The harmonic oscillator in a space with a screw dislocation

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HIGHLIGHTS

- Quantum-mechanical systems with screw dislocation are receiving considerable interest.
- The harmonic oscillator with screw dislocation is not completely separable.
- The screw dislocation removes the degeneracy.
- The variational method is useful for obtaining eigenvalues and eigenfunctions.
- The spectrum exhibits a rich structure of avoided crossings.

ARTICLE INFO

ABSTRACT

We obtain the eigenvalues of the harmonic oscillator in a space with a screw dislocation. By means of a suitable nonorthogonal basis set with variational parameters we obtain sufficiently accurate eigenvalues for an arbitrary range of values of the space-deformation parameter. The energies exhibit a rich structure of avoided crossings in terms of such model parameter.

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1. Introduction

Space dislocations have been useful for the description of a variety of physical phenomena. Among such applications we mention an analysis of the influence of frozen-in topological defects in a crystal on the long-wavelength quantum states of a particle [1], a study of electrons moving in a magnetic

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field in the presence of a screw dislocation [2], the scattering of electrons on a screw dislocation [3], an investigation of the quantum scattering of an electron by a screw dislocation with an internal magnetic flux [4], a geometric model for the explanation of the origin of the observed shallow levels in semiconductors threaded by a dislocation density [5], the influence of the Aharonov–Casher effect on the Dirac oscillator in three different scenarios of general relativity [6], an investigation of torsion and noninertial effects on a spin-1/2 quantum particle in the nonrelativistic limit of the Dirac equation [7], a study of ac electronic transport in semiconductor crystals with a screw dislocation [8], a two-dimensional electron gas on a cylindrical surface with a screw dislocation [9], a study of spin currents induced by topological screw dislocation and cosmic dispiration [10], an analysis of a relativistic scalar particle with a position-dependent mass in a spacetime with a space-like dislocation [11], a study of the influence of a screw dislocation on the energy levels and the wavefunctions of an electron confined in a two-dimensional pseudoharmonic quantum dot under the influence of an external magnetic field and an Aharonov–Bohm field [12] and the effect of a screw dislocation on an anharmonic oscillator [13].

The present paper is motivated by those of Filgueiras et al. [12] and Bakke [13] who solve the Schrödinger equation with a screw dislocation. In the former case the authors choose a deformed potential $V_d(\rho)$ and a scalar pseudoharmonic interaction $V_{conf}(\rho)$, $\rho^2 = x^2 + y^2$, so that the motion of the electron along the z-axis is free. Under these conditions the resulting eigenvalue equation is separable and exactly solvable. Later the authors consider that the electrons are confined by infinite walls at $z = 0$ and $z = d$ and claim that the eigenvalue equation is still separable. In the latter case the author chooses a potential $V(\rho)$ so that the motion of the particle is unbounded along the z direction and the spectrum continuous. Here we choose one of the simplest confining potentials, the three-dimensional harmonic oscillator, and obtain approximate eigenvalues of the resulting nonseparable deformed Schrödinger equation. In Section 2 we develop the main equations for the model, in Section 3 we first obtain approximate results by means of a simple variational ansatz that later use as the starting point of a more accurate Rayleigh–Ritz variational calculation. In this section we show results for different quantum numbers in a range of values of the dislocation parameter. Finally, in Section 4 we summarize the main results and draw conclusions.

2. The model

Some kind of topological defects are described by means of the line element

$$ds^2 = g_{ij}dy^i dy^j, \tag{1}$$

where g_{ij} are the elements of the metric tensor, $\{y^i\}$ is a suitable set of curvilinear coordinates and summation on repeated indices is assumed. The Laplacian in such a space is given by

$$\nabla^2 = \frac{1}{\sqrt{|\mathbf{g}|}} \partial_i \sqrt{|\mathbf{g}|} g^{ij} \partial_j, \tag{2}$$

where $|\mathbf{g}|$ is the determinant of the matrix $\mathbf{g} = (g_{ij})$, $\partial_i = \frac{\partial}{\partial y^i}$ and $g^{ij}g_{jk} = \delta^i_k$. Valanis and Panoskaltsis [14] derive expressions for a wide variety of deformations in a material body.

