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Effect of magnetic field on the formation of D^- ions in lens-shape quantum dots

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Abstract

We report a calculation of the ground state binding energies of the on- and off-axis neutral, D^0, and negatively charged, D^-, donors in an oblate lens-shaped InAlAs/GaAlAs quantum dot in the presence of a uniform magnetic field applied parallel to the dot axis. The calculations have been performed by using the adiabatic approximation for the electron, a Bastard-type trial function for the D^0, and the Hylleraas-type trial function for the D^- ion. Novel curves and contour plots for the energies of donors confined in a quantum lens as functions of the distance from the axis for several dot heights and magnetic field strengths are presented. We show that under strong magnetic field the on-axis D^- ion binding energy becomes larger than the corresponding value of the D^0 located in the peripheral region close to the barrier, making possible the formation of on-axis D^- centres in equilibrium via electron transfer from the peripheral donor to the on-axis D^0.

1. Introduction

A negatively charged donor, D^-, ion appears when a neutral donor, D^0, in the quantum well (QW) traps a second electron released into well by a barrier neutral donor [1]. The electron transferring between two neutral donors becomes possible because of the fact that the D^- ions located inside the well are more strongly bound than in bulk; meanwhile, the neutral donors D^0 located in the barrier close to the well are more weakly bound than in bulk. The stronger the confinement the larger is the ratio of the binding energy of the negatively charged well donor to the binding energy of the barrier neutral donors located close to the well and the more probable is the formation of D^- ions inside the well by means of trapping of the electron released into well by the barrier donor. This mechanism of formation of D^- ions in QWs has previously been analysed by Larsen [2]. One can expect that this process should be more pronounced in quantum dots (QDs), where the effect of the confinement is stronger than in QWs.

Recently, the Stranski–Krastanov growth technique [3] has been used to manufacture self-assembled quantum dots (SAQDs) with controlled thickness and relatively sharp interfaces whose shapes look alike, of pyramids, cones, discs, lenses or rings. Structural studies have shown that the SAQDs commonly are oblate because their heights are much smaller than the base sizes [3]. Spectra of the particles confined in QDs are strongly dependent on the structural properties such as size and morphology. Therefore, the capability to design and manufacture new opto-electronic devices is inextricably bound up with the knowledge of the energy spectrum of a few particles [4]. In consequence, reliable methods to calculate the electronic structure of few particle systems in QDs are required. This is the reason why many studies of QDs containing an exciton or two electrons have been fulfilled in the last two decades. Spectra of these systems have been analysed by using different methods, such as variational [5], diagonalization [6], finite elements [7], perturbation theory [8] and the adiabatic approximation [9].

Ground state binding energies of the on-centre D^0 and D^- confined in a spherical quantum dot (SQD) have been calculated in the papers [10] by using the series expansion and variational method, respectively. It has been shown that the ratio of the on-centre D^- binding energy to the on-centre D^0 binding energy in an SQD is essentially larger than in other types of heterostructures and it can reach the proportion 1:3. Off-centre D^0 binding energies in an SQD have been calculated in the paper [11] by using the diagonalization method. The energy levels of the ground and excited states of both the spin-singlet and spin-triplet configurations for the on-centre D^- confined in an SQD have been calculated by variational means and the conditions of binding for the excited states have been determined as functions of the potential-well depth and quantum-dot radius [12]. Recently, we have proposed a fractal dimension scheme [13] for calculating the ground state energies of the off-centre donors D^0 and D^- which gives results in excellent concordance with those obtained previously for a QW, cylindrical quantum wire and SQD by means of the Monte Carlo [14], diagonalization [11] and series expansion [10] methods.

A comprehensive analysis of the influence of the dot size and shape on the off-axis D^0 and D^- donor binding energies in SAQDs and the possibility of the electron transferring from the peripheral donor to the on-axis one has been done more recently [15] by using the fractal dimension procedure. On the other hand, the formation of D^- ions in QDs could be additionally reinforced under strong magnetic field, which reduces the separation between an electron and the donor located close to the axis, whereas this separation increases for the peripheral donor. In this paper we explore the conditions more relevant for the formation of the D^- ion in SAQDs in the presence of magnetic field. To this end, we extend the fractal-dimensional scheme [13] in the case of the oblate QDs with axial symmetry for calculating the ground state binding energies of D^0 and D^- in lens-shaped InAlAs–AlGaAs SAQDs with large base radius–height aspect ratio. The last condition permits us to take advantage of the adiabatic approximation, in order to separate the one-particle rapid motion along the z-axis from the slower lateral motion in the x–y plane and thus to make possible the application of the fractal-dimensional scheme.

This paper is organized as follows. In the next section we consider the theoretical model of the D^0 and D^- confinement in a lens-shaped SAQD. In section 3 we show how the wave equation for the electron in the SAQD can be reduced to a two-dimensional central force problem by using the adiabatic approximation. A short description of the fractal-dimensional scheme for calculating the binding energies of donors confined in lens-shaped SAQDs is given in section 4. The results of the D^0 and D^- energies as functions of the donor position, QD height and magnetic field strength and the discussion of the effect of the magnetic field on the formation of the D^- in SAQDs are presented in section 5. A summary is provided in section 6.

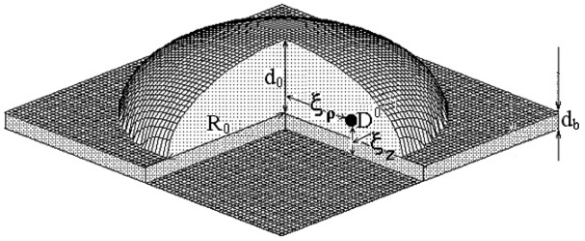

Figure 1. Schematic picture of a lens-shaped self-assembled quantum dot including a wetting layer as part of the QD.

The numerical procedures used for solving the two-dimensional central force problem and for calculating the binding energies are given in appendices A and B, respectively.

