Impurity-related electronic properties in quantum dots under electric and magnetic fields*

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This paper presents a systematic study of the ground-state binding energies of a hydrogenic impurity in quantum dots subjected to external electric and magnetic fields. The quantum dot is modeled by superposing a lateral parabolic potential, a Gaussian potential and the energies are calculated via the finite-difference method within the effective-mass approximation. The variation of the binding energy with the lateral confinement, external field, position of the impurity, and quantum-size is studied in detail. All these factors lead to complicated binding energies of the donor, and the following results are found: (1) the binding energies of the donor increase with the increasing magnetic strength and lateral confinement, and reduce with the increasing electric strength and the dot size; (2) there is a maximum value of the binding energies as the impurity placed in different positions along the z direction; (3) the electric field destroys the symmetric behaviour of the donor binding energies as the position of the impurity.

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1. Introduction

The understanding of the nature of impurity states in semiconductor nanostructures of different geometries turns out to be a very important task, since the presence of impurity can greatly modify the physical properties of the quantum devices. Shallow impurity-related properties of the quantum well (QW), quantum-well wires (QWWs), and quantum dots (QDs) have been largely studied in recent years.[1−9] The impurity binding energies of these quantum systems can be directly manipulated by choosing appropriate materials and geometries. Due to the electronic confinement, which increases as the size of the heterostructure decreases, the impurity binding energy may strongly depend on the position of the impurity along the heterostructures as well as on the typical dimensions of the heterostructures. Acceptor-related photoluminescence spectra on GaAs–(Ga,Al)As QWW have been theoretically studied and compared with laser-induced photoluminescence measurements on GaAs wire-shaped microcrystals.[10] Concerning to QDs, Li and Xia[11] calculate the electronic structures and binding energy of a hydrogenic impurity in a hierarchically self-assembled GaAs/(Ga,Al)As QD in the framework of effective-mass envelope-function theory. They found that acceptor impurity energy levels depend more sensitively on those of the QD than those of a donor impurity, on the other hand, they have also shown that the binding energy has a maximum value when the impurity is located below the symmetry axis along the growth direction.

The effects of magnetic field on the impurity states of donors in quantum systems have been reported in recent years.[12,13] The presence of a magnetic field, as it is well known, introduces another electronic confinement which superposes with the geometrical one. Depending upon the direction of the applied magnetic field (parallel or perpendicular to the interfaces), we find that some interesting physical phenomena can take place as it is the case of the induced magnetotransport in QWs.[14] The magnetic field dependence of the binding energy of a hydrogenic impurity in a parabolic QWWs has been studied by An and Liu.[15] Using strong-confinement approach, Ferreyra *et al.* studied the influence of the magnetic field on the binding energy of the impurity.[16]

The effects of an applied electric field on the electronic states of quantum heterostructures have been

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extensively studied. An electric field applied perpendicularly to the interfaces generates the formation of a triangular QW inducing an anisotropy on the spatial distribution of the electronic wave function which reflects itself in the physical properties of the system.[17,18] Such effects could be used, for instance, to modulate the output intensity of optoelectronic devices. Recently, Mendoza *et al.*[19] reported a detailed variational calculation of the binding energies of hydrogenic impurities in a cubic QD as a function of both the impurity position and an applied electric field. They found that the binding energy of the impurities highly depend on the impurity position, and the electric field splits the energy of the impurities at points in the box which are equivalent in the absence of the electric field. However, they adopted an infinite potential model in their calculations and only studied the case of equal edge length (cubic QDs).

In this work, we are concerned with the calculation of the ground state donor-binding energy in a QD as a function of the dot size in the presence of external electric and magnetic fields applied both along the z direction. The QD is modeled by superposing a Gaussian well potential defined in the z direction and a parabolic potential in the lateral direction. The emphasis here is placed on a detailed analysis of the interplay among the impurity position in the QD, the confinement due to the external fields, and the quantum-size confinement on the donor-binding energy. These calculations are done by using the finite-difference method within the one dimensional (1D) effective potential model. The paper is organized as follows: Section 2 introduces our theoretical model, our numerical results and discussion are presented in Section 3, and finally in Section 4 the conclusions obtained are summarized briefly.

