Physica E 66 (2015) 128–132

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Finite-difference calculation of donor energy levels in a spherical quantum dot subject to a magnetic field

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HIGHLIGHTS

- Donor states in a spherical quantum dot subject to a magnetic field are calculated.
- The effective-mass equation is numerically solved by the finite-difference method.
- Excellent agreement with the H atom is obtained by the Richardson extrapolation.
- Variational results may either underestimate or overestimate the binding energy.
- Transition energies in a realistic dot are given in terms of the field strength.

ARTICLE INFO

Article history:
Received 6 June 2014
Received in revised form
10 October 2014
Accepted 14 October 2014
Available online 23 October 2014

Keywords:
Quantum dot
Semiconductor
Impurity
Zeeman splitting

ABSTRACT

The ground and excited states of a donor impurity at the center of a spherical quantum dot subject to a magnetic field are calculated within the effective-mass approximation. The barriers are infinitely high and the differential equation is solved by combining the finite-difference method with the Richardson extrapolation. The binding and transition energies are more accurate than the available variational values, and excellent agreement is found with the hydrogen atom. The transition energies for a medium-size quantum dot are given.

1. Introduction

The theoretical study of nanometric pieces of semiconductor materials, called quantum dots, has been a valuable tool during the rise of nanoscience and nanotechnology. Most efforts have been devoted to the calculation of the electronic states, taking into account different shapes of the confining potential, the presence of inner and outer impurities [1], applied electric [2–4] and magnetic fields [5,6], excitonic states [7], electron–electron [8,9] and electron–phonon [10] interactions.

Several investigations of hydrogenic impurities in quantum dots subject to a magnetic field have been reported in the literature. Xiao et al. [11] have calculated the binding energy by assuming an infinite confining barrier. They followed a variational approach to calculate the energy of the donor states and the ground state of an electron in the absence of the impurity. Their results display the expected qualitative behavior of the binding energy as a function of the dot radius and the magnetic-field strength. A similar approach was used by Corella-Madueño et al. [12] and Seddik et al. [13], while Guimarães and Prudente [14] used a different variational procedure which is based on the finite-element method. Furthermore, Changa et al. [15] have dealt with the case of an off-center donor in a spherical quantum dot without the magnetic field. They found good agreement between perturbation-theory and finite-difference approaches.

The variational method is of intrinsic limited accuracy and may either under or overestimate the exact values of the binding and the transition energies. This is because such energies are differences between two approximate energy values. To overcome this difficulty, we perform a finite-difference calculation of the electronic states, both in the absence and the presence of the donor impurity. We deal with the binding energy of the 1s states and the $1s \rightarrow 2p^{\pm}$ transition energies. We hope this will pave the way for a

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http://dx.doi.org/10.1016/j.physe.2014.10.011
1386-9477/

more detailed description of the impurity states in the nanostructures under investigation.

The remainder of this paper is organized as follows: In Section 2, the Hamiltonian and the symmetry of the wave function are described. Section 3 contains the main finite-difference equations, the discretized boundary conditions and the Richardson extrapolation procedure. In Section 4, we present the numerical results for the 1s and several excited energy levels as a function of the quantum-dot radius and the magnetic-field strength. Finally, we summarize our findings in Section 5.

2. Theory

We consider an electron moving inside a spherical quantum dot, interacting with a positively charged impurity atom placed at the center of the dot, and subject to a magnetic field along the z-axis.

Conveniently, we choose the origin of coordinates at the impurity position and express lengths and energies in units of the effective Bohr radius a^* and the effective Rydberg Ry^* of the dot material, respectively. In these units, the dot radius is denoted as R. Moreover, the dimensionless parameter $\gamma = (a^*/\lambda)^2$ measures the magnetic-field strength, where $\lambda = \sqrt{\hbar/(eB)}$ is the Landau radius. The vector potential of the magnetic field is chosen in the symmetric gauge.

The effective-mass equation of the neutral donor, with the origin of energies at the bottom of the conduction band of the dot material, is given by

$$\hat{H}\Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi), \tag{1}$$

where r, θ and ϕ are the usual spherical coordinates: r is the electron-impurity distance, while θ and ϕ are the polar and azimuthal angles, respectively. The Hamiltonian operator has the following form:

$$\hat{H} = -\nabla^2 - i\gamma\frac{\partial}{\partial\phi} + \frac{\gamma^2 r^2 \sin^2(\theta)}{4} - \frac{2}{r}. \tag{2}$$

Assuming that the electron is strictly confined within the dot, the boundary condition $\Psi(R, \theta, \phi) = 0$ applies for all values of θ and ϕ. Moreover, according to the axial symmetry, the eigenfunctions of $\hat{H}$ have well-defined angular momentum along the z-axis. Its eigenfunctions may be written as

$$\Psi_m(r, \theta, \phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}\psi_m(r, \theta), \tag{3}$$

where m is an integer and $\psi_m(r, \theta)$ satisfies

$$\hat{H}_m\psi_m(r, \theta) = E_m\,\psi_m(r, \theta), \tag{4}$$

with

$$\hat{H}_m = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{m^2}{r^2\sin^2(\theta)} + m\gamma + \frac{\gamma^2 r^2\sin^2(\theta)}{4} - \frac{2}{r}. \tag{5}$$

Moreover, $\psi_m(R, \theta) = 0$ applies for all values of θ. Since $\hat{H}_{-m} - \hat{H}_m = -2m\gamma$, the eigenvalues E_m and eigenfunctions $\psi_m(r, \theta)$ may be chosen to satisfy $E_{-m} = E_m - 2m\gamma$ and $\psi_{-m}(r, \theta) = \psi_m(r, \theta)$.