2. Model

We consider a lens-shaped QD of height d_0 modelled as a part of an ellipsoid with circular base of radius R_0 on a wetting layer of thickness d_b. The structure's thickness, d, dependence on the distance from the axis, ρ, is defined by the function

$$d(\rho) = \begin{cases} d_b; & \rho > R_0 \\ d_b + d_0\sqrt{1-(\rho/R_0)^2}; & \rho < R_0. \end{cases} \tag{1}$$

A schematic picture of a lens-shaped QD given by these relations is shown in figure 1, where the parameters ξ_ρ and ξ_z give the distances from the donor to the axis and the bottom of the wetting layer, respectively. In what follows we consider the wetting layer as a part of the QD. The confining potential $V(\rho, z)$ inside the QD and the wetting layer ($0 < z < d(\rho)$) is equal to zero and it is equal to V_0 in the barriers ($z < 0$ or $z > d(\rho)$).

Neglecting the differences between the material parameters, the dielectric constant ε and the electron effective mass m^* of the well and those of the barriers, the dimensionless Hamiltonian of D^- ion S states in a QD in the presence of a uniform magnetic field, $\mathbf{B} = B\,\hat{\mathbf{z}}$ can be written as

$$\hat{H}(\mathbf{r}_1, \mathbf{r}_2, Z_1, Z_2) = \hat{H}_0(\mathbf{r}_1, Z_1) + \hat{H}_0(\mathbf{r}_2, Z_2) + 2Z_1Z_2/|\mathbf{r}_1 - \mathbf{r}_2|; \tag{2a}$$

$$\hat{H}_0(\mathbf{r}_i, Z) = -\nabla_i^2 + V(\rho_i, z_i) + \gamma^2\rho_i^2/4 - 2Z/|\mathbf{r}_i - \boldsymbol{\xi}|; \qquad i = 1, 2; \tag{2b}$$

where $\boldsymbol{\xi} = (\boldsymbol{\xi}_\rho, \xi_z)$ and $\mathbf{r}_i = (\boldsymbol{\rho}_i, z_i)$ designate the 3D position vectors of the ion and electrons 1 and 2, respectively. The effective Bohr radius $a_0^* = \varepsilon\hbar^2/m^*e^2$, the effective Rydberg $Ry^* = e^2/2a_0^*\varepsilon$ and the first Landau level expressed in R_y^*, $\gamma = e\hbar B/2m^*cRy^*$, have been taken as units of length, energy and the dimensionless magnetic field strength, respectively. One can see that the Hamiltonians (2*a*) and (2*b*) describe different situations for different sets of the parameters Z, Z_1 and Z_2. In particular, Z in the one-particle Hamiltonian (2*b*) is equal to zero for the free electron and one for the donor, the set $Z_1 = 1$ and $Z_2 = 1$ corresponds in (2*a*) to D^- whereas the set $Z_1 = 1$ and $Z_2 = 0$ in the Hamiltonian (2*a*) may be related to a hypothetical model of the non-interacting neutral donor D^0 and electron, both confined within the QD.

The ground state wavefunctions of a free electron, $f_0(\mathbf{r})$, a neutral donor, $\Psi_{D^0}(\mathbf{r})$, a negatively charged donor, $\Psi_{D^-}(\mathbf{r}_1, \mathbf{r}_2)$, and their corresponding lowest energies E_0, $E(D^0)$

and $E(\mathrm{D}^-)$ in a QD, can be found as solutions of the respective eigenvalue problems:

$$\hat{H}_0(\mathbf{r}, Z=0) f_0(\mathbf{r}) = E_0 f_0(\mathbf{r}) \tag{3a}$$

$$\hat{H}_0(\mathbf{r}, Z=1) \Psi_{\mathrm{D}^0}(\mathbf{r}) = E(\mathrm{D}^0) \Psi_{\mathrm{D}^0}(\mathbf{r}) \tag{3b}$$

$$\hat{H}(\mathbf{r}_1, \mathbf{r}_2, Z_1=1, Z_2=1) \Psi_{\mathrm{D}^-}(\mathbf{r}_1, \mathbf{r}_2) = E(\mathrm{D}^-) \Psi_{\mathrm{D}^-}(\mathbf{r}_1, \mathbf{r}_2). \tag{3c}$$

In order to analyse the problem of existence of bound states for neutral and negative donors in the QD their binding energies $E_b(\mathrm{D}^0)$ and $E_b(\mathrm{D}^-)$ have been defined in [12] as minimum energies required to liberate one electron from the bound state of the donors located in a single QD and transfer it into the barrier region. Once the donor ground state energies $E(\mathrm{D}^0)$ and $E(\mathrm{D}^-)$ are calculated, the binding energies according to this definition are given by

$$E_b(\mathrm{D}^0) = V_0 - E(\mathrm{D}^0); \qquad E_b(\mathrm{D}^-) = V_0 + E(\mathrm{D}^0) - E(\mathrm{D}^-). \tag{4a}$$

Another definition of the binding energies as a difference between the eigenvalues of the Hamiltonians $\hat{H}_0(\mathbf{r}, Z=0), \hat{H}_0(\mathbf{r}, Z=1)$ for the D^0 and $\hat{H}(\mathbf{r}_1, \mathbf{r}_2, Z_1=1, Z_2=0), \hat{H}(\mathbf{r}_1, \mathbf{r}_2, Z_1=1, Z_2=1)$ for D^- was used in [10, 11]. Since these differences can be considered as correlation energies related to the Coulomb interactions responsible for the trapping of the electron, in what follows we denote them as $E_c(\mathrm{D}^0)$ and $E_c(\mathrm{D}^-)$ for the neutral and negatively charged donors, respectively:

$$E_c(\mathrm{D}^0) = E_0 - E(\mathrm{D}^0); \qquad E_c(\mathrm{D}^-) = E_0 + E(\mathrm{D}^0) - E(\mathrm{D}^-). \tag{4b}$$

Detailed discussion of the physical meaning of the binding energy (4*a*) and the correlation energy (4*b*) was given in [12]. One can observe that the correlation energies given by the relations (4*b*) contain the refined information only about intrinsic properties of donors confined in the QD whereas the binding energies (4*a*) give joint information about properties of both the donor and the surroundings. To study a process of donor ionization related to transferring of the electron in the conduction band one can calculate $E_b(\mathrm{D}^0)$ and $E_b(\mathrm{D}^-)$, whereas to describe a process of electron transfer between donors located within the same QD it is preferable to use the correlation energies $E_c(\mathrm{D}^0)$ and $E_c(\mathrm{D}^-)$. In what follows we present the results of calculation of both the binding and correlation energies.

