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Energies and wave functions of an off-centre donor in hemispherical quantum dot: Two-dimensional finite difference approach and ritz variational principle

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ABSTRACT

Eigenvalues equation solutions of a hydrogen-like donor impurity, confined in a hemispherical quantum dot deposited on a wetting layer and capped by an insulating matrix, are determined in the framework of the effective mass approximation. Conduction band alignments at interfaces between quantum dot and surrounding materials are described by infinite height barriers. Ground and excited states energies and wave functions are determined analytically and via one-dimensional finite difference approach in case of an on-center donor. Donor impurity is then moved from center to pole of hemispherical quantum dot and eigenvalues equation is solved via Ritz variational principle, using a trial wave function where Coulomb attraction between electron and ionized donor is taken into account, and by two-dimensional finite difference approach. Numerical codes developed enable access to variations of donor total energy, binding energy, Coulomb correlation parameter, spatial extension and radial probability density with respect to hemisphere radius and impurity position inside the quantum dot.

1. Introduction

In the two last decades, low-dimensional system (LDS) based on semiconductor materials such as quantum wells (QW's), quantum well wires (QWW's) and quantum dots (QD's) gave rise to major theoretical and experimental research topics. The enthusiasm expressed to semiconductor QD's issue as well as the progress reached in crystal growth techniques, especially in soft chemistry processes of growth, has made it possible the fabrication of high-quality semiconductor QD's within a variety of geometries and a large range of sizes for different fields of applications such as optical encryption [1], multiplexing [2], solar energy harvesting [3], biology and medicine where QD's are used in the study of intracellular processes at single molecule level [4,5]. Semiconductor QD's are also used in high-resolution cellular imaging [6–9], in long term in vivo observation of cell trafficking, in tumor targeting and in disease diagnostics [10–13].

Hydrogen-like donors whose energy levels are close to conduction band edge are predisposed to play an important role in optical transitions occurring in QD's. So, large number of studies has been devoted to this topic. In this way, Assaid et al. determined all states energies and wave functions of an on-centre donor confined in lens-shaped QD's [14]. Ibral et al. investigated dielectric mismatch effect on exciton ground state energy [15,16]. They also studied dielectric mismatch and impurity position effects on ground state energy and wave function of an off-centre donor confined in core/shell QD's [16,17]. They showed that in case of intermediate and large size core/shell QD's, donor binding energy is larger than exciton binding energy for impurity positions near core surface. Nevertheless in small size core/shell QD's, off-centre donor is more stable than exciton for impurity positions near core centre. They expected that core surface effects would have great influence on optical properties of core/shell QD's by promoting non-radiative extrinsic transitions at the expense of radiative exciton transitions. Using finite elements method [18], Satori et al. calculated binding energy of shallow donor in spherical QD's [19] and investigated combined effects of pressure and

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impurity position on donor binding energy in cubic QD's [20]. In the case of spherical QD's, they found excellent agreement with former results obtained by Ritz variational method. As for cubic QD's, they showed that hydrostatic pressure is more perceptible for small size QD's and that donor binding energy is a decreasing function when impurity is moved from center to corner of the cube. Using one-dimensional finite difference approach with Richardson extrapolation, de Souza et al. calculated ground and excited states of an on-centre donor inside a spherical QD in presence of magnetic field [21]. They compared donor binding and transition energies to variational results available in literature and found excellent agreement with hydrogen atom for large dots and stated that finite difference results are more accurate than variational values for finite dot size.

In the present work, we determine ground and excited states energies and wave functions of hydrogen-like donor, confined in a hemispherical quantum dot (HQD) deposited on a wetting layer and capped by a host insulating matrix. HQD are promising nanostructures with outstanding properties. The sensitive dependence of their electronic, optical and magnetic properties on single dopant has given a large range of tunable phenomena to investigate and apply to devices such as single-spin devices or long-lived spin-based memory in the area of quantum information [22] or single-dopant transistors [23]. So, HQD are at the cutting edge of spintronics [22] and solotronics [24].

The present work may be broken into three sections. In the first one, energies and wave functions of hydrogen-like on-centre donor are determined exactly and their dependence versus HQD radius is investigated. In the second section, energies and wave functions of confined hydrogen like on-centre donor are determined via one-dimensional finite difference approach against QD radius and compared to results obtained via exact analytic resolution, perfect agreement between the results coming from the two methods is then raised. In the third section, donor impurity is moved from center to pole of HQD. Then, ground and excited states total energies, binding energies, wave functions, electron to ionized donor distance mean value and radial probability density are determined via Ritz variational principle and using two-dimensional finite difference approach.