2. Theory

The effective-mass Hamiltonian of a single hydrogenic impurity in a QD, in the presence of uniform magnetic (B) and electric (F) fields, both applied the $z$direction, can be written as

$$H = \frac{1}{2m_{\rm e}^*}\left(\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right)^2 - \frac{e^2}{\varepsilon\sqrt{\rho^2+(z-z_i)^2}} + |e|\,Fz + V_z(z) + V_{\rm p}(\rho), \quad (1)$$

where $m_{\rm e}^*$ and ε are the effective mass and the dielectric constant of the material of GaAs QDs respectively, $\boldsymbol{A}$ is the vector potential associated with the magnetic field. Using a cylindrical gauge, we take the vector potential as $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B}\times\boldsymbol{r}$. We consider z_i as the impurity position along the z axis and e being the electron charge. The $V_z(z)$ is the Gaussian model of the longitudinal confinement potential[20]

$$V_z(z) = -V_0\exp(-z^2/Z^2). \quad (2)$$

Here V_0 is the depth of the potential well and Z corresponds to the range of the longitudinal confinement. And the lateral potential $V_{\rm p}(\rho)$ is given by

$$V_{\rm p}(\rho) = \frac{1}{2}m_{\rm e}^*\omega_{\rm p}^2\rho^2, \quad (3)$$

in which $\omega_{\rm p}$ is a characteristic frequency associated with the intensity of the lateral confinement.

We have used the effective electron Bohr radius in QDs, $a_{\rm d} = \hbar^2\varepsilon/m_{\rm e}^*e^2$, as the unit of length and the effective electron Rydberg $R_{\rm d} = e^2/2\varepsilon a_{\rm d}$ as the unit of energy. In these units, the Hamiltonian (1) can be rewritten as

$$H = -\nabla^2 + \left(\frac{1}{4}\gamma_{\rm m}^2 + \gamma_{\rm p}^2\right)\rho^2 + \gamma_{\rm m}L_z - \frac{2}{\sqrt{\rho^2+(z-z_i)^2}} + |e|\,Fz + V_z(z). \quad (4)$$

Here L_z is the z component of the angular momentum operator of an electron (in unit of $\hbar$). The $\gamma_{\rm m}$ and $\gamma_{\rm p}$ are dimensionless measures of the magnetic field and the parabolic potential, respectively, which are defined as

$$\gamma_{\rm m} = \frac{e\hbar B}{2m_{\rm e}^*cR_{\rm d}} \quad \text{and} \quad \gamma_{\rm p} = \frac{\hbar\omega}{2R_{\rm d}}. \quad (5)$$

For the case of the ground state, when the eigenvalue of L_z is taken as zero, the potentials associated with the magnetic field and the lateral confinement play a similar role in the Hamiltonian. One must not lose sight of the fact that the former potential is concerned with a charge particle in a magnetic field while the last one is a consequence of the particular parabolic potential chosen to model the lateral confinement. The problem has a characteristic frequency given by $\omega^2 = \frac{1}{4}\omega_{\rm c}^2 + \omega_{\rm p}^2(\omega_{\rm c} = eB/m_{\rm e}^*c)$, and in the absence of the impurity potential the ground-state energy can be written as

$$E_{\rm GS}^0 = E_{\rm F}^0 + \hbar\omega, \quad (6)$$

with $E_{\rm F}^0$ being the ground state energy of the QW potential in the presence of the electric field.