3. Free electron ground state

Equation (3*a*) for a free electron in a QD does not completely separate and no exact solutions have been found. It is therefore of interest to consider the case $d_0 \ll R_0$ corresponding to a strongly oblate lens, which we call the adiabatic limit for the following reason. One can rescale the coordinates in the wave equation (3*a*) in such a way that displacements in z and radial directions become of the same order by using the substitutions $z = d_0\tilde{z}$ and $\rho = R_0\tilde{\rho}$. In these rescaled coordinates the electron motion is mainly restricted within the region $0 < \tilde{\rho}, \tilde{z} < 1$ and it is described by the wave equation

$$\begin{aligned} &-\frac{1}{d_0^2}\frac{\mathrm{d}^2 f_0(\tilde{\rho}, \tilde{z})}{\mathrm{d}\tilde{z}^2} - \frac{1}{R_0^2}\nabla_{\tilde{\boldsymbol{\rho}}}^2 f_0(\tilde{\rho}, \tilde{z}) + \tilde{V}(\tilde{\rho}, \tilde{z}) f_0(\tilde{\rho}, \tilde{z}) = E_0 f_0(\tilde{\rho}, \tilde{z}); \\ &\tilde{V}(\tilde{\rho}, \tilde{z}) = V(\tilde{\rho}, \tilde{z}) + \frac{\gamma^2 R_0^2 \tilde{\rho}^2}{4}. \end{aligned} \tag{5}$$

Equation (5) may be regarded as the Schrödinger equation describing two hypothetical particles, the light particle of mass d_0^2 and the heavy particle of mass R_0^2, interacting through the potential $\tilde{V}(\tilde{\rho}, \tilde{z})$. Since one of these masses is much larger than the other, we follow

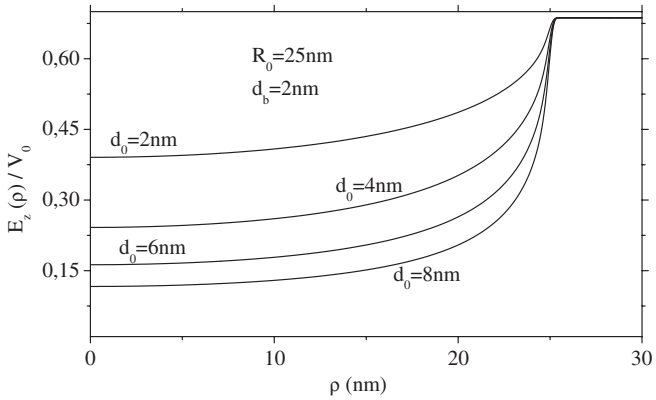

Figure 2. Normalized in-plane confining potential curves for QDs with different heights.

the well known adiabatic procedure of first solving the equation for the light particle motion along the z-axis:

$$-\frac{\mathrm{d}^2 f_z(z,\rho)}{\mathrm{d}z^2} + V(\rho,z) f_z(z,\rho) = E_z(\rho) f_z(z,\rho), \tag{6}$$

where ρ is treated as a parameter (cf electronic motion for fixed nuclear position in the molecular problem), and then for the heavy particle in-plane motion

$$-\nabla_{\boldsymbol{\rho}}^2 f_\rho(\rho) + \left[E_z(\rho) + \frac{\gamma^2 \rho^2}{4} \right] f_\rho(\rho) = E_0 f_\rho(\rho). \tag{7}$$

In equations (6) and (7) we return again to the initial coordinates. The dependence of the eigenvalue E_z on the distance from the axis, ρ, represents the potential curve for a two-dimensional central force given by equation (7).

Once the functions $f_z(z,\rho)$ and $f_\rho(\rho)$ are found, the function $f_0(\mathbf{r})$ can be obtained through

$$f_0(\mathbf{r}) = f_z(z,\rho) f_\rho(\rho). \tag{8}$$

Numerical procedures for calculating the free electron ground state energy in QD, $E_z(\rho)$, E_0, $f_z(z,\rho)$ and $f_\rho(\rho)$ are given in appendix A.

In figure 2 we display the potential curves, $E_z(\rho)$, for the in-plane electron motion in QDs with the base radius $R_0 = 25$ nm, the wetting layer thickness $d_b = 2$ nm and four different values of d_0: 2, 4, 6 and 8 nm. One can see that the barrier height for the in-plane motion decreases due to the confinement in the z-direction approximately by 48% as the QD thickness is equal to 6 nm, 56% for $d_0 = 4$ nm and 70% when $d_0 = 2$ nm. Generally, the smaller the QD height the larger is the decrease of the barrier height.

4. Neutral and negatively charged donor ground states

To find the ground state wavefunctions $\Psi_{D^0}(\mathbf{r})$ and $\Psi_{D^-}(\mathbf{r_1}, \mathbf{r}_2)$ corresponding to the lowest energies $E(D^0)$ and $E(D^-)$, we use the Bastard-type [16] trial functions:

$$\Psi_{D^0}(\mathbf{r}) = f_0(\mathbf{r}) \Phi_{D^0}(|\mathbf{r} - \boldsymbol{\xi}|); \qquad \Psi_{D^-}(\mathbf{r}_1, \mathbf{r}_2) = f_0(\mathbf{r}_1) f_0(\mathbf{r}_2) \Phi_{D^-}(|\mathbf{r}_1 - \boldsymbol{\xi}|, |\mathbf{r}_2 - \boldsymbol{\xi}|, r_{12}) \tag{9}$$

where the envelope functions, Φ_{D^0} and Φ_{D^-}, describe the alterations of the one- and two-particle wavefunctions, respectively, caused by the Coulomb interactions.

