Chemical Physics 493 (2017) 32–41

Contents lists available at ScienceDirect

Chemical Physics

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

Magnetic-field dependence of the impurity states in a dome-shaped quantum dot

E.C. Niculescu, C. Stan *, M. Cristea, C. Truscă

Department of Physics, "Politehnica" University of Bucharest, Romania

ARTICLE INFO

Article history:
Received 4 May 2017
In final form 10 June 2017
Available online 13 June 2017

Keywords:
Quantum dot
Wetting layer
Donor impurity
Magnetic field
Diamagnetic susceptibility

ABSTRACT

Using the finite element method, the effect of magnetic fields on the donor states and transition energies in a InAs/GaAs quantum dot coupled to its wetting layers is investigated. Results are obtained for different impurity locations. We found that the diamagnetic shift of the ground state energy increases monotonously with the applied field and can be described by a simple function which interpolates between the low and high magnetic-field behavior. Frequencies associated to the transitions between the *S*-like ground state and P_- (P_+) excited states range in terahertz region and show a magnetic field-induced red (blue) shift, irrespectively of the impurity position.

1. Introduction

Semiconductor quantum dots (QD) have been widely investigated in the last decades because of their potential applications in electronics [1], photo-detection and optoelectronics [2,3], quantum information [4,5], engineering [6] and medicine [7,8]. Of particular interest are self-assembled QDs since their special properties open new area of possibilities for high-performance optoelectronic devices. Due to the 3D confinement, QDs exhibit quantized states of energy with high lifetime for excited states. Moreover, these structures allow both *z*- and in-plane-polarization of the conduction intraband transitions so that Stranski-Krastanov growth method can be utilized to create QD-based devices in THz range [9,10]. These advantages make self-assembled QDs a subject of intensive study both experimentally [11–13] and theoretically [14–16].

Magnetic field is an important tool used to control and modulate the intensity output of the optoelectronic devices since it can be experimentally applied in a well controlled way. Many studies reported on the electronic properties as well as on the linear and nonlinear optical absorption of QDs induced by the externally applied magnetic fields [17–25].

Investigations of the effect of hydrogenic impurity in such configurations are also important, since their presence influences the electronic mobility and optical properties. Under the confinement, the dopant position can tailor the electronic and optical properties of the system. The impurity can be located on (off) the center of symmetry to get a symmetric (asymmetric) situation, or near the boundary of the QD to get surface-like states (edge states) of this system. An important number of theoretical and experimental researches focused on the impact of the impurity states on the quantum nanostructures properties, in the presence of external perturbations [26–34]. However, up to now, only few reports were involved in studying the external fields effect on the electronic states in QDs coupled to their wetting layers (WL). Sabaeian et al. [14] discussed the dependence of energy eigenvalues of *S*- and *P*-states and interlevel *P*- to -*S* transition energy on applied vertical electric field in a semi-spheroid-shaped InAs/GaAs QD coupled to its WL. Diamagnetic susceptibility of an off-center hydrogenic donor impurity confined by pyramid and cone-like GaAs/$Ga_{0.5}In_{0.5}As$ QD grown on a GaAs WL have been investigated in [35]. In our previous work, we analyzed the asymmetric Stark shift in an InAs/GaAs dome-shaped QD with WL for different impurity positions [16] and optical nonlinearities associated to hydrogenic impurities in InAs/GaAs self-assembled QD under applied electric fields [36]. Very recently [37], energy eigenvalues, transition energies, and transition dipole moments of impurity-free truncated pyramidal-shaped InAs/GaAs quantum dots under a vertical magnetic field were presented.

To the best of our knowledge, there are no reports on the electronic properties of donor impurity (on-surface or on-center) localized in self-assembled InGaAs/GaAs QDs subjected to a magnetic field. The present work attempts to fill this gap in the literature by a detailed investigation of the electronic probability density, energy levels, transition frequencies and diamagnetic susceptibil-

* Corresponding author.
E-mail address: cstan@physics.pub.ro (C. Stan).

http://dx.doi.org/10.1016/j.chemphys.2017.06.004
0301-0104/

ity of hydrogenic donors in a dome-shaped InAs/GaAs QD coupled to its WL and subjected to a magnetic field.

The outline of the paper is as follows. In Section 2 we describe the theoretical framework. The numerical results and discussion are presented in Section 3. A brief summary is given in Section 4.

2. Theory

In this study, a dome-shaped InAs/GaAs QD with radius $R = 7$ nm grown on a 2 nm wetting layer is considered (see inset of Fig. 1a). The z-axis which pierces the dot through its center and is perpendicular to the plane of the wetting layer represents a symmetry axis for the system.

