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# Far-infrared optical spectrum of donor impurities in quantum dots in a magnetic field

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We report calculations for far-infrared absorption in GaAs/$Ga_{1-x}Al_xAs$ quantum dots doped with shallow-donor impurities in the presence of a magnetic field. The wave functions and the eigenvalues are obtained in the effective-mass approximation by using a variational approach in which the ground and excited magneto-impurity states are simultaneously obtained. The allowed intra-donor transitions have been investigated by using far-infrared radiation circularly polarized in the plane perpendicular to the magnetic field. We present results for the absorption coefficient as a function of the photon energy for several field strengths and arbitrary impurity positions. We have found that, as a consequence of the quantum dot confinement the infrared magneto-absorption strongly depends on the position of the impurity in the dot.

**Introduction** Understanding of the effects of the quantum confinement on the impurity states in low dimensional structures is a very important subject in semiconductor physics. Electronic and optical properties of shallow impurities in quantum wells, quantum wires, and quantum dots are strongly modified with respect to the host materials due to the quantum-confinement effects [1–3]. The shallow-donor energy levels can be probed experimentally by far-infrared spectroscopy. Most of the experimental investigation of impurities states in heteroestructures has been carried out in the presence of an external magnetic field [4]. The additional induced magnetic confinement competes with the geometrical confinement of the nanostructures and the properties of the impurity spectrum can be dramatically modified by the field [5, 6].

We present here a theoretical study of the energy spectrum for shallow-donor impurities confined in a quantum dot in the presence of a magnetic field. We analyze the effects of the quantum-size confinement and magnetic confinement for impurities located in different positions in the quantum dot. In particular, we studied the infrared transitions between states of magneto-impurities confined in the quantum dot. The wave functions and the eigenvalues are obtained in the effective-mass approximation by using a variational approach in which the ground and excited magneto-impurity states are simultaneously obtained [7]. We perform calculations of the absorption coefficient for far-infrared radiation circularly polarized in the plane perpendicular to the magnetic field. We analyze the effects of the different mechanisms of confinement and the influence on the position of the impurity on the spectra. We have found that the absorption coefficient as a function of the photon energy presents interesting features when the impurity is displaced to off-center positions.

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**Theory** The effective-mass Hamiltonian for a donor impurity inside the quantum dot in the presence of a uniform magnetic field applied parallel to the disk axis, $\boldsymbol{B} = B\hat{\boldsymbol{z}}$, is written as

$$H = \frac{1}{2m^*}\left(\boldsymbol{p} + \frac{|e|}{c}\boldsymbol{A}_0\right) + V_{\rm dot}(\boldsymbol{r}) + \frac{e^2}{\epsilon_0|\boldsymbol{r} - \boldsymbol{r}_0|}\,, \tag{1}$$

in which $m^*$ is the electronic effective mass, $\boldsymbol{A}_0$ is the vector potential which is taken in the symmetric gauge, and $\epsilon_0$ is the GaAs dielectric function. The confining dot-potential is modelled by a superposition of a well potential along the $z$-direction and a lateral parabolic potential which in cylindrical coordinates is given by: $V_{\rm dot}(\rho, z) = V_0\,\Theta(|z| - L/2) + \frac{1}{2}\,m^*\omega_g^2\rho^2$, where $\Theta(x)$ is the Heaviside function and $V_0$ and $L$ are the barrier height and the well width, respectively. $\boldsymbol{r}_0$ gives the position of the impurity, and $\omega_g$ is the frequency associated with the lateral geometrical confinement. To solve the eigenvalue equation for the Hamiltonian (1) we expand the envelope function of the donor impurity, $F(\rho, \phi, z)$, in a finite set of basis functions. They are chosen as a product of a $z$-dependent solutions of the one-dimensional problem for an electron in a quantum well, $f_\ell(z)$, and a restricted set of radial Gaussian functions, with length parameters $\alpha_j$ fixed a priori to cover the relevant physical region and assure convergence [8],

$$F(\rho, \phi, z) = \sum_n \sum_{j,m} a^\ell_{j,m}\, {\rm e}^{-\frac{\rho^2}{\alpha_j}}\, \rho^{|m|}\, {\rm e}^{im\phi} f_\ell(z)\,. \tag{2}$$

The quantum number associated with the $z$-component of the orbital angular momentum operator, denoted by the index $m$ is a good quantum number for an impurity located on the axis of the quantum disk. For any other location of the impurity, the lateral confinement potential destroys the cylindrical symmetry and we should expand the quantum dot envelope function in terms of functions of different angular momenta. We have neglected the contribution of the continuum states and $\ell$ runs over all the discrete levels in a the quantum well.