We assume that the electron is in the ground state of transverse motion. The electron wave function for

this potential can be separated in cylindrical coordinates as[21]

$$\psi(r) = \psi_{\perp}(\rho,\varphi)\psi_{//}(z). \tag{7}$$

Where

$$\psi_{\perp}(\rho,\varphi) = \frac{(\frac{1}{4}\gamma_{\rm m}^2+\gamma_{\rm p}^2)^{1/4}}{\sqrt{\pi}} \times \exp\left[-\frac{1}{2}\sqrt{\frac{1}{4}\gamma_{\rm m}^2+\gamma_{\rm p}^2}\rho^2\right], \tag{8}$$

$$V_{\rm eff}(z) = 2\sqrt{\pi}\left(\frac{1}{4}\gamma_{\rm m}^2+\gamma_{\rm p}^2\right)^{1/4} \times{\rm erfcx}\left[\left(\frac{1}{4}\gamma_{\rm m}^2+\gamma_{\rm p}^2\right)^{1/4}|z|\right]. \tag{9}$$

Here ${\rm erfcx}(t) = \exp(t^2){\rm erfc}(t)$ is the exponentially scaled complementary error function, which can be calculated using standard numerical procedures, and ${\rm erfc}(t)$ is the complementary error function. We define the operator $H_{//}$ as the Hamiltonian for the longitudinal motion which satisfies the equation

$$H_{//}\psi_{//}(z) = \int \rho{\rm d}\rho{\rm d}\varphi\psi_{\perp}^{*}(\rho,\varphi)H\psi_{\perp}(\rho,\varphi)\psi_{//}(z). \tag{10}$$

Equation (10) yields

$$H_{//} = 2\sqrt{\frac{1}{4}\gamma_{\rm m}^2+\gamma_{\rm p}^2} - \frac{\partial^2}{\partial z^2} - V_{\rm eff}(z) + |e|\,Fz + V_z(z). \tag{11}$$

The eigenvalue problem for Hamiltonian (11) depends on only one coordinate. Therefore, it can be treated with the finite-difference method on a 1D mesh.

The ground-state binding energy $E_{\rm B}$ of the impurity is defined as the ground-state energy of the system without the impurity minus the ground-state energy with the impurity:

$$E_{\rm B} = E_{\rm GS}^{0} - E_{\rm min}, \tag{12}$$

where $E_{\rm min}$ is the minimum eigenvalue of $H_{//}$ in Eq. (11).

3. Results and discussion

All the numerical results have been performed for GaAs QDs and donor impurities. The values of the parameters used in our calculations are $V_0 = 200$ meV in the Gaussian confinement, $\varepsilon = 12.5$, and $m_{\rm e}^{*} = 0.067m_0$, where m_0 is the free-electron mass. With this set of parameters, the effective units correspond to $a_{\rm d} = 9.87$ nm and $R_{\rm d} = 5.83$ meV.

