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Magnetic properties of electrons confined in an anisotropic cylindrical potential

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ABSTRACT

In the present paper a theoretical model, describing the effects of external electric and magnetic fields on an electron confined in an anisotropic parabolic potential, is considered. The exact wave functions are used to calculate electron current and orbital magnetic dipole momentum for the single electron. Exact expressions, giving the force and energy of the dipole–dipole interaction, are also determined. Further, the system is coupled to a heat bath, and mean values and fluctuations of the magnetic dipole momentum, utilizing the canonical ensemble are calculated. Influences of the temperature, as well as the external magnetic field, expressed via the Larmor frequency are analyzed. We also include the dependencies of the magnetic dipole momentum and its fluctuations on the effective mass of the electron, considering some experimental values for low-dimensional systems, that are extensively studied for various applications in electronics. Our results suggest that the average momentum or its fluctuations are strongly related to the effective mass of the electron. Having on mind that parabolically shaped potentials have very wide area of application in the low-dimensional systems, such as quantum dots and rings, carbon nanotubes, we believe that the proposed model and the consequent analysis is of general importance, since it offers exact analytical approach.

1. Introduction

Modeling of real physical and chemical systems using various types of parabolic potentials is widely exploited in treating a broad class of phenomena in condensed matter physics, such as optical transitions in solids, molecular vibrations, phononic vibrations up to vibronic transitions, and excitonic transitions. On the other hand, the advancement of spectroscopic techniques for studying molecular vibronic transitions and excitonic transitions in solid state produces a large amount of experimental data (energy spectrum, Fermi surfaces, effective mass of confined electrons), providing a ground to develop reliable theoretical models and determine the limits of applicability of the known models. So far, it has been shown in a number of excellent papers that electronic structure, optical transition, absorption coefficients of newly fabricated low-dimensional quantum systems, such as quantum dots, quantum wires, quantum rings, where one deals with *N*-electrons, confined in one or three dimensions under various potential shapes are successfully modeled by parabolic potentials [1-14], to name but a few. These systems resemble many interesting electronic, optical and magnetic properties, thus development of theoretical models to rationalize and understand experimentally detected features is of crucial importance. In Ref. [14] electronic properties of anisotropic quantum dots are studied analytically, including the effects of the magnetic field magnitude and anisotropy on the energy levels. The theory and the modeling of anisotropic quantum systems have attracted much attention recently, because a series of interesting properties of anisotropic quantum dots have been found. For example, resonance Raman scattering in the anisotropic quantum dots subjected to magnetic field suggests that such a quantum dot could be used as a phonon modes detector [13,15]. In Ref. [11] *N*-electron quantum dots with several shapes of confining potentials at high magnetic fields are investigated in the frameworks of configurations interaction scheme with a multi-centered single-electron wave functions in Cartesian coordinates. In the paper, among the other shapes, the authors also consider anisotropic two-dimensional parabolic potential with Landau gauge and in order to verify the validity of the proposed method, comparison with isotropic three-dimensional parabolic potential is provided.

Undoubtedly, the model of linear harmonic oscillator (parabolic confining potential) with its simplicity is still an important

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reference for theoretical description of emerging quantum systems. Stating the Schrödinger equation for a class of systems, manifesting some common properties, such as harmonicity and anisotropy, and even more finding analytical solutions enable a general and systematic approach in treating, predicting and analyzing a broader class of problems. It is worth to emphasize here that the aforementioned properties could not be extrapolated from the bulk properties, thus finding exact forms of single-electron wave functions is of great importance, since it provides a basis set for expanding N-electron wave functions describing the aforementioned few-electron nanostructures.

In our previous work we have stated an analytically solvable model for an axially symmetrical anisotropic quantum oscillator in the presence of electric and magnetic fields, obtaining the non-degenerate energy spectrum and normalized wave functions, as well as selection rules in dipole approximation for the considered system [16]. A perturbation theory approach, utilizing the derived basis set, was also applied to inspect the effects of symmetry removal in the presence of external fields. In the present work we extend this model, by investigating also magnetic properties of a system that could be described as anisotropic cylindrical oscillator. Assuming the applicability of this theoretical model in investigation of the low-dimensional structures, such as quantum wires, dots and rings, we here adopt effective mass approximation and consider the motion of electron in anisotropic parabolic potential. We use the previously derived analytical solutions by our group [16] to carry out calculations of the electron current density in electric and magnetic fields that are further utilized to obtain orbital magnetic dipole momentum. It is worth to be mentioned here that the orbital magnetic momentum is predominant over a spin one in some of the emerging novel materials, such as carbon nanotubes for example [17]. Obtaining normalized basis set and calculating the current density are also very important to analyze the edge states in quantum dots [12]. We further consider statistical mean values of the magnetic dipole momentum and its fluctuations within a canonical ensemble approach. An extensive analysis of the dependence of the magnetic fluctuations on the temperature and the external magnetic field is provided. We have also obtained exact expression for the magnetic dipole–dipole interaction of the confined electrons that could be further used to perturbatively analyze the effects of long-range interactions of electrons. As we mentioned above, the potential area of application of such a model is wide, considering that the effective model Hamiltonians of electrons in low-dimensional structures often contain a parabolic potential.

