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Impurity binding energies in quantum dots with parabolic confinement

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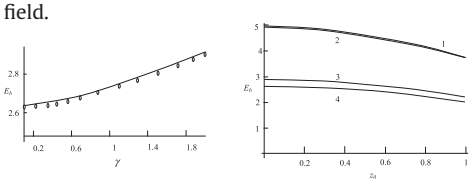
HIGHLIGHTS

- We consider hydrogen-like impurity states in quantum dot with parabolic confinement.
- New approach to calculation of impurity binding energy is developed.
- Electron wave function is determined as expansion over 1D harmonic oscillator states.
- Binding energy as function of the impurity position and magnetic field strength are presented and discussed.

GRAPHICAL ABSTRACT

We present an effective numerical procedure to calculate the binding energies and wave functions of the hydrogen-like impurity states in a quantum dot with parabolic confinement in the presence of magnetic field.



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ABSTRACT

We present an effective numerical procedure to calculate the binding energies and wave functions of the hydrogen-like impurity states in a quantum dot (QD) with parabolic confinement. The unknown wave function was expressed as an expansion over one-dimensional harmonic oscillator states, which describes the electron's movement along the defined z-axis. Green's function technique used to obtain the solution of Schredinger equation for electronic states in a transverse plane. Binding energy of impurity states is defined as poles of the wave function. The dependences of the binding energy on the position of an impurity, the size of the QD and the magnetic field strength are presented and discussed.

1. Introduction

Quantum dots (QDs) are artificial structures in which the motions of the charge carriers are limited to three directions. The type of confinement potential used determines their possible states, such as the band structure and the basic physical properties of the QDs. Two important factors are the impurity states (IS) and the external field, without which it would be difficult to practically implement QDs in electronics and they can affect the band structure. Since Bastard first calculated [1] the impurity binding energy in a quantum well (QW), many works have been published on this subject. Over the last three decades, new calculation methods have been developed to determine the IS in QWs and QDs, by assuming the form of the confinement potential [2–5], the features of the band structure [5–9] and the types of impurity model–hydrogen- [1–9] or helium-like [10–15]. The form of the confinement potential is a significant characteristic. In particular, (as mentioned in Ref. [16]) the advantages of devices based on QDs (compared with QWs) have become possible because of the synthesis of QDs that satisfy the rigid requirements of size, shape, uniformity and density, which ultimately affect the choice of the potential used to confine the charge carriers in the QDs. Although the most widely used model for QDs has a spherical symmetry potential, allowing for simple and convenient (for the following analysis) solutions, it only provides a qualitative picture, because there are many factors that reduce the symmetry, making the

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problem very complicated. In this sense, a model with a parabolic potential and a low symmetry is more adequate. The practicality of this model has been demonstrated in many studies (see Ref. [5] and the references therein).

A study of the effect of an external field on the energy spectrum of low-dimensional structures also led to the work performed by Bastard [17], where the electron eigenstates in a QW under an electric field were calculated.

In QDs, only discrete energy levels for the electron states are possible, unlike in QWs where the electron energy levels are quantized for the movement along growth axis of the QW. Thus, applying a magnetic field to the structure is an efficient tool to study the energy spectrum of a QD. Studies of the magnetic field effect on the electron states in a QD have been performed over the past three decades using various methods, where variational techniques [18], a perturbation approach [19], numerically solving the Schrödinger equation [20], and strong-confinement approaches [21] have been developed. The variational approach is one of the most exploited methods used to study the energy spectra of QDs. For some particular cases of QDs size variational results were confirmed with calculations, according to the perturbation theory [19,22]. The well-known limitations of the variational approach are: the accuracy of the method cannot be estimated and a trial wave function needs to be constructed for each IS. Other disadvantages for the above techniques include the difficulty of the calculation methods and/or the specific conditions (as for the magnetic field, QD size) of their applicability. These problems are absent in the approach proposed below.

In the present study, the problem of the hydrogen-like IS in QDs with parabolic confinement, under a magnetic field is considered and solved. Our approach has allowed formulating the problem as a system of algebraic equations, where variables determine the wave function of the electron, and the condition of solvability of the system leads to a direct calculation of the binding energy. The approach did not use any additional (non-physical) parameters, allowing for the control of the accuracy of the results obtained. This approach allows calculates both the ground and the excited states.