The Hamiltonian operator for a particle of mass m moving in such a space under the effect of a potential-energy function $V(\mathbf{r})$ is

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}). \tag{3}$$

In order to solve the Schrödinger equation for H it is convenient to choose a convenient set of units. We choose a set of dimensionless coordinates $\mathbf{r}' = \mathbf{r}/L$, where L is an arbitrary length, and rewrite the Hamiltonian operator in dimensionless form as

$$\frac{2mL^2}{\hbar^2}H = \nabla'^2 + v(\mathbf{r}'), \quad v(\mathbf{r}') = \frac{2mL^2}{\hbar^2}V(L\mathbf{r}'), \tag{4}$$

where $\nabla'^2 = L^2 \nabla^2$

Following Filgueiras et al. [12] and Bake [13] we choose the screw dislocation

$$ds^2 = d\rho^2 + \rho^2 d\phi^2 + (dz + \eta d\phi)^2,$$ (5)

where $\rho = \sqrt{x^2 + y^2}$, $\phi = \arctan(y/x)$ and η characterizes the torsion field (dislocation). In this case the Laplacian is

$$\nabla^2 = \frac{1}{\rho}\partial_\rho \rho \partial_\rho + \partial_z^2 + \frac{1}{\rho^2}\left(\partial_\phi - \eta\partial_z\right)^2.$$ (6)

If we choose a harmonic interaction

$$V(r) = \frac{k}{2}r^2 = \frac{k}{2}\left(\rho^2 + z^2\right),$$ (7)

and the length unit $L = \sqrt{\frac{\hbar}{m\omega}}$, $\omega = \sqrt{\frac{k}{m}}$, the dimensionless Schrödinger equation becomes

$$\left[-\frac{1}{\rho}\partial_\rho \rho \partial_\rho - \partial_z^2 - \frac{1}{\rho^2}\left(\partial_\phi - \lambda\partial_z\right)^2 + \rho^2 + z^2\right]\psi = \mathcal{E}\psi,$$

$$\mathcal{E} = \frac{2mL^2}{\hbar^2}E, \ \lambda = \frac{\eta}{L},$$ (8)

where we have omitted the primes in ρ' and z'.

If we write

$$\psi(\rho, z, \phi) = F(\rho, z)e^{im\phi}, \ m = 0, \pm1, \pm2, \ldots$$ (9)

then we are left with an equation for $F(\rho, z)$

$$\left[-\frac{1}{\rho}\partial_\rho \rho \partial_\rho - \left(1 + \frac{\lambda^2}{\rho^2}\right)\partial_z^2 + \frac{2im\lambda}{\rho^2}\partial_z + \frac{m^2}{\rho^2} + \rho^2 + z^2\right]F(\rho, z) = \mathcal{E}F(\rho, z).$$ (10)

Note that this equation is invariant under the transformations $(m \to -m, \ z \to -z)$ and $(\lambda \to -\lambda, \ z \to -z)$, therefore the eigenvalues depend on m^2 and λ^2.

When $\lambda = 0$ the equation is fully separable $F_{nkm}(\rho, z) = f_{nm}(\rho)g_k(z)$ and the energy eigenvalues $\mathcal{E}_{nkm}(0)$ are g_{nkm}-fold degenerate, where

$$\mathcal{E}_{nkm}(0) = 4n + 2k + 2|m| + 3, \ n, k = 0, 1, \ldots,$$

$$g_{nkm} = \frac{1}{2}\left(4n + 2k + 2|m|\right)\left(4n + 2k + +2|m| + 1\right).$$ (11)

Note that the dislocation removes almost all the degeneracy leaving only that coming from the z-component of the angular momentum. In what follows we use the quantum numbers n, k and $|m|$ to label the eigenvalues of the nonseparable Schrödinger equation for $\lambda > 0$. Obviously, only m is a good quantum number.

3. Variational approach

In this section we try to obtain approximate eigenvalues to Eq. (10). Our starting point is the simple (unnormalized) variational function for the states with $n = k = 0$:

$$\varphi(\rho, z) = \rho^s \exp\left(-\rho^2/2 - bz^2\right),$$ (12)

where s and b are variational parameters. A straightforward calculation shows that the minimum of

$$W(s, b) = \frac{\langle\varphi|H|\varphi\rangle}{\langle\varphi|\varphi\rangle},$$ (13)