The impurity energies and wave functions are obtained by solving a linear set of coupled equations for the coefficients of the expansion, $a^\ell_{jm}$. All the numerical calculations have been performed for a quantum dot obtained confining laterally a GaAs/$Ga_{0.7}Al_{0.3}$As quantum well. The dielectric constant is given by $\epsilon_0 = 12.58$ and the effective mass is $m^* = 0.067m_0$. To represent the geometrical lateral confinement we define a quantum disk radius $r_D$ in terms of the expectation value of the in-plane coordinate $\rho^2$ in the ground state, $r_D = \sqrt{\langle\rho^2\rangle} = \sqrt{\hbar/m^*\omega_g}$.

In Figure 1 we present a plot which illustrates the behavior of the low-lying impurity energies as a function of the magnetic field for a quantum dot with parameters $L = 60$ Å, and $r_D = 100$ Å. Figure 1a displays the case of an on-center impurity and Fig. 1b the case for an impurity located in $r_0 = 25$ Å. Because for an on-center donor the impurity states are eigenstates of the angular-momentum operator in the field direction, we have labelled the different states with an hydrogen-like notation 1s, 2p, etc. We can observe the Zeeman splitting of the 2p and 3p states as the magnetic field increases. For an off-center impurity the azimuthal symmetry is broken and the states with different angular momentum become mixed by the impurity potential. We can see in Fig. 1b as the degeneracy of the p states is split even for zero magnetic field.

To study the far-infrared magneto-optical absorption of an impurity confined in a quantum dot, we have calculated the absorption coefficient for far-infrared radiation circularly polarized in the plane perpendicular to the magnetic field. The oscillator strength for transitions from ground state to excited impurity states in the dipolar approximation, is proportional to $|\langle F_f|\,\hat{\boldsymbol{\epsilon}}\cdot\left(\boldsymbol{p} + \frac{e}{c}\,\boldsymbol{B}_0\right)|F_i\rangle|^2$, where $\hat{\epsilon}$ denotes the photon polarization vector. The absorption coefficient is given by

$$\alpha(\omega) = \frac{\alpha_0}{\omega}\sum_{n',n}\sum_{j',j}\sum_{m,m'} a^n_{j,m}a^{n'}_{j',m'}\delta_{n,n'}\delta_{m,m'\pm1}G^{m,m'}_{j,j'}\,\delta(\Delta E_{f,i} - \hbar\omega) \tag{3}$$

where

$$G^{m,m'}_{j,j'} = \left(\frac{1}{\alpha_j} - \frac{a_0^{*2}}{2\ell_B^2}\right)\frac{(M)!}{\alpha_{jj'}^{M+1}} + \frac{(M-1)!}{\alpha_{jj'}^{M}}\,(m \pm |m'|)$$

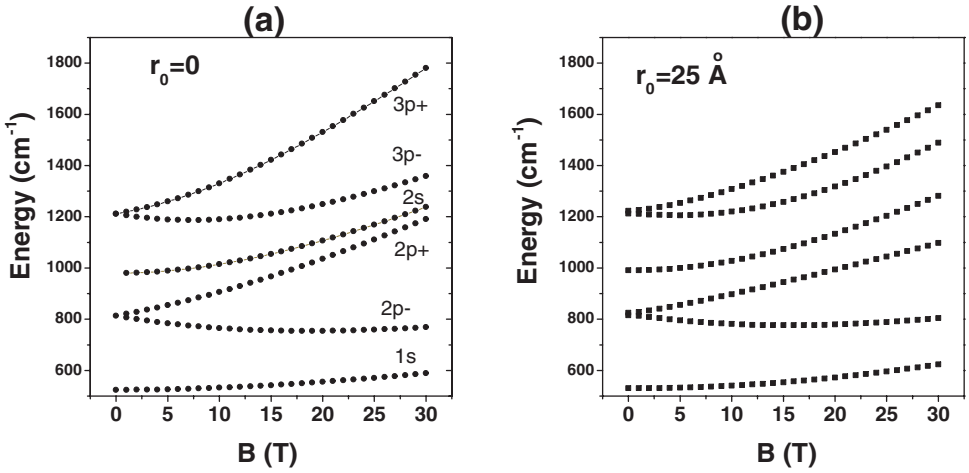


**Fig. 1** Low-lying impurity energies as a function of the magnetic field for a quantum dot with parameters $L = 60$ Å, and $r_D = 100$ Å; a) for an on-center impurity and b) for an impurity located in $r_0 = 25$ Å.

with $\alpha_0$ being a constant, and $M = (|m| + |m'| + 1)/2$. The parameter $\alpha_{jj'} = (\alpha_j + \alpha_{j'})/\alpha_j\alpha_{j'}$ and $\Delta E_{f,i}$ is the energy difference between the final and initial donor states. $a_0^* = \dfrac{4\pi\hbar^2\varepsilon}{m^* e^2}$ is the effective Bohr radius and $\ell_B = \sqrt{hc/eB}$ denotes the Landau radius. The $\delta$ function has been replaced with a Lorentzian line shape of width 0.1 meV, in the computation of the absorption coefficient.