2. Theoretical framework

Let's consider a donor impurity confined in a narrow band gap HQD deposited on a wide band gap wetting layer and capped by an insulating matrix (see Fig. 1). The bottom of dot conduction band is below the bottoms of layer and matrix conduction bands. Due to this well-like band profiles, charge carriers are confined in HQD.

2.1. Electron and hydrogen-like donor Hamiltonians in atomic units

To simplify expressions of different Hamiltonians involved, we use as unit of length donor effective Bohr radius in bulk material $a_D^* = \varepsilon\hbar^2/e^2m_e^*$ and as unit of energy absolute value of donor ground state energy in bulk material $R_D^* = m_e^*e^4/2\varepsilon^2\hbar^2$, e is the elementary charge, m_e^* is the electron effective mass and ε is HQD dielectric constant. In the framework of envelope function approximation and assuming isotropic, parabolic and non-degenerated bands, the Hamiltonians of confined electron, on-centre and off-centre donors are:

$$H_e = -\Delta_e + V_{we}(r_e, \theta_e) \tag{1}$$

$$H_{D^0}^{on-centre} = -\Delta_e - \frac{2}{r_e} + V_{we}(r_e, \theta_e) \tag{2}$$

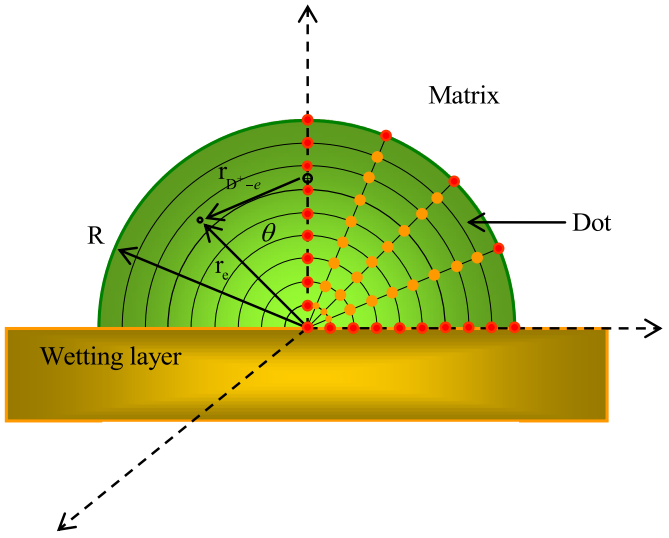

Fig. 1. Sketch of Hemispherical Quantum Dot (HQD) deposited on wetting layer and capped with insulating matrix. According to layer, dot and matrix conduction bands lineup electron is completely confined in HQD. The dots correspond to $M \times N$ uniformly separated nodes of two-dimensional grid used to discretize HQD. Red dots are nodes corresponding to grid borders where boundary conditions must be applied. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$H_{D^0}^{off-centre} = -\Delta_e - \frac{2}{\sqrt{r_e^2 + d^2 - 2r_e d\ \cos(\theta_e)}} + V_{we}(r_e, \theta_e) \tag{3}$$

r_e is the electron radial distance from the origin O. θ_e is the polar angle between the zenith ($\vec{z}$ axis) and the position vector $\vec{r_e}$ (see Fig. 1). The electron confining potential inside HQD $V_{we}(r_e, \theta_e)$ is:

$$V_{we}(r_e, \theta_e) = \begin{cases} 0, & 0 < r_e < R \ \&\ 0 < \theta_e < \pi/2 \\ \infty, & outside \end{cases} \tag{4}$$

For a donor placed on z-axis, d is the nucleus distance to the dot centre (see Fig. 1).

2.2. Exact solutions of hydrogen-like on-centre donor eigenvalues equation

In case of a QD presenting spherical symmetry such as spherical QD's or core/shell QD's, electron and on-centre donor Hamiltonians are invariant with respect to all rotations, i.e. they present rotational symmetry. Thus, these Hamiltonians are simultaneously diagonalizable with L_z and L^2. As a consequence, total separation of angular and radial variables may be achieved in Hamiltonians as well as in wave functions which may be expressed as a product of a radial part $R^{n,l}(r_e)$ with a spherical harmonic $Y_{l,m}(\theta_e, \varphi_e)$ standing for angular part. n is the principal quantum number, l and m are the orbital and the magnetic quantum numbers.

In case of HQD, confining potential $V_{we}(r_e, \theta_e)$ may be separated into radial $V_{we}(r_e)$ and angular $V_{we}(\theta_e)$ operators as long as the potential outside the dot is infinite:

$$V_{we}(r_e, \theta_e) = V_{we}(r_e) + V_{we}(\theta_e) \tag{5-a}$$

where

$$V_{we}(r_e) = \begin{cases} 0, & 0 < r_e < R \\ \infty, & R < r_e \end{cases} \tag{5-b}$$

and