As has been demonstrated in [13], the trial functions (9) satisfy the Schrödinger variational principle, if the envelope functions Φ_{D^0} and Φ_{D^-} are solutions of wave equations for the hydrogen atom H and negatively charged ion H^-, respectively, with modified Laplacian in which the radial part of the Jacobian r^2 is replaced by the expression $J(r) = r^2 \int f_0^2(\mathbf{r}')\delta(|\mathbf{r}'| - r)\,\mathrm{d}\mathbf{r}'$. Once the free electron wavefunction (8) is defined, the dependence of the Jacobian on r may then be found in a straightforward way by means of a numerical estimation of this integral, which for the wavefunction (8) in cylindrical coordinates can be found as [13]

$$\begin{aligned} &J(r) = r\int_0^{2\pi} \mathrm{d}\varphi \int_{-r}^{r} \mathrm{d}z\, f_z^2(z+\xi_z, |\boldsymbol{\rho}+\boldsymbol{\xi}_\rho|) f_\rho^2(|\boldsymbol{\rho}+\boldsymbol{\xi}_\rho|); \\ &|\boldsymbol{\rho}+\boldsymbol{\xi}_\rho| = \sqrt{r^2 - z^2 + \xi_\rho^2 + 2\xi_\rho\sqrt{r^2-z^2}\cos\varphi}. \end{aligned} \tag{10}$$

The function $\Phi_{D^0}(r)$ is the solution of the following wave equation [13]:

$$-\frac{1}{J(r)}\frac{\mathrm{d}}{\mathrm{d}r}\left[J(r)\frac{\mathrm{d}\Phi_{D^0}(r)}{\mathrm{d}r}\right] - \frac{2}{r}\Phi_{D^0}(r) = [E(D^0) - E_0]\Phi_{D^0}(r). \tag{11}$$

In order to estimate $E(D^-)$ we use for Φ_{D^-} the following simple three-parametric Hylleraas trial function [17]:

$$\Phi_{D^-}(r_1, r_2, r_{12}) = \left[1 + \beta(r_1 - r_2)^2 + \eta r_{12}\right]\exp(-\alpha(r_1 + r_2)), \tag{12}$$

which permits us to find the variational energy $E(D^-, \alpha, \beta, \eta)$ as a function of three parameters α, β and η. The estimated upper limit of the negatively charged donor then can be found as

$$E(D^-) = \min_{\alpha,\beta,\eta\in(0,1)} E(D^-, \alpha, \beta, \eta). \tag{13}$$

Some details of our numerical procedure used for calculating $E(D^0)$ and $E(D^-)$ are given in appendix B.

5. Results and discussion

In what follows we present the results of calculation for heterostructures of $In_{0.55}Al_{0.45}As/Ga_{0.65}Al_{0.35}As$ where the values of a_0^* and Ry^* are equal to 8.86 nm and 6.40 meV, respectively, and the barrier height $V_0 \approx 40\ Ry^*$ [18]. It should be noted that the heterostructures of $GaAs/Ga_{0.7}Al_{0.3}As$ have a set of parameters close to these values and therefore the results presented below are also applicable with a slight variation to these heterostructures. The donor position in a QD with axial symmetry given by the vector $\boldsymbol{\xi}$ is described by means of two parameters, ξ_ρ, the distance from the axis, and ξ_z, the distance from the wetting layer bottom.

We calculate the correlation and the binding energies of the D^0 and D^- centres located in different parts of QDs with the base radius 25 nm, the wetting layer thickness 2 nm and different heights, d_0, 2, 4, 6 and 8 nm, with and without external magnetic field. The calculation results are presented in figures 3–6. First, we have performed a numerical calculation of the correlation and the binding energies of donors with different distances from the axis, ξ_ρ, and located on the edge of the wetting layer, $\xi_z = d_b$. Donor ground state correlation energies as a function of ξ_ρ in QDs with different heights are shown in figures 3(a) and (b). Similar dependences for the binding energies are shown in the insets. The decrease

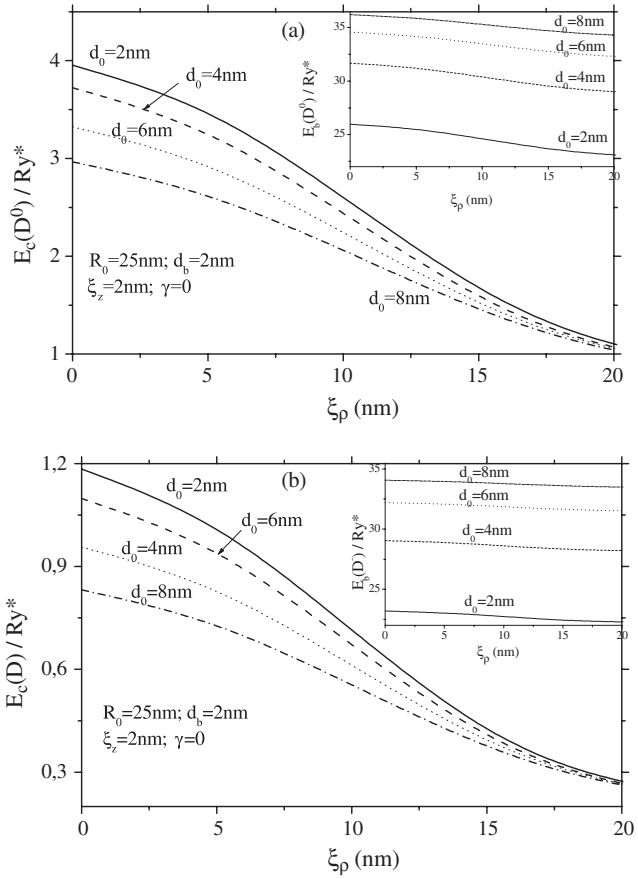

Figure 3. The correlation energy of D^0 (a) and D^- (b) as a function of the distance from the axis of the QDs with different heights. In the inset the donor binding energy is plotted. The same curve conventions are used as in the main figure.

of the correlation and the binding energies as the donor is removed from the axis can be easily observed. It is due to the fact that the motion of the electron is mainly restricted in the region close to the axis, independently of the donor position. Therefore, as the donor is removed from the axis, the mean distance between the electrons and ion increases while the binding energy decreases. It is also seen from figures 3(a) and (b) that the orders of the curves for different QD heights in the main figure and in the inset are inverted. The correlation energies of both neutral and negative donors in the main figures decrease as the height of the quantum dot increases, whereas curves with larger binding energies in the insets correspond to donors located in QDs with larger heights. As the QD height reduces the donor binding energies decrease due to the fact that all energy levels, of the electron and the neutral and negative donors, climb up toward the conduction band bottom. On the other hand, this rise of the energy levels is accompanied by the enhancement of the distances between them determined by the Coulomb correlation energy.

