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Magnetic field effect on the polarizability of shallow donor in cylindrical quantum dot

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Abstract

Using a variational method in the effective mass approximation and considering a noninteracting model, we have calculated the binding energy and the polarizability of shallow donor impurities in cylindrical GaAs quantum dot under an applied magnetic field. We have considered an infinite and finite confinement model to describe the barriers on the dot boundaries. We present our results as function of the size of the dot and several values of the magnetic field strength. It is found that the polarizability decreases as the dot radius R decreases, reaches a minimum at a certain value of R and then increases as the radius becomes smaller. The magnetic field increases the binding energy and strongly reduces the polarizability. The finite barrier-height effects are important for smaller dot widths. For higher field strength and large dot, the magnetic field effects are predominant.

Keywords: Quantum dot; Donor; Polarizability; Binding energy; Magnetic field

1. Introduction

With the recent improvements in microfabrication technology of nanostructures, the growth of semiconductor systems with reduced dimensionality has been actively pursued in recent years as consequence of their promising technological applications. Quantum dots (QD) have been constituted one of the intensely studied semiconductor nanostructure from theoretical [1–5] and experimental [6–8] point of view due to the extreme degree of confinement of the electrons. The effect of an applied electric field on the binding energy has been the subject of intensive investigation [9–11]. When an electric field is applied to a nanostructure, this originates the polarization of the distribution of carriers and a shift of the energy of quantum states. An electron bound to an impurity state at the center of a large QD is never influenced by the boundary, and behaves as a three-dimensional (3D) electron bound to an impurity in a GaAs/$Ga_{1-x}Al_xAs$ structure. For intermediate QD size (of the order of the effective Bohr radius a^*), the electron confinement due to the potential barrier cane be greater than the confinement due to the impurity, and the electron behaves as quasi-0D system, therefore, the binding energy increases and the polarizability decreases. For much smaller sizes, the

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infinite-well model fails strongly because tunneling effects become very important and the electron leaks out as 3D electrons in $Ga_{1-x}Al_xAs$ bound to impurities and is weakly perturbed by the potential well, therefore the binding energy restarts to decrease and the polarizability increases; while for an infinite barrier potential model, the electron bound to the impurity ion stays inside the dot, thus increasing the binding energy.

There are several reports on the polarizabilities of shallow donor impurities in quantum well (QW) and quantum well wire (QWW) [12–15]. Recently, Duque et al. [16], have studied the effect of applied electric field on the binding energy and polarizability of shallow donor implanted in rectangular cross section $GaAs/Ga_{1-x}Al_xAs$ QWWs. They have found that, for larger dimensions of QWW, both the binding energy and the polarizability decreases with the increasing electric field intensity, while for the smaller dimensions the variation of the binding energy is very small and the polarizability stays constant. The effects of the interaction electron phonon on the polarizability of a shallow donor in QWW have been studied by Filali et al. [17]. They have reported that the polaronic effects significantly decrease the polarizability and increase with increasing wire size. Murillo et al. [18] have calculated the binding energy of a donor impurity in $GaAs/Ga_{1-x}Al_xAs$ spherical quantum dot with parabolic confinement and with an applied electric field. They have found that the binding energy decreases with increasing electric field intensity for even radii of the dot.

The application of a magnetic field to a crystal changes the dimensionality of electronic levels and leads to a redistribution of the density of states. In the Refs. [19,20] the authors have studied the hydrogenic impurity binding energy in QWWs and QDs in the presence of a magnetic field by using a variational approach. Zhigang et al. [21] have calculated the binding energy of the ground state of a hydrogenic donor in a cylindrical wire in the presence of a magnetic field parallel to the wire axis as a function of the wire radius and the magnetic field intensity. Recently Niculescu et al. [22] have calculated the binding energy of a shallow donor in a cylindrical GaAs QWW in the presence of an axial magnetic field. They have adopted an infinite confinement potential and taken into account the impurity position in the wire. The effect of the magnetic field on the polarizability of the shallow donor in the spherical QD has been analyzed by Feddi et al. [23] using an infinite confinement potential case.

In a previous paper [24], we have studied the polarizability of a magneto-donor in a quantum wire. It has been found that the magnetic field reduces strongly the polarizability. The finite barrier-height effect is important for small well widths. For higher fields and a large wire, the magnetic field effects are predominant and the barrier potential is a small perturbation.

