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Energy spectra of D^- centres quantum dots in a Gaussian potential

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Abstract

We explore D^- centres quantum dot in a Gaussian confining potential. By means of numerical matrix diagonalization within the effective-mass approximation we obtain the energy spectrum and show that the property of the ground and low-lying states of the quantum dot is rather sensitive to the strength of the confinement potential. The energy deviation of the ground and the first excited states of the D^- centres confined in Gaussian and harmonic-oscillator potential is analyzed explicitly.

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1. Introduction

Quantum dots are structures in which the charge carriers are confined in all three dimensions [1,2]. These QDs are often referred to as artificial atoms in which the atomic potential is replaced by the artificial dot potential. In a typical structure the number of electrons can be well controlled and a small number of electrons per dots has been achieved experimentally [3,4]. The number of electrons is increased by changing the gate voltage and charging the dot with an additional single electron. The experimental study of semiconductor QDs is expanding rapidly, and electron–electron interaction and correlation effects are shown to be of great importance in such systems [5,6]. From a theoretical point of view, these few-body systems represent a challenging problem. The standard tools of the condensed-matter physicist, such as the many-body techniques relying on Hartree–Fock approximations are often not sufficient, since the exchange and correlation energies can be far from negligible [7]. A fully quantum mechanical treatment is needed. An example is the promble of a strictly two-dimensional D^- centre QD. A negative hydrogenic donor center (D^-) in semiconductors consists of a single positive ion and two electrons which are bound to the posi-

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tive ion. It is analogous to a negative hydrogen ion (H^-) [8]. D^- centres are one of the simplest many-body electronic systems, which cannot be solved exactly. Recently, there has been much experimental and theoretical interest in the existence of D^- centre in quasi-two-dimensional systems. The existence of D^- centre in the center-doped GaAs/Al_xGa_{1-x}As multiple quantum wells was first reported by Huant et al. [9]. Xie calculated the binding energy spectra of a D^- centre QD with a parabolic potential by using the method of few-body physics with a magnetic field [10–12].

The lateral confinement can be considered as two-dimensional [13]. In most investigations, a harmonic oscillator potential were used to describe the lateral confinement. However, the parabolic potential possesses infinite depth and range. It is inappropriate to describe the experimentally measured charging of the QD by the finite number of excess electrons [14]. Some experimental results suggest that the real confining potential is nonparabolic and possesses a well-like shape. When a dot is small (i.e., when its radius is comparable to the characteristic length of the variation of the lateral potential near the edge), a good approximation offers simple smooth potentials, such as Gaussian potential well, $V(r) = -V_0 \exp(-r^2/2R^2)$ [13]. This model potential is smooth and possesses a finite depth V_0 and a characteristic finite radius R. About three years ago Adamowski et al. [15] studied two electrons confined in QDs under an assumption of a Gaussian confining potential well and its parabolic approximation. Xie calculated the energies of two interacting electrons in a QD with Gaussian confining potential [16]. In the present Letter we study the properties of D^- centre QD in Gaussian confining potential in terms of the method of numerical matrix diagonalization. Such calculations are valid mainly for a QD with radius R comparable to the exciton Bohr radius a_B ($a_B \sim 10$ nm).

In this Letter, we will propose a procedure to calculate energy spectrum of D^- centres in disk-like QDs with a Gaussian confining potential by using the method of few-body physics. We will investigate the energy levels of the ground and low-lying states of the D^- centres as a function of the QD size. We will also study the energy deviations of the ground and the first excited states of the D^- centreconfined in Gaussian and harmonic oscillator.

2. Theoretical model

The D^- centre in a disk-like QD can be described as a system composed of two electrons and a positively charged donor impurity located at the center of the disk potential-well region. We assume the validity of the effective-mass approximation and neglect the difference of the electron band masses and dielectric-constant between the QD region and the surrounding medium. It is reasonable for the case of the strong confinement and small dielectric-constant difference. However, we should point out that if there is a significant penetration into the barrier, then the effect of the electronic effective masses can be important, and that the effect of the discontinuity of the dielectric instants on the D^- states should be considered for large differences.With the effective-mass approximation, the Hamiltonian of two electrons bound to an ionized donor located in the center of a disk-like parabolic QD can be written as

$$H = \sum_{i=1,2}\left[\frac{p_i^2}{2m_e^*} + V(r_i) - \frac{e^2}{\epsilon r_i}\right] + V \tag{1}$$

with

$$V(r_i) = -V_0 \exp\left(-\frac{r_i^2}{2R^2}\right), \tag{2}$$

$$V = \frac{e^2}{\epsilon r_{12}}, \tag{3}$$

$\vec{r}_i$ ($\vec{p}_i$) is the position vector (the momentum vector) of the ith electron originating from the center of the dot, m_e^* is the effective mass of an electron, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the electron–electron separation and ϵ is the dielectric constant of the QD, V_0 is the height of the potential well and $V_0 > 0$; and R is the range of the confinement potential, which corresponds to a radius of the QD. For $r/R \ll 1$, Gaussian potential can be approximated by the parabolic potential.

Throughout the present Letter, we use the donor Rydberg $Ry^* = m_e^* Ry/\epsilon^2$ as a unit of energy, and the donor Bohr radius $a^* = \epsilon a_B/m_e^*$ as a unit of length, where Ry is the atomic Rydberg, a_B is the atomic Bohr radius. For a disk-like QD, the Hamiltonian has cylindrical symmetry with respect to the QD axis, i.e., z-axis, which implies that the total orbital angular momentum, L, and the z-component of the total orbital angular momentum L_z, are a conserved quantity, i.e.,