In figure 4 we present similar dependences of the donor correlation and binding energies in a QD with height $d_0 = 4$ nm, base radius $R_0 = 25$ nm and wetting layer thickness $d_b = 2$ nm for several magnetic field strengths. It is seen from the main figures 4(a) and (b)

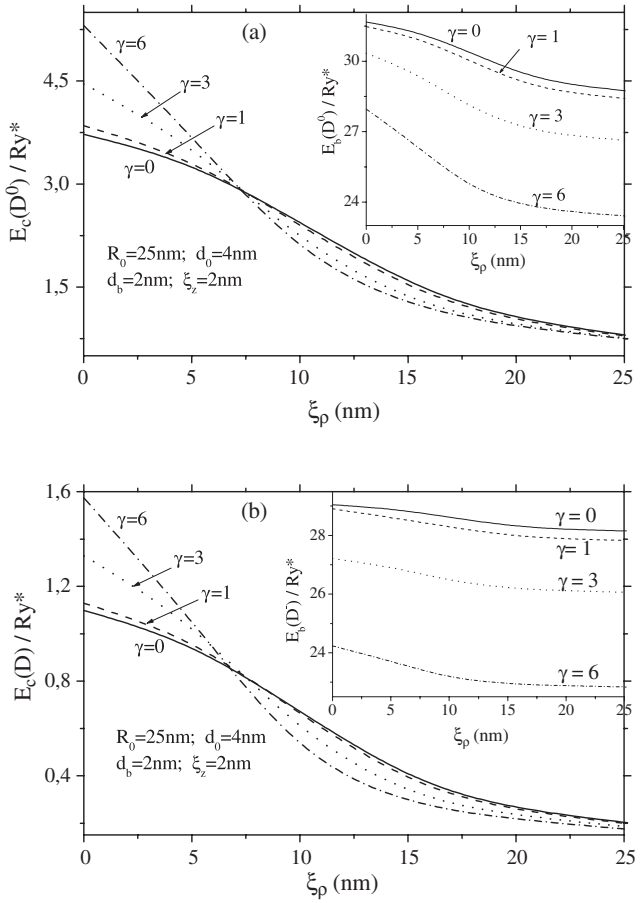

Figure 4. The correlation energy of D^0 (a) and D^- (b) as a function of the distance from the axis of QDs under different magnetic fields. In the inset the donor binding energy is plotted. The same curve conventions are used as in the main figure.

that under magnetic field the correlation energies of donors located close to the axis increase while the correlation energies of donors located far from the axis decrease. In consequence, all curves cross at the same point, where the correlation energy remains unchanged. The external magnetic field provides an additional confinement which restricts the electron motion in the radial direction, making more probable their location close to the axis. Due to such variation of the charge distribution under magnetic field, the separation between electrons and ions for donors located close to the axis decreases, providing the increase of the Coulomb correlation energy, and inversely this separation increases when donors are situated far from the axis.

In order to achieve a better understanding of the dimensional characteristics of the D^0 and D^- centres in QD, we present in figure 5 the ratio $\sigma = E_c(D^-)/E_c(D^0)$ as a function of the distance of the donor from the axis for different QD heights (a) and for different magnetic field strengths (b).

For the unconfined 3D and 2D cases, the ratio σ is respectively equal to 0.0506 and 0.086 in the present work (by using the Hylleraas three-parameter trial function) and 0.056 and 0.128 in the paper of Louie and Pang [14] (by using the diffusion Monte Carlo method). As established previously the limit values of σ for on-centre donors in an SQD [10, 13]

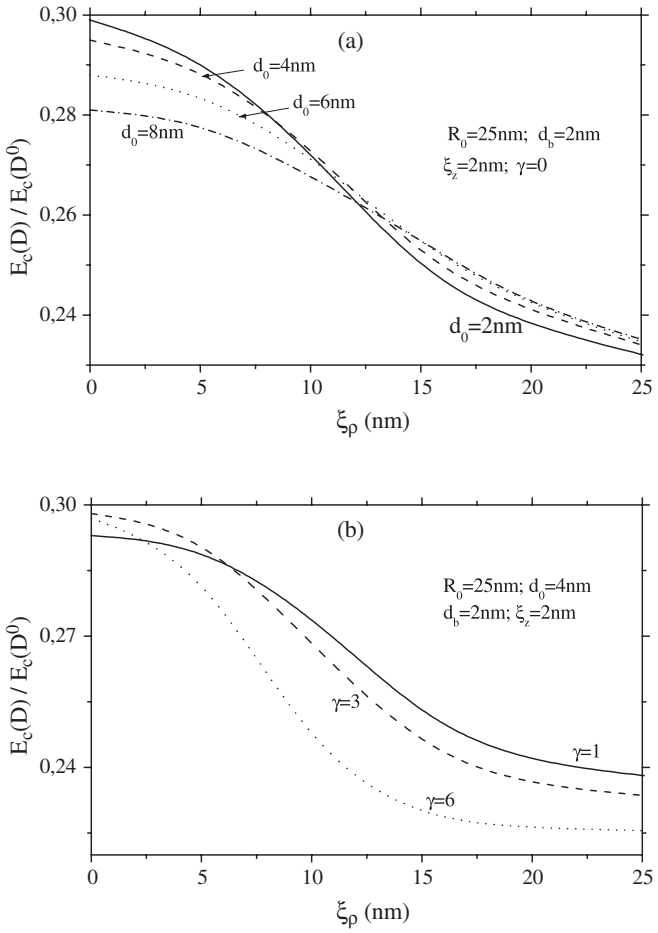

Figure 5. Ratio $\sigma = E_c(D^-)/E_c(D^0)$ as a function of the distance of the donor from the axis of the dot for different QD heights (a) and for different magnetic field strengths (b).

and a cylindrical quantum well-wire [13] with the barrier height $40Ry^*$ are about 0.3 and 0.2, respectively. Consequently, one can expect that typical values of σ for 0D, 1D and 2D heterostructures are respectively about 0.3, 0.2 and 0.1. Indeed, as seen from figure 5, the limit value, $\sigma \cong 0.3$, for an SQD is also valid for donors located close to the axis of the lens-shaped QD independently of the presence of the magnetic field. When the donor is removed far from the axis σ is reduced and tends monotonically toward the 1D limit, 0.2, demonstrating that both D^0 and D^- configurations adopt a nearly linear geometrical shape with the electrons located mainly close to the axis and the ion displaced in the peripheral region. As seen from figure 5(b), under strong magnetic field the σ 1D limit is achieved more rapidly with removing the donor position in the peripheral region. This is due to the fact that under magnetic field the electron motion becomes more restricted in the vicinity of the axis and with the donor displacement from the axis the electron orbit becomes more elongated.