2. Numerical procedure

Here we consider an isolated donor in a QD with parabolic confinement, $V_c(R, z)$, under a magnetic field. The corresponding Hamiltonian in cylindrical coordinates (R, z, θ) can be written as

$$H = -\frac{\hbar^2}{2m^*}\left[\frac{d^2}{dR^2} + \frac{1}{R}\frac{d}{dR} + \frac{1}{R^2}\frac{d^2}{d\theta^2} + \frac{d^2}{dz^2}\right] - \frac{i\hbar eB}{2m^*}\frac{\partial}{\partial\theta} + \frac{e^2B^2R^2}{8m^*} + V_c(R, z) + U(R, z), \quad (1)$$

where m^* is the effective mass of an electron. $V_c(R, z)=m^*\omega^2(R^2+z^2)$, where ω is the angular frequency of the parabolic confining potential, B is the magnetic field, $U(R, z) = -(e^2/4\pi\kappa\kappa_0)(2/\sqrt{R^2 + (z - z_0)^2})$ is the Coulomb interaction between an electron and an impurity ion, e is the unit charge, κ is the permittivity, κ_0 is the dielectric constant, and z_0 is the position of the impurity atom. Because of the axial symmetry of the system, the projection of the angular momentum onto the z-axis was conserved, $L_z=\hbar m$ ($m=0, \pm1, \pm2, \ldots$ and is the magnetic quantum number) and their eigenfunctions ($exp(imz)$) determine the dependence of the unknown electron wave function $\psi(R,\theta,z)$ at an angle, θ: where $\psi(R, \theta, z) \equiv \exp(im\theta)\psi(R, z)$. By solving the one-dimensional Schrödinger equation for the unknown functions, $\varphi(z)$

$$\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + m^*\omega^2z^2\right)\varphi(z) = \varepsilon\varphi(z),$$

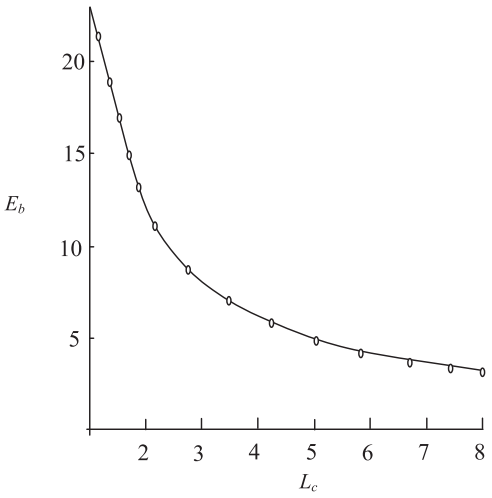

Fig. 1. Binding energy versus QD size L_c (circles–perturbation calculation [19], solid–our results).

the basis for an expansion of the wave function can be obtained

$$\Psi_m(z, \vec{\rho}) = \exp(im\theta)\sum_n f_n^m(R)\varphi_n(z). \quad (2)$$

The same approach has been used for impurities in an inversion layer [23] and in QWs. [24, 25] By substituting Eq. (2) into Eq. (1) and using the dimensionless variables

$$a_b = \frac{4\pi\varepsilon\varepsilon_0\hbar^2}{m^*e^2},\ R^* = \frac{\hbar^2}{2m^*a_b^2},\ \beta^2 = \frac{m^*\omega^2a_b^2}{R^*},\ \gamma = \frac{\hbar}{2m^*Ry}\frac{eB}{}$$

which are the units of distance (Bohr radius, a_b) and energy (Rydberg, R^*), the magnitude of the confining potential (β^2) and the magnetic field (γ), a system of differential equations was obtained

$$\left[\frac{d^2}{dR^2} + \frac{1}{R}\frac{d}{dR} + E - \varepsilon_N - \gamma m - \frac{m^2}{R^2} - \beta^2R^2\right]f_N(R) = \sum_n U_{Nn}(R)f_n(R), \quad (3)$$

where $U_{Nn}(R) = \int\varphi_N^*(z)\ U(R, z)\ \varphi_n(z)\ dz,\ N = 1, 2, 3, \ldots$.

Since a_b is a unit of distance, β^2 can be considered as the inverse of the dimensionless length L_c, i.e. $\beta^2=1/L_c^2$, where L_c, corresponds to the size of the QD [19].

In the following, to find a solution to Eq. (3) Green's function, $G_N(R, R')$ was introduced through the definition

$$\left[\frac{d^2}{dR^2} + \frac{1}{R}\frac{d}{dR} - \frac{m^2}{R^2} - \frac{\gamma R^2}{4}\right]G_N(R, R') = \frac{\delta(R - R')}{R},$$

which does not depend on energy.

Table 1
Binding energy for the various calculation parameters.

$\gamma=2$, $z_0=0$			$\gamma=0.5$, $z_0=1$		
Number of QD level	$N_R \times \Delta R$	E_b	Number of QD level	$N_R \times \Delta R$	E_b
5	120×0.050	4.962	5	80×0.050	3.730
7	120×0.035	4.972	6	120×0.035	3.745
7	180×0.025	4.990	6	150×0.030	3.745
7	220×0.025	4.988	7	150×0.030	3.754
9	180×0.025	4.993	8	180×0.025	3.757