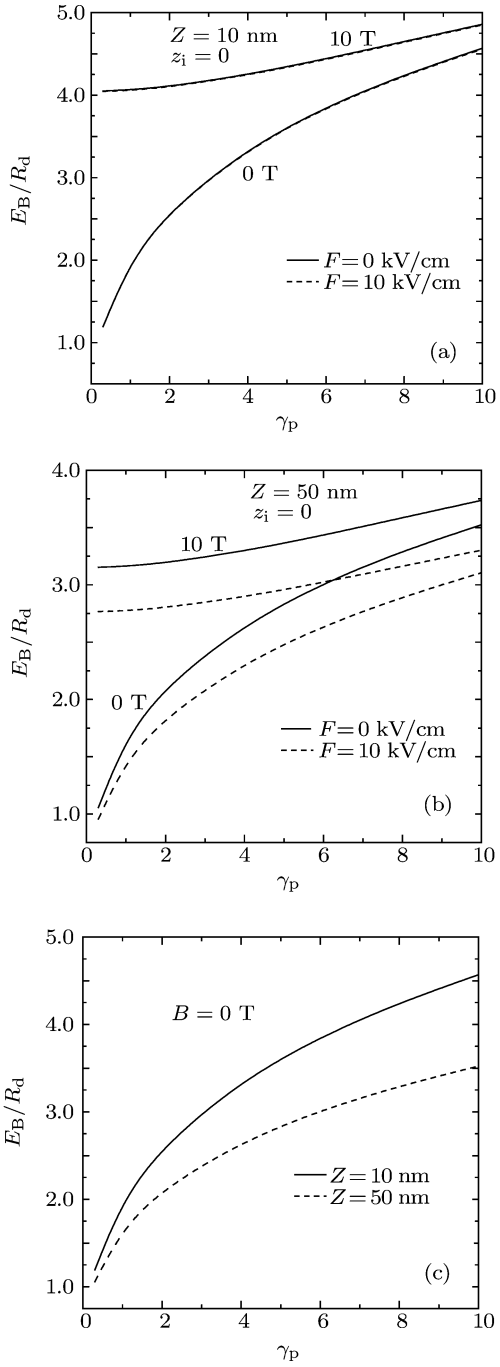


Fig. 1. Binding energies of an on-centre donor impurity in a GaAs QDs as a function of the lateral confinement for different values of the applied fields, for (a) $Z = 10$ nm, (b) $Z = 50$ nm, (c) $B = 0$ T.

Figure 1 shows the binding energy of an on-centre donor in a QD as a function of the lateral confinement for different values of the external magnetic and electric fields, corresponding to two particular well sizes which are $Z = 10$ nm and $Z = 50$ nm respectively. The binding energy exhibits a similar dependence on the lateral confinement for both well sizes. It increases with increasing parabolic potential, which confines the electron close to the donor. In the weak confinement

regime, in which the lateral confinement energies are lower than the binding energy of a donor in the bulk ($\gamma_{\rm p} < 1$), a linear behaviour with the characteristic frequency ω is expected, since in this limit the lateral confinement potential can be considered as a small perturbation. For zero magnetic and electric field, the binding energy is in fact linear with $\gamma_{\rm p}$ and the same slope is obtained for $Z = 10$nm and $Z = 50$ nm. It is worth noticing that in the limit of $\gamma_{\rm p}$ the result is suitable for the binding energy of donors in a QW. For a strong lateral confinement, one would expect a binding energy less sensitive to the increase of the parabolic confining potential. In that regime, the Coulomb interaction is governed by the complex interplay determined by the QD size and the external fields. This behaviour is more obvious for $Z = 50$ nm when an electric field is applied. The results presented in Fig. 1(b) for a $Z = 50$ nm QD, clearly show that the increase of the electric field decreases the sensitivity of the binding energy to the increase of lateral confinement. In that case, there is an additional electronic confinement in the z direction due to the formation of a triangular potential.

In Fig. 1 it also shows that the influence of the electric field on the binding energies is more sensitive to the dot size than that of the magnetic field, which can be seen from the comparison between Figs. 1(a) and 1(b). The binding energies in $F = 10$ kV/cm are almost the same as those in the zero electric field in Fig. 1(a) for $Z = 10$ nm, but the splitting originated by the presence of an electric field is obvious in Fig. 1(b) for $Z = 50$ nm. While, the splitting originated by the magnetic field is almost the same for different dot sizes.

In order to have a clear picture about the interaction between the dot size and the lateral confinement, we draw the binding energies as functions of the lateral confinement for different dot sizes in the same picture Fig. 1(c). It shows that the influence of the lateral confinement is stronger for $Z = 10$ nm than that for $Z = 50$ nm. It is very different from the interaction between electric field and dot size. This is because the electric field has effects on the z direction, along the well. When the dot size decreases, which means the increasing confinement, the interaction between the electron and ion will be difficult to change, so that the effect of the electric field can be seen as a small perturbation. However, the lateral confinement is perpendicular to the well. When the electron is confined in the z direction, the Coulomb interaction will be more sensitive to the lateral confinement, which is the reason why the binding energy is more sensitive to lateral confinement potential in small dot size than in large one. Because the magnetic field also has effects on the lateral direction, the influence of the dot size on it has the same trend as the lateral confinement, shown in Fig. 2(c).