In order to facilitate the interpretation of the calculation results for off-axis D^0 and D^- centres, we show the contour plots in figure 6, which correspond to the level lines of the $E_c(D^0)$ and $E_c(D^-)$ of donors with different positions along a cross section through the axis

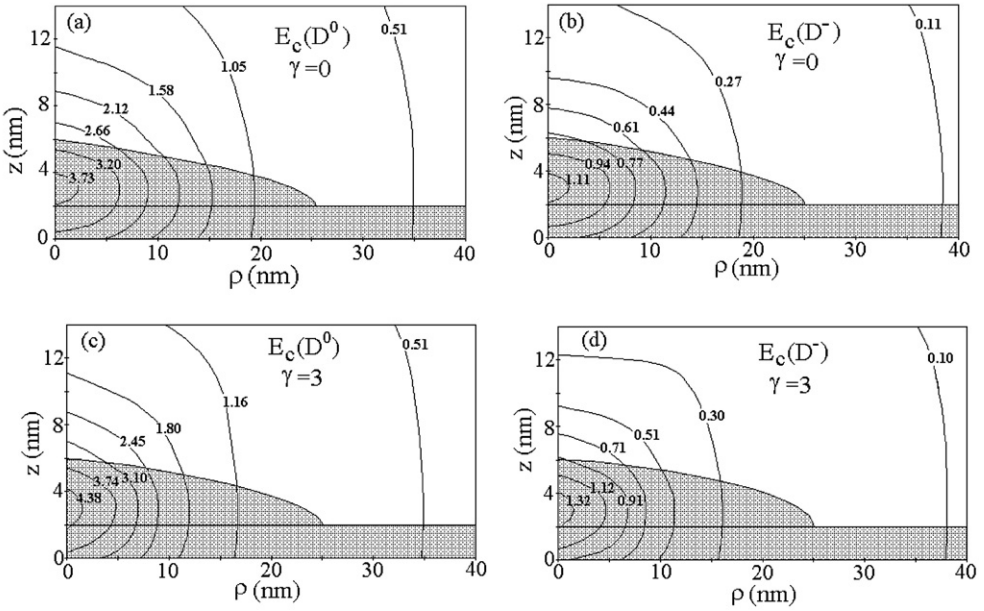

Figure 6. Contour plots of the correlation energies of D^0 and D^- in a plane through the axis of symmetry of the quantum lens with base radius 25 nm, height 4 nm and wetting layer of thickness 2 nm for $\gamma = 0$ (figures 6(a) and (b)) and $\gamma = 3$ (figures 6(c) and (d)).

of symmetry of the lens for $\gamma = 0$ (figures 6(a) and (b)) and $\gamma = 3$ (figures 6(c) and (d)). The shadowed parts indicate the cross section of the QD with the base radius 25 nm, height 4 nm and wetting layer thickness 2 nm. The numbers on the contour plot lines indicate the donor correlation energies in Ry^*. Due to the squeezing by the applied magnetic field the particles become more centred in the middle of the dot and the level lines in the lower contour plots (figures 6(c) and (d)) for $\gamma = 3$ become more compressed along the ρ direction than those in the upper contour plots (figures 6(a) and (b)) for $\gamma = 0$. It is also seen that the behaviour of the level lines for the D^0 and D^- centres, in general, is similar, and in both cases the correlation energies under magnetic field increase for donor locations close to the axis and they decrease for peripheral locations.

Comparing the contour plots for the D^0 and D^- centres presented in figures 6(a) and (b) one can see that the correlation energies of the D^- located close to the axis are larger than the correlation energies of the peripheral D^0, i.e. the peripheral D^0 are more weakly bound than the D^- ions located close to the axis. For example, the on-axis D^- correlation energy in figure 6(b) is about 1.11 Ry*, whereas the correlation energies of the peripheral D^0 in figure 6(a) distant from the axis more than 20 nm are less than 1.05 Ry*. This means that the transferring of the electron from the peripheral D^0 to the D^0 located close to the axis is energetically favourable. In consequence, a significant population of D^- ions can appear in equilibrium close to the axis. Additionally, one can observe in figures 6(c) and (d) that in the presence of the magnetic field the difference between the correlation energies of the D^- located close to the axis and those of the peripheral D^0 increases, and therefore the process of the formation of D^- ions under strong magnetic field becomes significantly reinforced.

The probability that a neutral on-axis donor, D^0_{on}, will convert to a D^-_{on} ion, trapping the electron released from the peripheral donor, D^0_{off}, according to the charge exchange reaction