Depending on the symmetry of the wavefunction, additional boundary conditions apply [16]. In fact, ψ_m satisfies $\psi_m(r, \pi - \theta) = \sigma\psi_m(r, \theta)$, where $\sigma = 1$ ($\sigma = -1$) corresponds to symmetric (anti-symmetric) states along the z-axis direction. For instance, $\sigma = 1$ ($\sigma = -1$) applies to 1s-like and $2p^{\pm}$-like ($2p^0$-like) states. In this sense, one may restrict the numerical calculations to the range $0 \le \theta \le \pi/2$.

3. Numerical procedure

The donor energy levels in the quantum dot are calculated by the finite-difference technique. This is done over a rectangular and uniform mesh in the computational domain given by $0 \le r \le R$ and $0 \le \theta \le \pi/2$, with spacing $h = R/(M+1)$ and $k = \pi/(2N+2)$, respectively, where R is the dimensionless quantum-dot radius and M, N are sufficiently large integer numbers. Hence, the mesh is given by $(r_i, \theta_j) = ((i-1)h, (j-1)k)$, with $1 \le i \le M+2$ and $1 \le j \le N+2$.

The node values of the wavefunction are denoted by $G_{i,j} = \psi_m(r_i, \theta_j)$, and the second-order discretization of Eq. (4) leads to

$$-\frac{1}{h^2}\left(G_{i+1,j} - 2G_{i,j} + G_{i-1,j}\right) - \frac{1}{h\,r_i}\left(G_{i+1,j} - G_{i-1,j}\right) - \frac{1}{k^2 r_i^2}\left(G_{i,j+1} - 2G_{i,j} + G_{i,j-1}\right) - \frac{\cot(\theta_j)}{2kr_i^2}\left(G_{i,j+1} - G_{i,j-1}\right) + V_{i,j}\,G_{i,j} = E_m(M, N)G_{i,j}, \tag{6}$$

where

$$V_{i,j} = m\gamma + \frac{m^2}{r_i^2\sin^2(\theta_j)} + \frac{\gamma^2}{4}r_i^2\sin^2(\theta_j) - \frac{2}{r_i} \tag{7}$$

and $E_m(M, N)$ is the finite-difference estimate of the energy level E_m.

The boundary conditions are discretized up to second order. The confinement of the electron within the dot, i.e, $\psi_m(R, \theta) = 0$, leads to $G_{M+2,j} = 0$. When $\sigma = -1$ ($\sigma = 1$), the function (the partial derivative on θ) should vanish at $\theta = \pi/2$, i.e., $G_{i,N+2} = 0$ ($G_{i,N} - 4G_{i,N+1} + 3G_{i,N+2} = 0$). Moreover, smoothness at the polar axis of states with $m \neq 0$ ($m=0$) requires the function (the derivative with respect to θ) to vanish at $\theta = 0$, i.e., $G_{i,1} = 0$ ($3G_{i,1} - 4G_{i,2} + G_{i,3} = 0$). The last boundary condition refers to $\psi_m(0, \theta)$. Since every node of the form $(0, \theta_j)$ maps into the dot center, one has $G_{1,j} = G_{1,1}$. Moreover, the coefficient of $G_{1,j}$ in Eq. (6) is $(1/h - 1/r_2)/h = 0$. This means $G_{1,1}$ is not relevant in our finite-difference calculation of the energy levels.

When the boundary values are put into Eq. (6), the system of linear equations may be written as

$$\mathbf{\Lambda}\vec{G} = E_m(M, N)\vec{G}, \tag{8}$$

where $\vec{G}$ is a linear arrangement of length MN containing the values of $G_{i,j}$ for $2 \le i \le M+1$, $2 \le j \le N+1$. Approximate values of the energy levels are given by the eigenvalues of the matrix $\mathbf{\Lambda}$.

To improve the accuracy of the calculated energy levels, it is desirable to approach the limit $M \to \infty$, $N \to \infty$. Therefore, we use quite large values for M and N, namely, $M_1 = N_1 = 100$ and $M_2 = N_2 = 200$, for $R \le 10$, but $M_1 = N_1 = 300$ and $M_2 = N_2 = 600$ when $R=30$. Thus, the smallest matrix size is $10\,000 \times 10\,000$ and the largest one is $360\,000 \times 360\,000$. By fixing the ratio $M/N = 1$, the numerical values of $E_m(N, N)$ may be fitted by a simple law of the form $E_N = \alpha + \beta/N^2$. A quadratic Richardson extrapolation