Nevertheless, to the best of our knowledge, there is no study on the effect of a magnetic field on the polarizability of a donor in cylindrical quantum dot (CQD). In the present Letter, we propose to calculate the polarizability of a shallow donor placed at the center of a CQD, with infinite and finite barrier, as a function of the dot sizes and for various values of the magnetic field. This Letter is organized as follows: in Section 2, we present the general formalism; we deduce the expression of the donor binding energy and its polarizability in the presence of an uniform magnetic field. The numerical results and discussions are presented in Section 3 with application to a CQD made out of GaAs.

2. General formalism

We consider a system consisting of a GaAs cylindrical quantum dot (CQD) with radius R and length H, surrounded by $Ga_{1-x}Al_xAs$ with an electron bound to a shallow donor placed at the center of the dot. In the presence of an applied electric field and a magnetic one along the z-direction, which is taken as the axis of the dot. In the effective mass approximation, the Hamiltonian is given by

$$H = -\nabla^2 - \frac{2}{\sqrt{\rho^2 + z^2}} + \eta z + \frac{\gamma^2}{4}\rho^2 + \gamma L_z + V(\rho, z), \tag{1}$$

where

$$V(\rho, z) = \begin{cases} 0 & \text{for } \rho < R \text{ and } |z| < \frac{H}{2}, \\ V_0 & \text{for } \rho > R \text{ and } |z| < \frac{H}{2}, \\ V_0 & \text{for } |z| > \frac{H}{2} \end{cases} \tag{2}$$

is the electron confining potential, ρ and z are the electron coordinates in the plane perpendicular and along the cylinder axis, respectively. L_z is the z component of the angular momentum operator. We use the effective Bohr radius $a^* = \frac{\hbar^2\varepsilon_0}{m^*e^2}$ and the effective Rydberg constant $R^* = \frac{m^*e^4}{2\hbar^2\varepsilon_0^2}$ as the units of length and energy. $\eta = \frac{ea^*F}{R^*}$ is a dimensionless measure of the electric field, $\gamma = \frac{\hbar\omega_c}{2R^*}$ is a dimensionless measure of the magnetic field and ε_0 is the dielectric constant. m^* is the electron band effective mass which is given by [25]

$$m^* = \begin{cases} m_1^* = 0.067\,m_0 & \text{in GaAs,} \\ m_2^* = (0.067 + 0.083\,x)m_0 & \text{in Ga}_{1-x}\text{Al}_x\text{As,} \end{cases} \tag{3}$$

where m_0 is the free electron mass and x is the Al concentration. The value of the potential heights are determined from the Al concentration x in $Ga_{1-x}Al_xAs$ through the expression of the energy band-gap discontinuity at the interfaces, $\Delta E_g = (1.04\,x + 0.47\,x^2)$ eV, the value of V_0 is taken to be 60% of ΔE_g [15].

First, we study the much simpler case of infinite potential barrier in Section 2.1; the case of finite potential barrier is presented in Section 2.2.

2.1. Infinite potential barrier case

We assume that a single donor impurity is located at the center of the CQD and we suppose an infinite confinement potential (i.e., $V_0 = \infty$). Since the Schrödinger equation cannot be solved exactly, we follow the Hass variational method. We choose the trial wave function in the form:

$$\psi_i(\rho, z) = \psi_0(\rho, z)(1 + \beta z), \tag{4}$$

where β is a variational parameter (which takes into account the presence of the weak electric field) and $\psi_0(\rho, z)$ is the wave function in the absence of electric field ($\eta = 0$) given by

$$\psi_0(\rho, z) = N J_0\left(\theta_0 \frac{\rho}{R}\right) \cos\left(\frac{\pi z}{H}\right) \times \exp\left(-\left(\frac{\rho^2}{8b^2} + \frac{z^2}{8a^2}\right)\right), \tag{5}$$

where J_0 is the Bessel function of zero order; $\theta_0 = 2.4048255577$ is its first zero, a and b are variational parameters and N is the normalization constant. The single parameter trial wave function used by El Said et al. [12] is certainly not adequate since it preserves the spherical symmetry of the hydrogen-like wave function; it does the not take into account the anisotropy effects introduced by the external magnetic field (i.e., the compression of the wave function in the x- and y-direction). In previous work we have used a linear combination of a cylindrical wave function and an oscillating one which is valid at all magnetic field value [26,27].