is given by

$$s = \sqrt{b\lambda^2 + m^2}, \ \left(4b^2 - 1\right)\sqrt{b\lambda^2 + m^2} + 4b^2\lambda^2 = 0,$$ (14)
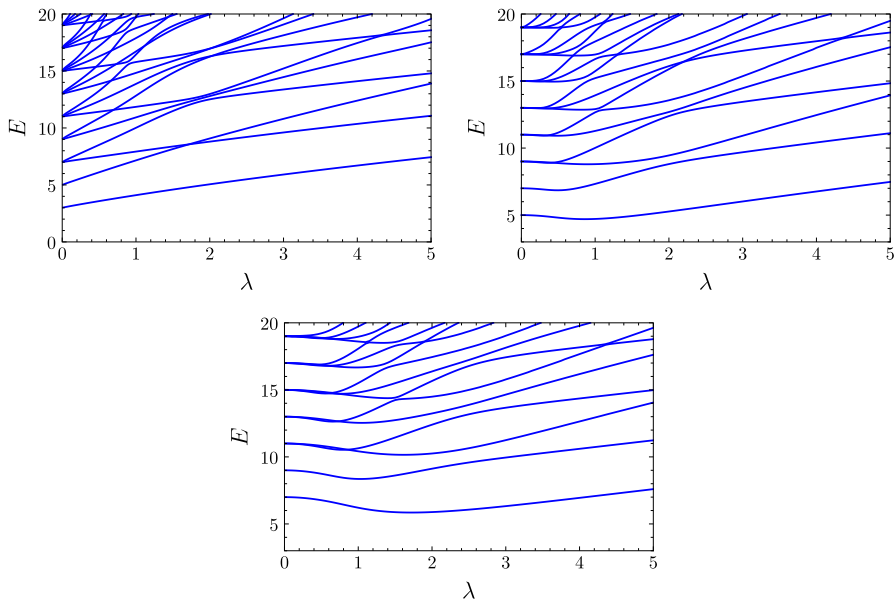
Fig. 1. Lowest eigenvalues with $|m| = 0, 1, 2$.

and the upper bound to the lowest energy for a given value of $|m|$ is

$$W = \frac{8b\sqrt{b\lambda^2 + m^2} + 4b^2 + 8b + 1}{4b}. \tag{15}$$

In order to improve the accuracy of the results and obtain the excited-state energies we apply the Rayleigh–Ritz variational method with the nonorthogonal basis set

$$\varphi(\rho, z) = \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} c_{ij} \rho^{i+s} z^j \exp\left(-\rho^2/2 - bz^2\right), \tag{16}$$

where s is given by Eq. (14). In this case we obtain the minimum of the variational integral (13) with respect to the linear parameters c_{ij} and to the nonlinear one b.

Fig. 1 shows the lowest eigenvalues $\mathcal{E}_{nkm}(\lambda)$ for $|m| = 0, 1, 2$ in the interval $0 \le \lambda \le 5$. We appreciate that the energies exhibit a rich structure of avoided crossings. Such avoided crossings take place because eigenvalues with the same quantum number m do not cross. The arguments for the noncrossing rule are similar to those for the states with the same symmetry already discussed by several authors [15–18].

Some of the avoided crossings shown in those figures may appear to be actual crossings because the eigenvalues approach each other quite closely. In order to illustrate this point, Fig. 2 shows the avoided crossings between eigenvalues in the multiplets $(\mathcal{E}_{102}, \mathcal{E}_{022})$, $(\mathcal{E}_{112}, \mathcal{E}_{032})$ and $(\mathcal{E}_{202}, \mathcal{E}_{122}, \mathcal{E}_{042})$ in somewhat more detail.

The first pair of subfigures in Fig. 2 show the eigenvalues $(\mathcal{E}_{102}, \mathcal{E}_{022})$ stemming from $\mathcal{E}(0) = 11$. The right subfigure is just an enlargement of that part of the left one corresponding to the avoided crossing. The second pair of subfigures illustrate the same feature for the pair of eigenvalues $(\mathcal{E}_{112}, \mathcal{E}_{032})$ stemming from $\mathcal{E}(0) = 13$. The last subfigure shows the triplet of states stemming from $\mathcal{E}(0) = 15$.