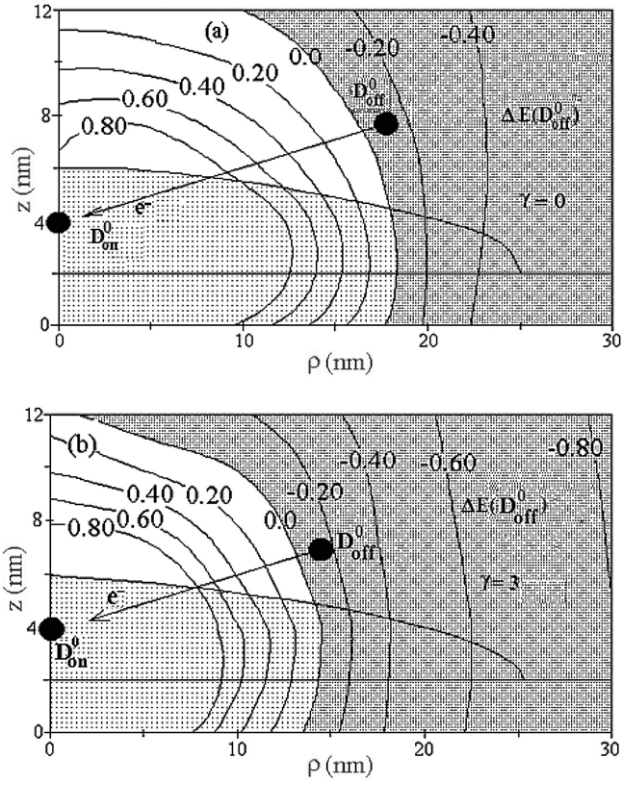

Figure 7. Contour plots of the energies ΔE required for the charge exchange between the on- and off-axis donors for different off-axis donor positions in a plane through the axis of symmetry of the lens without (a) and with (b) magnetic field. The dark-shadowed parts of the figures indicate the positions of the off-axis donors for which the charge exchange with the on-axis donor is exothermic.

$D^0_{on} + D^0_{off} \rightarrow D^-_{on} + D^+_{off}$, is significant only if the energy ΔE, required to remove the electron from the off-axis donor and place it on the on-axis donor, is negative, i.e. this reaction is exothermic. One can estimate the value of ΔE as the difference between the energy required in order to separate the electron from the peripheral donor, $E_c(D^0_{off})$, and the energies gained due to the correlation of the electron by the on-axis donor, $E_c(D^-_{on})$, and due to the electrostatic attraction between two ions formed in this reaction, U_a:

$$\Delta E = E_c(D^0_{off}) - E_c(D^-_{on}) - U_a. \tag{14}$$

The energies $E_c(D^0_{off})$ and ΔE depend strongly on the off-axis donor position. Therefore, in order to find the donor positions for which the charge exchange with the on-axis donor is exothermic, we present in figure 7 the contour plots of the energies ΔE required to remove the electron to the on-axis donor, located on the middle of the lens axis ($\xi_z = 0, \xi_\rho = d_b + d_0/2$), from D^0_{off} with different positions along a cross section in a plane through the axis of symmetry of the lens, for $\gamma = 0$ (figure 7(a)) and $\gamma = 3$ (figure 7(b)). The dark-shadowed parts of the figures indicate the positions of the neutral donors for which the energies ΔE are negative and the reaction of the formation of the on-axis D^- centre is exothermic.

We estimate U_a as the interaction energy between the point charge $+e$, located at the off-axis donor position, and the charge $-e$, homogeneously distributed within a sphere

of the radius $1/\alpha$ (α is the variational parameter of the Hylleraas trial function given by equation (12)) and centred at on-axis donor location ($\xi_\rho = 0, \xi_z = d_b + d_0/2$). It is seen from the contour plots presented in figure 7 that the energy required for the formation of the D^-_{on} falls off rapidly as the D^0_{off} is removed from the axis turning into negative (dark shadowed parts of the contour plots) as D^0_{off} is far from the on-axis donor more than 18 nm without magnetic field and 13 nm as $\gamma = 3$. Comparing the contour plots in figures 7(a) and (b) it is easy to observe that the increase of the magnetic field provides an expansion of the region with peripheral donor positions for which ΔE is negative, reinforcing the process of the formation of on-axis D^- ion.

6. Conclusions

In order to study the positional and the magnetic field dependences of the ground state correlation and binding energies of the neutral and negatively charged donors in oblate lens-shaped quantum dots, a numerical calculation has been performed by using the fractal dimension method [13]. It is found that the enhancement of the neutral and negative donor correlation energies for on-axis donors as a result of the confinement is accompanied by a significant increment of the ratio $\sigma = E_c(D^-)/E_c(D^0)$, very similar to one established previously for an SQD. We have calculated the σ for different donor positions within the lens-shaped QD in the presence of the magnetic field oriented along the axis of symmetry. It is pointed out that in the zero-magnetic-field case σ decreases from a typical value for zero-dimensional structures of about 0.3 up to a typical value for one-dimensional structures of about 0.2 as the donors are removed from the axis to the barrier region. We ascribe this variation of σ to the change of the electron distribution density configuration from nearly spherical around the donor position for the on-axis donor up to linearly elongated for the barrier donor. This results in the correlation energy of the on-axis D^- being larger than the correlation energies of the D^0 located far from the axis, and the formation of on-axis D^- ions by means of charge exchange between these two donors becomes very probable. We found that external magnetic field increases σ for the on-axis donors and decreases its value for the donors located far from the axis, making more probable the process of formation of on-axis D^- ions.

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Appendix A. Numerical procedure for calculating the free electron ground state energy and wavefunction in QL

The function $f_z(z, \rho)$ and the associated lowest energy $E_z(\rho)$ can be found exactly as the well known analytical solution of the one-particle wave equation (6) for a quantum well of width $d(\rho)$ with barrier height V_0 considering ρ as a fixed parameter. Once $f_z(z, \rho)$ and $E_z(\rho)$ are found, the ground state wavefunction $f_\rho(\rho)$ may then be obtained numerically in a straightforward way as a solution of the two-dimensional central force problem with field

potential $E_z(\rho)$. To solve equation (7) for S states, it can be written as

$$-f''_\rho(\rho) - \frac{1}{\rho}f'_\rho(\rho) + \left[E_z(\rho) + \frac{\gamma^2\rho^2}{4}\right] f_\rho(\rho) = E_0 f_\rho(\rho). \tag{A.1}$$