The corresponding energy is given by

$$E(\beta) = E_k + E_{\text{coul}} + E_m + E_e, \tag{6}$$

where

$$\begin{aligned} E_k &= \langle\psi_i| - \nabla^2|\psi_i\rangle \\ &= \left(\frac{\theta_0}{R}\right)^2 + \frac{1}{2b^2} - \frac{1}{2b^2}\frac{\theta_0}{R}\frac{I_{10}^2}{I_{00}^1} - \frac{1}{16b^2}\frac{I_{00}^3}{I_{00}^1} \\ &\quad + \left(\frac{\pi}{H}\right)^2 + \frac{1}{4a^2} + \frac{A + \beta^2 B}{\bar{I}_{02}^0 + \beta^2\bar{I}_{02}^2}, \end{aligned} \tag{6a}$$

$$E_{\text{coul}} = \langle\psi_i| - \frac{2}{\sqrt{\rho^2+z^2}}|\psi_i\rangle = \frac{G + \beta^2 H}{\bar{I}_{02}^0 + \beta^2\bar{I}_{02}^2}, \tag{6b}$$

$$E_m = \langle\psi_i|\frac{\gamma^2}{4}\rho^2 + \gamma L_z|\psi_i\rangle = \frac{\gamma^2}{4}\frac{I_{00}^3}{I_{00}^1}, \tag{6c}$$

where the matrix element $\langle\psi_i|\gamma L_z|\psi_i\rangle = 0$.

$$E_e = \langle\psi_i|\eta z|\psi_i\rangle = \frac{2\beta\bar{I}_{02}^2}{\bar{I}_{02}^0 + \beta^2\bar{I}_{02}^2}\eta \tag{6d}$$

with

$$A = -\frac{\pi}{2Ha^2}\bar{I}_{11}^1 - \frac{1}{16a^4}\bar{I}_{02}^2,$$

$$B = 2\frac{\pi}{H}\bar{I}_{11}^1 + \frac{1}{2a^2}\bar{I}_{02}^2 - \frac{\pi}{2Ha^2}\bar{I}_{11}^3 - \frac{1}{16a^4}\bar{I}_{02}^4,$$

$$G = -\frac{2}{I_{00}^1}\int_0^R\int_0^{H/2}\frac{\rho}{\sqrt{\rho^2+z^2}}J_0^2\left(\theta_0\frac{\rho}{R}\right)\exp\left(-\frac{\rho^2}{4b^2}\right) \times \cos^2\left(\frac{\pi z}{H}\right)\exp\left(-\frac{z^2}{4a^2}\right)d\rho\,dz,$$

$$H = -\frac{2}{I_{00}^1}\int_0^R\int_0^{H/2}\frac{\rho z^2}{\sqrt{\rho^2+z^2}}J_0^2\left(\theta_0\frac{\rho}{R}\right)\exp\left(-\frac{\rho^2}{4b^2}\right) \times \cos^2\left(\frac{\pi z}{H}\right)\exp\left(-\frac{z^2}{4a^2}\right)d\rho\,dz,$$

$$I_{mn}^{p} = \int_{0}^{R} \rho^{p} J_m\left(\theta_0 \frac{\rho}{R}\right) J_n\left(\theta_0 \frac{\rho}{R}\right) \exp\left(-\frac{\rho^2}{4b^2}\right) d\rho,$$

$$\bar{I}_{mn}^{p} = \int_{0}^{H/2} z^{p} \sin^{m}\left(\frac{\pi z}{H}\right) \cos^{n}\left(\frac{\pi z}{H}\right) \exp\left(-\frac{z^2}{4a^2}\right) dz.$$

In the absence of electric field ($\eta = 0,\ \beta = 0$), the binding energy of donor is defined as the ground state energy of the system without Coulomb term minus the ground state energy in the presence of the Coulomb term

$$E_i = E_{\text{sub}} - \min_{[a,b]}\bigl(E(\beta = 0)\bigr). \tag{7}$$

The polarizability of the shallow donor confined in the CQD is defined in terms of the dipole moment by [15]

$$\alpha = -\frac{E_e}{\eta^2}. \tag{8}$$

We note that the linear contribution to the energy E_e which is proportional to the permanent dipole moment is equal to zero due to the spherical symmetry of the donor. The value of β that minimizes the energy expression $E(\beta)$ is calculated and substituted in Eq. (6). The final results are obtained by numerical minimization of the energy expression with respect to the parameters a and b. Then theses values are used to deduce the polarizability given by Eq. (8).