In the presence of a hydrogenic impurity and under magnetic fields, the Hamiltonian of the system is given by

$$H_0 = \frac{1}{2m^*}(\vec{p} + e\vec{A})^2 + V(x,y,z) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r} - \vec{r}_i|} \tag{1}$$

where

$$m^*(x,y,z) = \begin{cases} m^*_{\mathrm{InAs}}, & \text{in QD} \\ m^*_{\mathrm{GaAs}}, & \text{elsewhere} \end{cases} \tag{2}$$

is the effective mass, and

$$V(x,y,z) = \begin{cases} 0, & \text{in QD} \\ \Delta E_c, & \text{elsewhere} \end{cases} \tag{3}$$

is the potential energy. ΔE_c is the conduction band offset between the InAs and GaAs and the last term in Eq. (1) is the Coulomb interaction between the electron and the hydrogenic donor located at $\vec{r}_i$. We assume a vertical magnetic field $\vec{B} = B\hat{z}$ (see Fig. 1). Using the Coulomb gauge $\vec{A} = (B/2)(-y\hat{x} + x\hat{y})$ the Hamiltonian becomes:

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m^*} + \frac{eB}{2m^*}(y\hat{p}_x - x\hat{p}_y) + \frac{e^2B^2}{8m^*}(x^2 + y^2) + V(x,y,z) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r} - \vec{r}_i|}. \tag{4}$$

We note the presence of two different terms related to magnetic field in the Hamiltonian operator: a liniar Zeeman term that couples the motions along directions perpendicular to the magnetic field (sometimes called paramagnetic term [32]) and a parabolic magnetic potential, which enhances the confinement of the electronic wave functions in the transverse plane, usually called diamagnetic term.

Fig. 1 shows the shape of the potential energy profile without (a) and with (b) applied magnetic field, including the Coulomb interaction associated to an on-center impurity. A sketch of the geometry of the nanostructure: (QD + WL + GaAs matrix) is inserted in Fig. 1a. The $S \to P$ transition – studied in the following – is also indicated in both cases. In our computations, the position of the impurity atom is considered either on z-axis or on x-axis.

The Schrödinger equation with the Hamiltonian given by Eq. (4) is numerically solved using the finite element method. The mesh

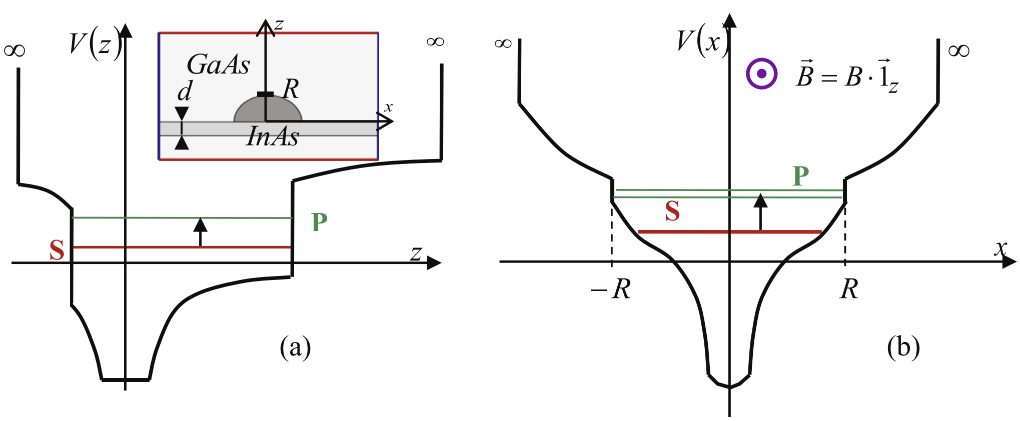

Fig. 1. Confinement potential including the Coulomb interaction associated to on-center impurity for InAs/GaAs QD without (a) and with applied magnetic field (b). Inset is a sketch of the InAs QD with its WL (darker gray) imbedded in a GaAs matrix (light gray).

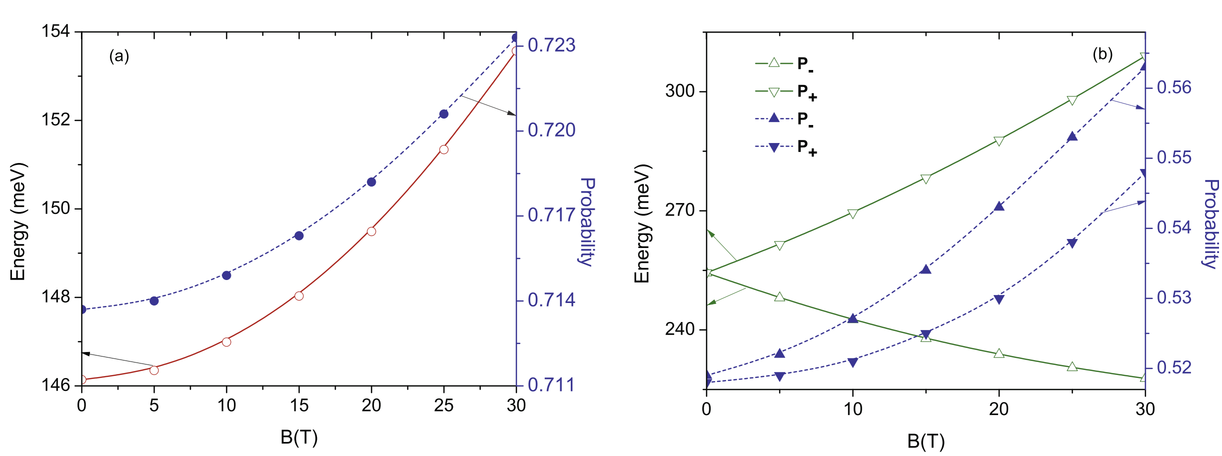

Fig. 2. The energy levels (continuous lines, left scale) and the probability of finding the electron inside the dome (dashed lines, right scale) versus the magnetic field: (a) S – state; (b) P_- and P_+ states, respectively. Results are for a QD without impurity.