What is interesting in this model is that the eigenvalues of a given multiplet with a fixed value of $|m|$ exhibit avoided crossings among themselves for sufficiently small values of λ (for example $0 < \lambda < 1$). For greater values of λ there are avoided crossings between eigenvalues of different multiplets as shown in Fig. 1.
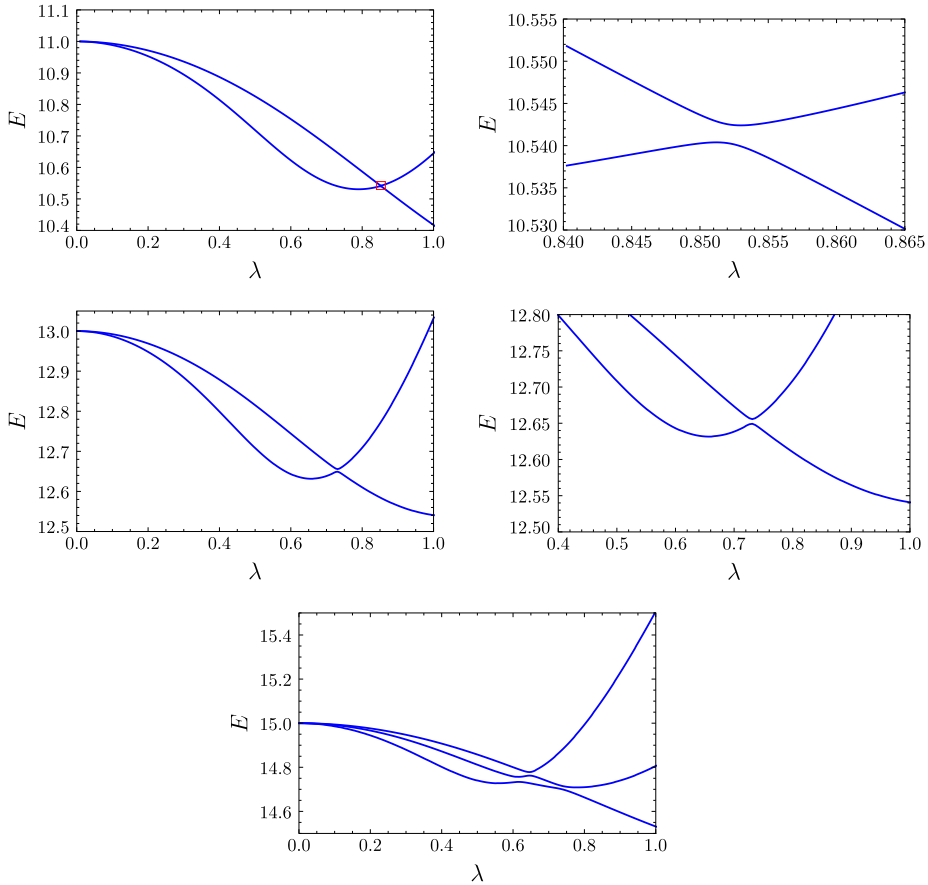
Fig. 2. Some multiplets of eigenvalues with $|m| = 2$.

4. Conclusions

As stated in the introduction this paper is motivated by those of Filgueiras et al. [12] and Bakke [13]. The main difference is that the models chosen by those authors are separable and do not reveal the possibility of avoided crossings. In addition to this, in those models the motion of the particle is unbounded in the z direction and the corresponding spectra are continuous. Filgueiras et al. [12] attempted to confine the electron in the z axis by means of a square-well potential but they did not take into account the correct boundary conditions. Their wavefunctions satisfy $\psi(\rho, \varphi, d) = e^{i\ell\pi}\psi(\rho, \varphi, 0)$, where $\psi(\rho, \varphi, 0) \neq 0$, and, consequently, their results apply to a problem with boundary conditions $\psi(\rho, \varphi, d) = \pm\psi(\rho, \varphi, 0)$ and not to the box confinement. If the walls of the square well are located at $z = 0$ and $z = d$ then the Schrödinger equation with the correct boundary conditions $\psi(\rho, \varphi, 0) = \psi(\rho, \varphi, d) = 0$ is not separable.

In this paper we have chosen a harmonic-oscillator potential in order to investigate the effect of space dislocation on the spectrum. The reason for this choice is that this potential is well known and facilitates the calculation of the matrix elements necessary for the application of the variational method. Besides, the Schrödinger equation is exactly solvable when there is no dislocation and we can therefore easily appreciate how the dislocation breaks the degeneracy. Although this model may not have a clear physical application it nevertheless shows what one may expect from a realistic model

with a confining potential and screw dislocation. Most probably such model will also exhibit some kind of structure of avoided crossings. The screw dislocation not only breaks the degeneracy but also gives rise to avoided crossings between energy levels.

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