Physics Letters A 382 (2018) 139–140

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Remark on Landau quantization, Aharonov–Bohm effect and two-dimensional pseudoharmonic quantum dot around a screw dislocation

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ARTICLE INFO

Article history:
Received 6 August 2017
Received in revised form 12 November 2017
Accepted 15 November 2017
Available online 21 November 2017
Communicated by R. Wu

Keywords:
Screw dislocation
Eigenvalue equation
Dirichlet boundary conditions
Periodic boundary conditions

ABSTRACT

We investigate 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 inside a dot and Aharonov–Bohm field inside a pseudodot. Filgueiras et al. (2016) [1] showed that the Schrödinger equation is separable in cylindrical coordinates when the motion along the z axis is unbounded. We show that it is not separable under box confinement as those authors claim but it is separable in the case of periodic boundary conditions along that axis.

In a recent paper Figueiras et al. [1] investigate 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 inside a dot and Aharonov–Bohm field inside a pseudodot. They show that the Schrödinger equation is separable in cylindrical coordinates when the motion of the electron is unbounded along the z axis and later they confine the electron into a square well with infinite walls on this axis. The purpose of this letter is to analyze the conditions for the separability of the Schrödinger equation in such physical models.

To make this letter as concise as possible we refer to the main results of Figueiras et al. [1]. The Schrödinger equation for the system is [1]

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\left(\frac{\partial}{\partial\varphi}-\beta\frac{\partial}{\partial z}+\delta\right)^2\right]\psi + \left[\frac{ieB\hbar}{2m}\left(\frac{\partial}{\partial\varphi}-\beta\frac{\partial}{\partial z}+\delta\right)+\frac{e^2B^2\rho^2}{8m}\right]\psi + \left[V_d(\rho)+V_{\mathrm{conf}}(\rho)\right]\psi = E\psi \tag{1}$$

where

$$V_d(\rho)=\frac{\hbar^2}{2ma^2}\frac{b^2}{4\pi^2\rho^2}\left(2+a^2\frac{\partial^2}{\partial z^2}\right),\qquad V_{\mathrm{conf}}(\rho)=V_0\left(\frac{\rho}{\rho_0}+\frac{\rho_0}{\rho}\right)^2 \tag{2}$$

The meaning of the parameters β, δ, B, etc is given in that paper [1]. The authors solve equation (1) by means of the ansatz

$$\psi(\rho,\varphi,z)=Ce^{il\varphi}e^{ikz}R(\rho) \tag{3}$$

where $l=0,\pm1,\pm2,\ldots$, $k\in\Re$ and C is a normalization constant. In this way we are left with an eigenvalue equation for $R(\rho)$:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{1}{\rho^2}(l-\beta k+\delta)^2-k^2\right]R(\rho) + \left[\frac{e^2B^2\rho^2}{8m}-\frac{eB\hbar}{2m}(l-\beta k+\delta)+V_0\left(\frac{\rho}{\rho_0}+\frac{\rho_0}{\rho}\right)^2\right]R(\rho) + \frac{\hbar^2}{2ma^2}\frac{b^2}{4\pi^2\rho^2}\left(2+a^2k^2\right)R(\rho)=ER(\rho) \tag{4}$$

Note that the motion of the electron along the z-axis is not bounded and the spectrum is therefore continuous as shown by the kinetic-energy term $\hbar^2k^2/(2m)$, where $-\infty<k<\infty$.

After solving this equation and discussing some of the properties of the solution the authors add another feature to the problem: "At this point, we consider the electrons on an flat interface,

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https://doi.org/10.1016/j.physleta.2017.11.014
0375-9601/

with thickness d, around a screw dislocation. They are confined by an infinite square well potential in the z-direction $(0 \leq z \leq d)$. This way, we have $k = \ell\pi/d$, where $\ell = 1, 2, \ldots$." Such confinement will obviously lead to a completely discrete spectrum. However, a square well potential with infinite walls at $z = 0$ and $z = d$ leads to the Dirichlet boundary conditions $\psi(\rho, \varphi, 0) = \psi(\rho, \varphi, d) = 0$, whereas the eigenfunction derived by the authors satisfies $\psi(\rho, \varphi, d) = e^{i\ell\pi}\psi(\rho, \varphi, 0)$, where $\psi(\rho, \varphi, 0) \neq 0$. In other words, the results derived by the authors apply to a problem with boundary conditions $\psi(\rho, \varphi, d) = \pm\psi(\rho, \varphi, 0)$ and not to the intended confinement inside a square well.

If we are going to impose Dirichlet boundary conditions on the system at $z = 0$ and $z = d$ we have to do it in equation (1) but the consequence is that the Schrödinger equation is not fully separable. In fact, the ansatz would be of the form $\psi(\rho, \varphi, z) = Ce^{il\varphi}F(\rho, z)$, where $F(\rho, 0) = F(\rho, d) = 0$. In this case we have to choose a suitable approximate method for the solution of the Schrödinger equation and we expect the eigenvalues to exhibit a more or less complicated behaviour with respect to the parameter that measures the degree of the dislocation. For example a simple harmonic oscillator in a space with a screw dislocation shows a rich structure of avoided crossings [2].

However, the treatment carried out by the authors is suitable for other type of boundary conditions; here we suggest periodic boundary conditions along the z axis: $\psi(\rho, \varphi, z + d) = \psi(\rho, \varphi, z)$. On choosing the same ansatz (3) we would have $\psi(\rho, \varphi, z + d) = e^{ikd}\psi(\rho, \varphi, z)$ so that $k = 2\pi\ell/d$, $\ell = 0, \pm 1, \pm 2, \ldots$. It is clear that all the results derived by Figueiras et al. [1] apply straightforwardly to this problem if one just substitutes $2\pi\ell/d$ for k.

Summarizing: the model proposed by Figueiras et al. [1] is separable when the motion of the electron is unbounded along the z axis and also in the case of periodic boundary conditions as argued above. The Schrödinger equation is not separable when the electron is confined within a box and the eigenfunctions an eigenvalues should be obtained approximately as in the case of the harmonic oscillator in a space with a screw dislocation [2]. If one resorts to the variational method the basis set should be chosen carefully.

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