2.2. *Finite barrier potential case*

For a finite barrier height V_0, we choose the trial wave function of the form

$$\psi_i(\rho, z) = \psi_0(\rho, z)(1 + \beta z), \tag{9}$$

where

$$\psi_0(\rho, z) = N\phi(\rho)\phi(z) \exp\left(-\left(\frac{\rho^2}{8b^2} + \frac{z^2}{8a^2}\right)\right), \tag{10}$$

$$\phi(\rho) = \begin{cases} J_0(k_{1\rho}\rho) & \text{for } \rho < R, \\ A_\rho K_0(k_{2\rho}\rho) & \text{for } \rho > R, \end{cases} \tag{10a}$$

J_0 and K_0 are, respectively, the zero-order Bessel function and the modified Bessel function. $k_{1\rho}$ and A_ρ are constants determined by the boundary condition at $\rho = R$, which is given by

$$A_\rho = \frac{J_0(k_{1\rho}R)}{K_0(k_{2\rho}R)}, \tag{10b}$$

$$\frac{k_{1\rho}}{m_1^*}\frac{J_1(k_{1\rho}R)}{J_0(k_{1\rho}R)} = \frac{k_{2\rho}}{m_2^*}\frac{K_1(k_{2\rho}R)}{K_0(k_{2\rho}R)}. \tag{10c}$$

The corresponding energy is given by

$$E_\rho = \frac{\hbar^2 k_{1\rho}^2}{2m_1^*} \tag{10d}$$

and

$$k_{2\rho} = \left(\frac{2m_2^*}{\hbar^2}(V_0 - E_\rho)\right)^{1/2}. \tag{10e}$$

$$\phi(z) = \begin{cases} \cos(k_{1z}z) & \text{for } |z| < \frac{H}{2}, \\ A_z \exp\bigl(-k_{2z}|z|\bigr) & \text{for } |z| > \frac{H}{2}, \end{cases} \tag{11a}$$

k_{1z} and A_z are determined by the boundary conditions at $|z| = \frac{H}{2}$:

$$A_\rho = \cos\left(k_{1z}\frac{H}{2}\right) \exp\left(k_{2z}\frac{H}{2}\right), \tag{11b}$$

$$\mathrm{tg}\left(k_{1z}\frac{H}{2}\right) = \frac{m_1^*}{m_2^*}\frac{k_{2z}}{k_{1z}}. \tag{11c}$$

The corresponding energy is given by

$$E_z = \frac{\hbar^2 k_{1z}^2}{2m_1^*} \tag{11d}$$

and

$$k_{2z} = \sqrt{\frac{2m_2^*}{\hbar^2}(V_0 - E_z)}. \tag{11e}$$

To minimize the energy and deduce the polarizability, we have used the same procedure as in Section 2.1.

3. Results and discussion

Using a variational method in the effective mass approximation and considering a noninteracting model, we have calculated the polarizability and the binding energy of a shallow donor placed at the center of a cylindrical quantum dot (CQD). We apply this model to CQDs made out of GaAs surrounded by $Ga_{1-x}Al_xAs$. The physical parameters used in this work are given by: $R^* = 5.8$ meV, $a^* = 98.7$ Å and

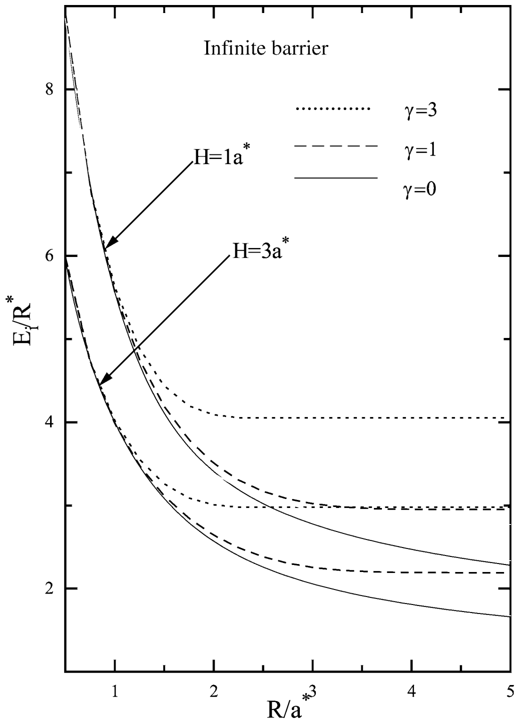

Fig. 1. The binding energy as a function of the dot radius for two values of the length and several values of the magnetic field γ (infinite barrier case).

