a new variable $x=\cos\theta$ to simplify the calculations. Thus, it becomes

$$\frac{\mathrm{d}^2\Theta(x)}{\mathrm{d}x^2}+\frac{(\alpha-1)x}{x^2-1}\frac{\mathrm{d}\Theta(x)}{\mathrm{d}x}-\frac{m_\alpha^2}{x^2-1}\Theta(x)=0. \tag{7}$$

The solutions of this differential equation can be represented in terms of the Gegenbauer polynomials $C_n^\nu(x)$ (Appendix A), i.e.

$$\Theta(\cos\theta)=C_n^{\frac{\alpha}{2}-1}(\cos\theta), \tag{8}$$

where $m_\alpha^2=n(n+\alpha-2)$, i.e., $n=-(\frac{\alpha}{2}-1)+\sqrt{(\frac{\alpha}{2}-1)^2+m_\alpha^2}$. For planar oscillator $\alpha=2$ ($m_\alpha=m_l$ – magnetic quantum number) we obtain $n=|m_l|$ and $\Theta(\theta)\to\Phi(\varphi)=e^{\imath m_l\varphi}$, where φ is the azimuthal coordinate. For spherical oscillator $\alpha=3$ ($m_\alpha^2=l(l+1)$, l-orbital quantum number) we obtain $n=l$ and $\Theta(\theta)=C_l^{\frac{1}{2}}(\cos\theta)=P_l(\cos\theta)$, where $P_l(x)$ are the Legendre polynomials [29].

Remark 1. This result can be obtained by introducing the substitution $z=\frac{1-x}{2}$. Thus, Eq. (7) yields a hypergeometric equation (Appendix C)

$$z(1-z)\frac{\mathrm{d}^2\Theta(z)}{\mathrm{d}z^2}+\left[\frac{\alpha-1}{2}-(\alpha-1)z\right]\frac{\mathrm{d}\Theta(z)}{\mathrm{d}z}+m_\alpha^2\Theta(z)=0, \tag{9}$$

which solution, by using relation (49), is given by

$$\begin{aligned}\Theta(x)&=F\left(-n,n+2\left(\frac{\alpha}{2}-1\right);\left(\frac{\alpha}{2}-1\right)+\frac{1}{2};\frac{1-x}{2}\right)\\&=\mathrm{Const}\cdot C_n^{\frac{\alpha}{2}-1}(x),\end{aligned} \tag{10}$$

where $n=-(\frac{\alpha}{2}-1)+\sqrt{(\frac{\alpha}{2}-1)^2+m_\alpha^2}$, i.e. $m_\alpha^2=n(n+\alpha-2)$.

Now, we address our discussion, in the next sections, for the solution of the radial equation when different forms of the potential energy function $U(r)$ are considered. The situation characterized by $U(r,\theta)$ will be also considered.

2.1. Harmonic oscillator

Let us first consider the solution of (5) for the harmonic oscillator potential energy function, i.e., $U(r)=M\omega^2r^2/2$, where ω is the classical frequency of the oscillator. Such potential energy function is used in the analysis of spreading of the wave packet of a time fractional Schrödinger equation in noninteger dimensions [6]. By substituting in Eq. (5), one obtains

$$\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\frac{\alpha-1}{r}\frac{\mathrm{d}R(r)}{\mathrm{d}r}+\left(\mathcal{A}-\frac{m_\alpha^2}{r^2}-\mathcal{B}r^2\right)R(r)=0, \tag{11}$$

where $\mathcal{A}=2ME/\hbar^2$ and $\mathcal{B}=M^2\omega^2/\hbar^2$. Representing the radial function as $R(r)=r^\sigma F(r)$, where $\sigma=-(\frac{\alpha}{2}-1)$ we obtain differential equation of form

$$\frac{\mathrm{d}^2F(r)}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}F(r)}{\mathrm{d}r}+\left[\mathcal{A}-\frac{m_\alpha^2+(\frac{\alpha}{2}-1)^2}{r^2}-\mathcal{B}r^2\right]F(r)=0. \tag{12}$$

The solution for this equation is [30]

$$F(r)=\mathcal{N}\frac{n_r!\Gamma(n+\frac{\alpha}{2})}{\Gamma(n_r+n+\frac{\alpha}{2})}r^{n+\frac{\alpha}{2}-1}e^{-\frac{1}{2}\frac{r^2}{r_0^2}}L_{n_r}^{(n+\frac{\alpha}{2}-1)}\left(\frac{r^2}{r_0^2}\right), \tag{13}$$

where $n=-(\frac{\alpha}{2}-1)+\sqrt{(\frac{\alpha}{2}-1)^2+m_\alpha^2}$, n_r is the radial quantum number having the values $n_r=0,1,2,\ldots$, $r_0^2=1/\sqrt{\mathcal{B}}=\hbar/(M\omega)$, $\mathcal{N}$ is the normalization constant, and $L_n^{(m)}(x)$ are Laguerre

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