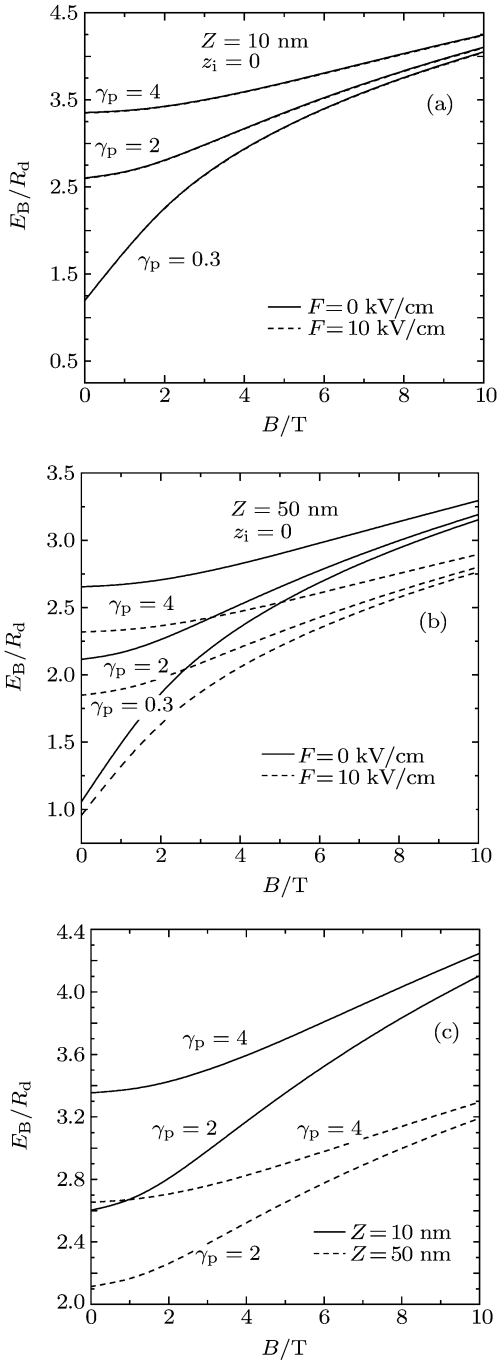


Fig. 2. Magnetic field dependence of the impurity binding energies of an on-centre donor in a GaAs QD for $F = 0$ and $F = 10$ kV/cm,$\gamma_{\rm p} = 0.3$, $\gamma_{\rm p} = 2$, and $\gamma_{\rm p} = 4$.

Figure 2 displays the dependence of the on-centre donor-binding energy on the applied magnetic field for

fixed values of electric field and dot sizes. One must take into account that now the lateral confinement is controlled by changing the magnetic field. It can be seen in Fig. 2(b), as expected, that the reduction of the electron cyclotron radius by applied magnetic fields up to 10 T is not competitive with the lateral confinement defined by $\gamma_{\rm p} = 4$, this fact leads to nearly magnetic-field-independent binding energies.

Figure 3 shows the on-centre donor-binding energies as a function of the applied electric field for different lateral confinement and magnetic field values.

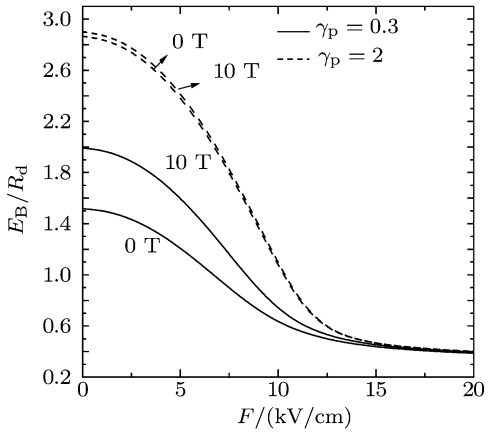


Fig. 3. Electric field dependence of an on-centre donor impurity in a GaAs QD for $B = 0$ and $B = 10$ T, and different values of $\gamma_{\rm p}$.

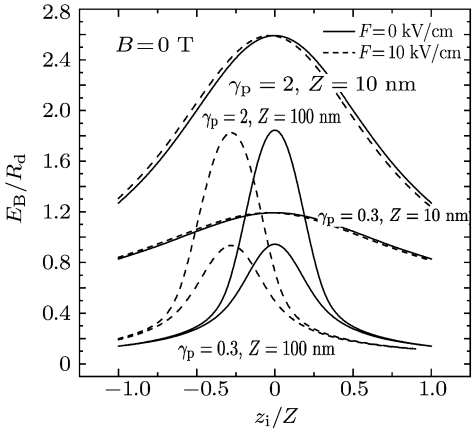


Fig. 4. Binding energies of a donor in a GaAs QD as a function of the impurity position along the z direction for $B = 0$ T, for $F = 0$ kV/cm and $F = 10$ kV/cm, and different values of $\gamma_{\rm p}$ and Z.