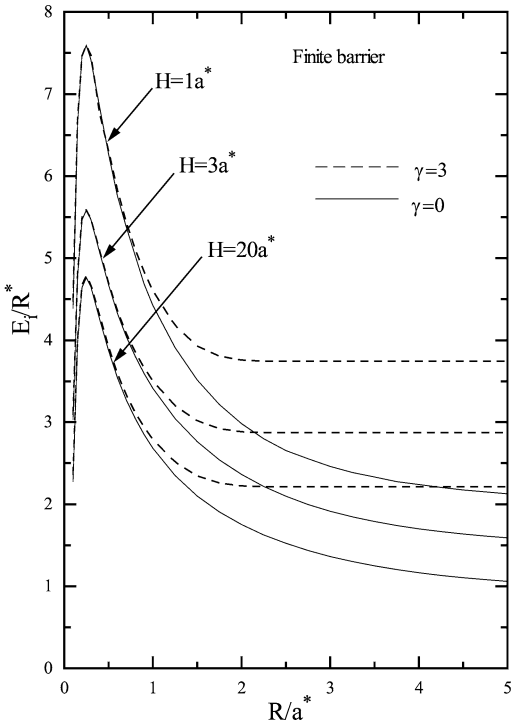

Fig. 2. The binding energy as a function of the dot radius for various values of the length and for two values of the magnetic field γ (finite barrier case).

$\varepsilon_0 = 12.5$. For the finite barrier case, we will use one value of the barrier-height equal to 219.2 meV (i.e., corresponding to $x = 0.30$). Our results for the polarizability are obtained for a very small intensity of an electric field ($\eta = 0.01$).

For the infinite barrier case, we have reported in Fig. 1, the donor binding energy as a function of the radius of the dot for two values of length ($H = 1a^*$, $3a^*$) and for different intensity of a magnetic field ($\gamma = 0, 1, 3$ where $\gamma = 3$ corresponds to $B \approx 20$ T).

This figure reflects the competition between the magnetic field effect and the spatial confinement effect. For a very small radius R, the strong geometric confinement leads the electronic wave function to be more compressed in the CQD. The binding energy is significant and relatively insensitive to the magnetic fields since the electron spatial localization prevails over the magnetic field confinement. To the vicinity of $1a^*$, the effect of the magnetic field begins to be apparent and the curves corresponding to different strength of the magnetic field tend to deviate from each other, as the dot radius rises, reaching asymptotically to the quantum well values case. For the large values of the radius, ($R > 1a^*$), the magnetic field governs the behavior of the binding energy because it overcomes the spatial localization. Furthermore, for given values of R and γ, the binding energy increases when the length of the dot decreases which reflects the increasing confinement.

In Fig. 2, we present the binding energy of the CQD in the case of finite height potential barrier ($V_0 = 219.2$ meV) as a function of the radius of the dot for several values of length ($H = 1a^*$, $3a^*$, $20a^*$) and for two values of magnetic field intensity ($\gamma = 0, 3$). For each value of length, the binding energy increases with increasing radius of the dot, reaches a maximum value and finally decreases monotonically. The effect of the magnetic field becomes remarkable only in the large radius region, as an infinite barrier case. In addition, we should signal that with our model, we can describe any low-dimensional structure going from 2D (two-dimensional) to 0D (zero-dimensional) by taking into

Table 1
Binding energies (in effective Rydbergs) of a shallow donor in (CQD) ($R = 5a^*$, $H = 20a^*$) for several values of the magnetic field intensity

	γ	0	0.5	1	1.5	2
$E_i\,(R^*)$	Present	1.0973	1.2803	1.5438	1.7536	1.9272
	Ref. [22]		1.3822	1.6196		1.9663