One should take into account that the potential $E_z(\rho)$ in the region $\rho \geqslant R_0$ is constant and equal to V_0, and therefore the solution of equation (A.1) outside the QD can be found analytically:

$$f_0(\rho) = C\exp\left(-\frac{\gamma\rho^2}{4}\right) U\left(\frac{1}{2} + \frac{V_0 - E_0}{2\gamma}, 1, \frac{\gamma\rho^2}{2}\right); \qquad R_0 \leqslant \rho < \infty \tag{A.2}$$

where $U(a, 1, x)$ is the general form of the confluent hypergeometric function [17] which remains finite, as $x \to \infty$. Within the QD, equation (7) by using substitution $g(\rho) = f'_0(\rho)/f_0(\rho)$ is reduced to the Cauchy problem for the Riccati equation:

$$g'(\rho) + g^2(\rho) + g(\rho)/\rho + \left[E_0 - E_z(\rho) - \gamma^2\rho^2/4\right] = 0; \qquad 0 < \rho < R_0; \quad g(0) = 0, \tag{A.3}$$

where E_0 is considered as a fixed parameter. One can define a function $g(R_0, E_0)$ as the solution of problem (A.3) at the point $\rho = R_0$, which can be found for each value of E_0 by using for example the Runge–Kutta method. Then sewing together this function with the solution (A.3) at the point $\rho = R_0$ one can obtain the following transcendental equation for the ground state energy E_0:

$$g(R_0, E_0) = -\frac{\gamma R_0}{2} - \gamma R_0\left(\frac{1}{2} + \frac{V_0 - E_0}{2\gamma}\right) \times U\left(\frac{3}{2} + \frac{V_0 - E_0}{2\gamma}, 2, \frac{\gamma R_0^2}{2}\right) \Big/ U\left(\frac{1}{2} + \frac{V_0 - E_0}{2\gamma}, 1, \frac{\gamma R_0^2}{2}\right), \tag{A.4}$$

where we have used the relation [19] $U'(a, c; x) = -aU(a + 1, c + 1; x)$.

Appendix B. Numerical procedure for calculating the ground state energies and the wavefunctions of the neutral and negatively charged donors in QL

To solve equation (11) let us to rewrite it in the following form:

$$\begin{aligned} &-\Phi''_{D^0}(r) - w(r)\Phi'_{D^0}(r) - \frac{2}{r}\Phi_{D^0}(r) = [E(D^0) - E_0]\Phi_{D^0}(r); \\ &w(r) = \left[\frac{2}{r} + (\ln P(r))'\right] \end{aligned} \tag{B.1}$$

where we use the notation $J(r) = r^2 P(r)$ taking into account that the behaviour of the Jacobian (10) for small values of r is almost parabolic. As the solution of equation (B.1) at the point $r = 0$ should be an analytical function, one can derive the following initial condition: $\Phi'_{D^0}(0)/\Phi_{D^0}(0) = -1$.

By using the substitution $\tan\vartheta(r) = \Phi'_{D^0}(r)/\Phi_{D^0}(r)$ one can reduce (B.1) to the Cauchy problem for the first order differential equation:

$$\vartheta'(r) + \sin^2\vartheta(r) + w(r)\sin\vartheta(r)\cos\vartheta(r) + \left[E(D^0) - E_0 + \frac{2}{r}\right]\cos^2\vartheta(r) = 0; \tag{B.2}$$
$$\vartheta(0) = -\pi/4.$$

Here the function $w(r)$ and the value E_0 are known from the previously solved free electron problem and the donor energy $E(\mathrm{D}^0)$ can be considered as a fixed parameter. For each value of this parameter the Cauchy problem can be solved numerically by using, for example, the Runge–Kutta method and the solution $\vartheta(r, E(\mathrm{D}^0))$ at any point r can be found. From the physical significance of the envelope function $\Phi_{\mathrm{D}^0}(r)$ it should tend to zero for large electron–ion separations r. One can also see from definition (9) that the behaviour of the envelope for large separation does not essentially affect the donor ground state function because of the presence of the predominant factor $f_0(\mathbf{r})$, which exponentially decreases for large separations r. For this reason one can choose a sufficiently large limit value for electron–ion separations $R_{\max}$ where we can put $\Phi_{\mathrm{D}^0}(R_{\max}) = 0$. This condition provides the following transcendental equation with respect to unknown donor energy $E(\mathrm{D}^0)$:

$$\vartheta(R_{\max}, E(\mathrm{D}^0)) = -\pi/2 \tag{B.3}$$

where $\vartheta(R_{\max}, E(\mathrm{D}^0))$ is the solution of the Cauchy problem (B.2) at the point $r = R_{\max}$.

To find the variational energy $E(\mathrm{D}^-, \alpha, \beta, \eta)$ as a function of three parameters α, β and η one can use the well known procedure of calculation of the multiple integrals in coordinates of Hylleraas [17] in an isotropic three-dimensional space where the radial part of the Jacobian r^2 is substituted by the function $r^2 P(r)$. One can then obtain the following explicit expression for the variational energy as a function of the parameters α, β and η:

$$E(\mathrm{D}^-, \alpha, \beta, \eta) = 2E_0 + 2\alpha^2 + \frac{\int_0^\infty \mathrm{e}^{-2\alpha s}\,\mathrm{d}s \int_0^s P\left(\frac{s+t}{2}, \boldsymbol{\zeta}\right) P\left(\frac{s-t}{2}, \boldsymbol{\zeta}\right) R_1(s,t)\,\mathrm{d}t}{\int_0^\infty \mathrm{e}^{-2\alpha s}\,\mathrm{d}s \int_0^s P\left(\frac{s+t}{2}, \boldsymbol{\zeta}\right) P\left(\frac{s-t}{2}, \boldsymbol{\zeta}\right) R_0(s,t)\,\mathrm{d}t}, \tag{B.4}$$

$$\begin{aligned} R_1(s,t) = {} & 2(s-t)[(s^2-t^2)(1+\beta t^2)^2 + 4\beta\eta s^2 t^2 + 2\alpha\eta s t^2(1+\beta t^2)] \\ & + (s^2-t^2)\{2s\alpha\eta^2 t^2 - 4s(1+\beta t^2)^2 + (s^2-t^2)[4\beta^2 t^2 + 2\eta(1+\beta t^2) + \eta^2]\} \\ & - \frac{2\eta}{3}(s^3-t^3)[4\beta t^2 + 2s(4+\alpha)(1+\beta t^2) \\ & - \eta(s^2-t^2)] - \eta^2 s(s^4-t^4)(\alpha+2) \end{aligned} \tag{B.5}$$

$$R_0(s,t) = (s^2-t^2)\left[\frac{1}{2}(s^2-t^2)(1+\beta t^2)^2 + \frac{2\eta}{3}(s^3-t^3)(1+\beta t^2) + \frac{\eta^2}{4}(s^4-t^4)\right].$$

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