As it was pointed out before, the electric field effects are only manifested for QW lengths for which the electric field energy is greater than the QW energy. This is clearly shown in Fig. 1(a) where the binding energy is almost insensitive to the strength of the electric field for the range of values displayed. A completely different behaviour takes place for a $Z = 100$ nm QD in which case the electric field pushes the electron to the opposite barrier, takes it apart from the impurity centre. For on-centre impurities, this effect leads to a decrease of the binding energies as a function of the electric field.

For impurities placed next to the electronic distribution, confined by the electric field, an enhancement of the binding energy is found. This can be seen in Fig. 4, where the donor binding energies as a function of the impurity position along the z direction are presented. For an electric field of 10 kV/cm, a departure from the typical symmetric behaviour exhibited by the binding energy in the absence of an applied electric field, can be clearly observed. For that field, the binding energy exhibits a maximum when the impurity is placed in $z_i = 0.3Z$ for a $Z = 100$ nm dot. It also exhibits that as the increas of the dot size the maximum place is away from the center of the dot. For strong electronic confinement, although the binding energies also exhibit a large spread as a function of the impurity position, the effects of the electric field are less important.

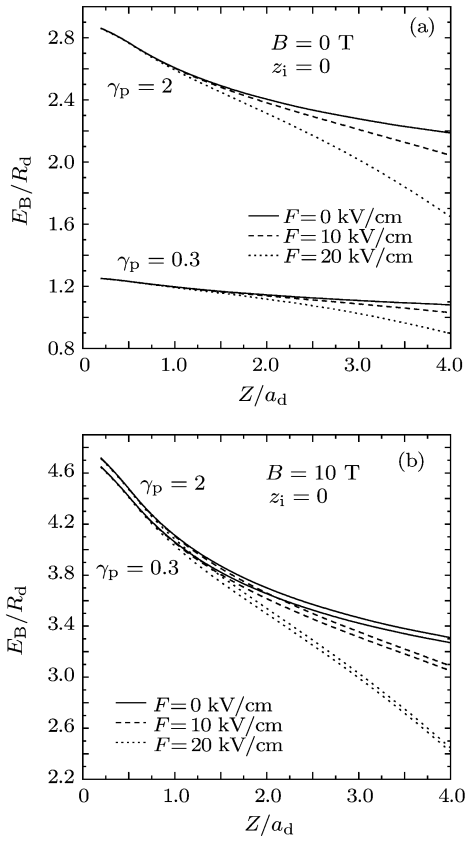


Fig. 5. Binding energies of an on-centre donor in a GaAs QD as a function of the QD size for different values of the applied fields and $\gamma_{\rm p}$.

Finally, in Fig. 5, we present the results for the impurity binding energy of an on-centre donor in a QD as function of the well width. A large range of binding energies is covered and a pronounced shift for increasing values of the applied electric field can be noticed. In fact, crossover regions in the spectrum of the donor-binding energy are exhibited in Fig. 5(b) reflecting the interplay among different confinement mechanisms. Figure 5 summarizes many of the features obtained for the on-center impurity binding energies for the different regimes considered. In particular, the onset of the spread of the binding energy due to the electric field is clearly evidenced.

4. Conclusions

The binding energies of the ground state of a hydrogenic impurity in a GaAs QD have been calculated by using the finite-difference method. We have considered the effects of external field, quantum-size confinements and donor places on the impurity ground state. The complex interplay of these effects leads to a complicated dependence of the binding energies on these factors. Our results also emphasize the importance of including the correct impurity profile in order to describe quantitatively an experiment performed in a particular doping condition. Although to our knowledge, there are no available experimental data to compare with our theoretical results, we believe that they provide an indication so that a tailored procedure can easily be used to change electronic properties of doped nanostructures. The theoretical model of the QD and the calculation method can be extended to other low-dimensional quantum systems.

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