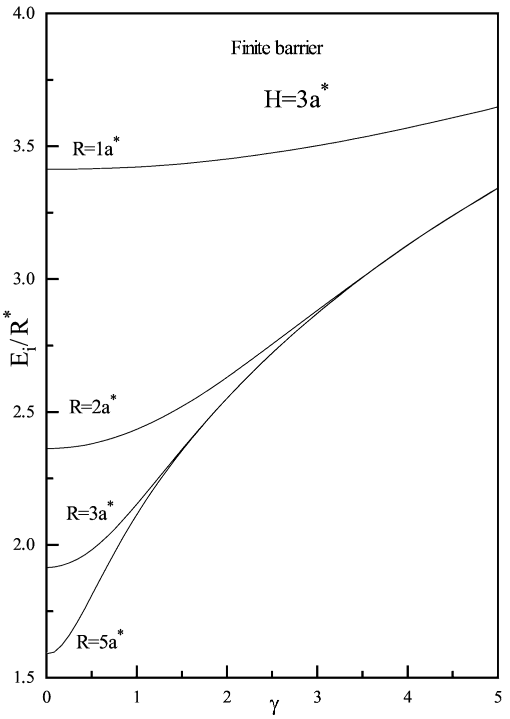

Fig. 3. The binding energy as a function of the magnetic field intensity γ for several values of the dot radius and for the length $H = 3a^*$ (finite barrier case).

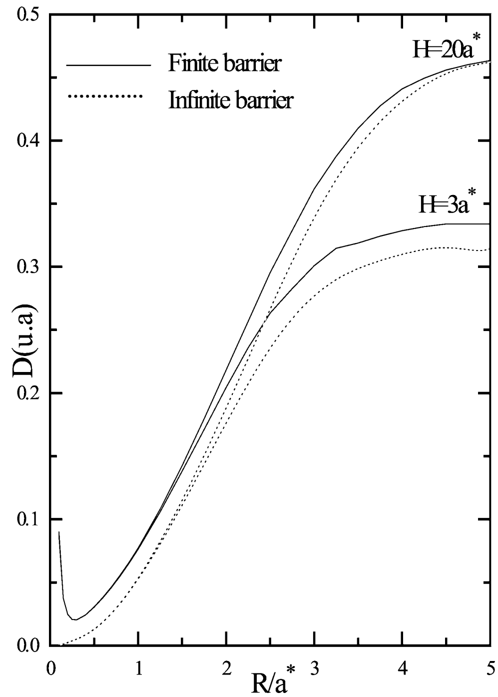

Fig. 4. Variation of the diamagnetic coefficient versus the dot radius for two values of length H and for $\gamma = 0.1$.

account the ratio between the length and the radius of the structure, that is $(H/R) \ll 1$ for a QW (2D), $(H/R) \gg 1$ for a QWW (1D) and $(H/R) \cong 1$ for QD (0D).

We present in Table 1, the binding energies of a shallow donor for a CQD ($R = 5a^*$, $H = 20a^*$) and for several values of magnetic field intensity. Our model gives good results for high intensity, a comparison has been made with Niculescu et al. [22].

The Fig. 3 shows the dependence of the binding energies upon the magnetic field for several values of R and for $H = 3a^*$. We see that at low magnetic fields the shift of the energy is diamagnetic, $\Delta E_i \sim \gamma^2$, and increases approximately linearly with the magnetic field at high γ. This result agrees well with previous results in QWW (see Niculescu et al. [22]). For weak magnetic field intensity, the energy can be written as $E(\gamma) = E(0) + \gamma^2 D$ where D is the diamagnetic coefficient. In Fig. 4, we report D as function of R (for $\gamma = 0.1$); we remark that D decreases with decreasing R and tends to zero in the case of infinite barrier potential. A similar behavior has been reported in Ref. [23]. In contrast, for the case of finite barrier, D reaches a minimum value and increases as R becomes smaller. This result is reasonable, since when R decreases, the electronic orbital is more and more localized and it becomes insensitive to the influence of magnetic field, and D tends to zero for the case of infinite barrier. For the