2. Methodology and calculations

Let us first give the statement of the model. We consider an anisotropic parabolic potential energy function of the form [18,20,21]

$$U^{(H)}=\frac{m^*}{2}(\omega_0^2\rho^2+\omega_z^2z^2), \tag{1}$$

where for the mass of the oscillator we use the effective mass m^* of the electron, and ω_0 and ω_z are the classical angular frequencies in the aforementioned potential. The effective mass approximation with such potentials has been used in many papers treating various shapes of semiconducting low-dimensional structures. For example, parabolically shaped confining potential is used in Ref. [1] to investigate the linear and the nonlinear optical absorption of quantum dots and rings made of GaAs. Intersubband transitions in semiconducting materials and the optical properties with parabolically shaped potential plus some additional terms are also studied in Ref. [2,3]. Similar but isotropic case is considered in Ref. [4]. Third harmonic generation in GaAs/AlAs cylindrical quantum dots within the frameworks of such models is investigated in Ref. [6–8]. In Ref. [9,10] the electronic states of narrow band gap semiconductor microcrystal, as well as interband transitions and absorption coefficients in cylindrical quantum dots made of GaAs, are studied. It is worth to mention that the effective mass of electrons and holes in solids is usually $(0.01–10)m_0$, where m_0 stands for the free electron mass, e.g. in GaAs it is $0.067m_0$ [22].

Further, the considered oscillator exhibits influence from external electric and magnetic fields and their explicit forms are provided below:

$$\mathbf{E}=E_z\mathbf{e}_z,\quad \mathbf{B}=B_0\mathbf{e}_z. \tag{2}$$

The Hamiltonian of this system, taking into account the influences of external fields, is given by

$$\hat{H}_0=\frac{1}{2m^*}(-i\hbar\nabla-qA)^2+U^{(H)}-q\cdot z\cdot E_z, \tag{3}$$

where q represents the charge of the electron. It is worth to mention here that the first statements of such Hamiltonians and valuable results, widely applicable also to emerging low-dimensional quantum systems, date back to seminal works of Fock and Darwin [18,19]. The corresponding Schrödinger equation has the following form:

$$\hat{H}_0\Psi(\rho,\phi,z)=E^{(0)}\Psi(\rho,\phi,z). \tag{4}$$

The potential function (1) is invariant by rotation around z-axis. Likewise, both external fields are of form which does not destroy the initial cylindrical symmetry of the oscillator. This fact naturally imposes to solve Schrödinger equation in cylindrical coordinates. A suitable choice for the vector potential $\mathbf{A}$ which enables analytical solution of the Schrödinger equation is the following: $\mathbf{A}=(B_0/2)\rho\mathbf{e}_\phi$, here $\mathbf{e}_\phi$ is an ort vector in azimuthal direction. This vector potential meets both required conditions div $\mathbf{A}=0$; rot $\mathbf{A}=\mathbf{B}$. As it is shown in Ref. [16] the exact wave function is given by the following expression:

$$\psi(\rho,\varphi,z)=C_{n_\rho,|m_l|,n_z}\cdot e^{im_l\varphi}\cdot\rho^{|m_l|}\cdot\exp\left[-\frac{1}{2}\left(\frac{\rho^2}{\rho_0^2}+\alpha_z\left(z-\frac{\beta}{2\alpha_z^2}\right)^2\right)\right]\times L_{n_\rho}^{(|m_l|)}\left(\frac{\rho^2}{\rho_0^2}\right)\cdot H_{n_z}\left[\sqrt{\alpha_z}\left(z-\frac{\beta}{2\alpha_z^2}\right)\right], \tag{5}$$

with normalization constant:

$$C_{n_\rho,|m_l|,n_z}=\left(\frac{\alpha_z}{\pi^3 2^{2n_z}}\right)^{1/4}\cdot\frac{1}{\rho_0^{|m_l|+1}}\cdot\left[\frac{n_\rho!}{n_z!\Gamma(n_\rho+|m_l|+1)}\right]^{1/2}. \tag{6}$$

Regarding notation, we have introduced the following labels: $\lambda=(2m^*E^{(0)}/\hbar^2$; $\alpha_0=(m^*\omega_0)/\hbar$; $\alpha_z=(m^*\omega_z)/\hbar$; $\beta=(2m^*qE_z)/\hbar^2$; $\rho_0^4=[\alpha_0^2+(q^2B_0^2)/(4\hbar^2)]^{-1}$, where m_l is the magnetic quantum number with allowed values $0, \pm1, \pm2\ldots$ Both quantum numbers n_z and n_ρ are allowed to values $0, 1, 2, \ldots$ Eigenenergies, calculated analytically as well, are of the following form [16]:

$$E^{(0)}_{n_\rho,n_z,m_l}=\hbar[\sqrt{\omega_0^2+\omega^2}(2n_\rho+|m_l|+1)-m_l\omega+\omega_z(1/2+n_z)]-(q^2E_z^2)/(2m^*\omega_z^2), \tag{7}$$

where we have introduced the Larmor frequency $\omega=qB_0/2m^*$.

2.1. Current density in electric and magnetic fields. Magnetic dipole momentum calculation

Knowing the exact quantum states in this potential as well as eigenenergies we are able to proceed finding analytical expressions of quantities related to the magnetic dipole momentum. A particle with charge q and effective mass m^* creates current