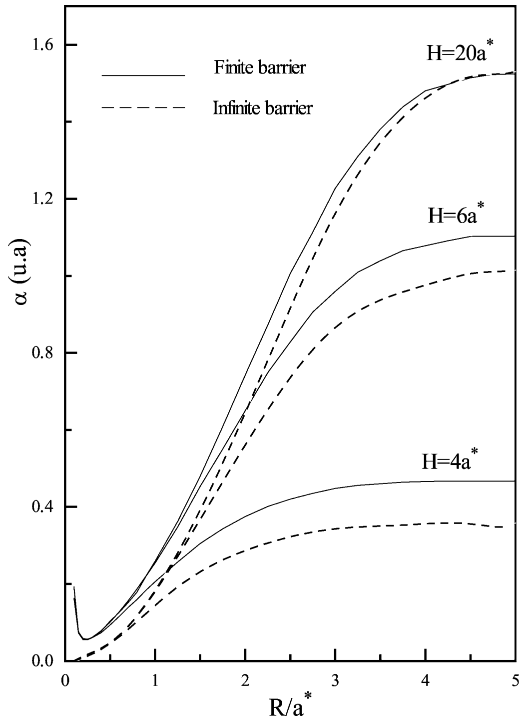

Fig. 5. The polarizability values as a function of the dot radius and several values of length (finite and infinite barrier).

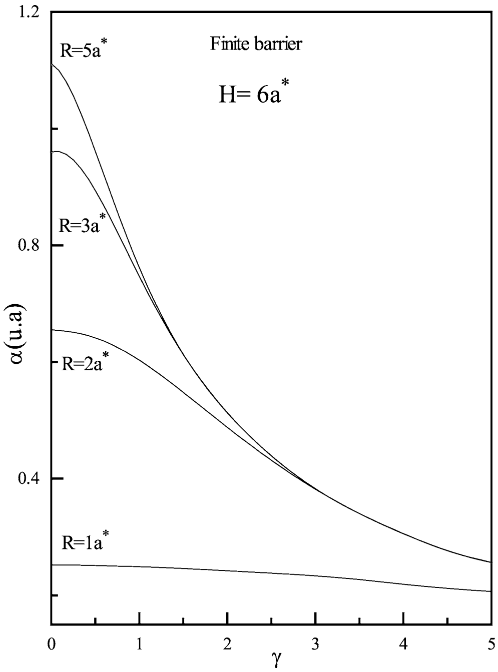

Fig. 6. The polarizability as a function of the magnetic field intensity γ for several values of the radius R and for the length $H = 6a^*$ (finite barrier case).

case of finite barrier and for very small R, the orbital escapes out towards the barrier material.

In Fig. 5, we have reported the effect of finite barrier height using two values of the barrier: $V_0 = 219.2$ meV and $V_0 = \infty$. From this figure we remark that the polarizability decreases with the decreasing of the size of the dot. In the finite barrier potential case, the polarizability reaches a minimum value at a certain value of R ($R \cong 0.25\,a^*$) and then increases as R becomes smaller. In order to explain this behavior, we notice that due to confining potential barrier the bound-electron wave function becomes compressed, reducing in this way the polarizability. When the width of the dot becomes very small the tunneling effects become very important, so the wave function escapes out of the dot towards the material barrier and then the polarizability starts to increase. Also, this figure shows, that the difference between the results for the finite and infinite barrier is important for average well length (see, for example the curves corresponding to $H = 4a^*$).

In Fig. 6, we present the results of the polatizability as a function of the magnetic field for a length $H = 6a^*$ and for various radius R. This figure reflects correctly the effect of the magnetic field, which confines more the electron and reduces the polarizability. For larger radial dimension of the CQD, the polarizability decreases as the magnetic field intensity increases, while for the smaller dimension ($R < 1a^*$) the polarizability is nearly independent of the magnetic field. This fact is in agreement with our discussion above on the strong confinement of the impurity, so it is not possible to further compress the impurity wave function. In contrast, for a strong magnetic field (i.e., $\gamma > 3$) and for large dot ($R \geqslant 2a^*$), the three upper curves coincide, so the spatial confinement is negligible and the magnetic field effects are predominant.

In conclusion, we have studied the effect of the magnetic field on the polarizability and the binding energy of a shallow donor in a GaAs CQD. Our results indicate that the polarizability and he binding energy of the donor depend strongly on the quantum confinement and strongly on the applied magnetic field. The effects of the electron–phonon interactions on the polarizability of a magneto-donor in CQD are in progress.

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