Figure 2 shows the calculated absorption coefficient as a function of the photon energy for a set of magnetic field values running from 0 to 24 T. The quantum dot geometric parameters are $L = 60$ Å, and $r_D = 100$ Å. Figure 2a corresponds to a an on-center impurity and Fig. 2b to an impurity located in $r_0 = 20$ Å. As expected, the absorption spectra of on-center impurities present well defined peaks which can be assigned as $1s{-}np_{\pm1}$ transitions allowed by the angular-momentum selection-rules $\Delta m = \pm 1$. These transitions degenerate in $B = 0$, split into $1s{-}np_{-1}$ and $1s{-}np_{+1}$ as the field increases (only the transitions with $n = 2, 3$ are displayed in the figures). When the impurity is dis-

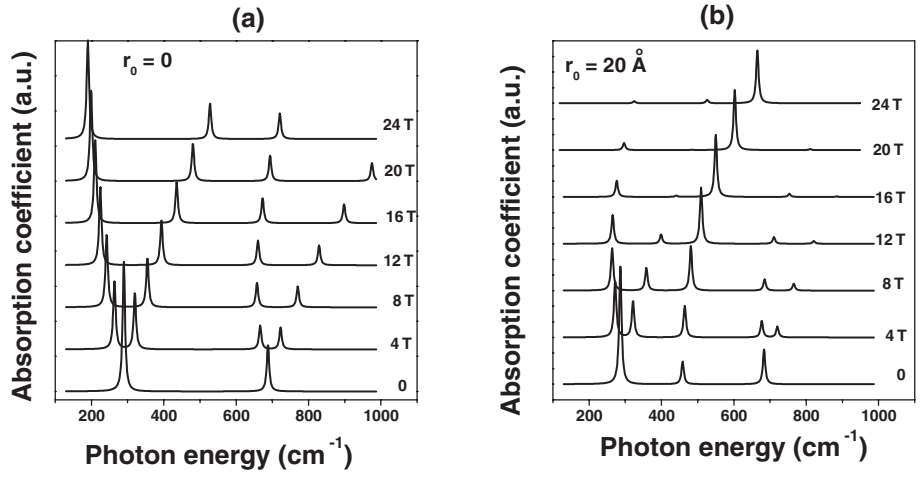


**Fig. 2** Absorption coefficient versus photon energy for magnetic field values from 0 to 24 Tesla. The quantum dot geometric parameters are $L = 60$ Å, and $r_D = 100$ Å; a) for an on-center impurity and b) for an impurity located in $r_0 = 20$ Å.

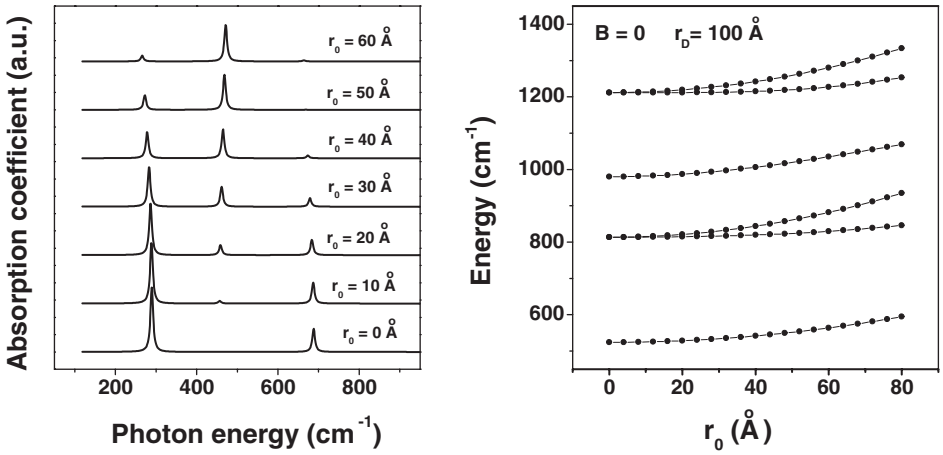


**Fig. 3** For the same quantum dot parameters as in Fig. 2 and for a zero magnetic field; a) absorption coefficient versus photon energy for several values of the impurity lateral-position and b) low-lying impurity energies as a function of the impurity lateral-position.

placed to off-center positions the spectra show remarkable differences compared to the case of an on-center donor. The most prominent feature is the apparition, for $B = 0$, of a clear peak between the two transitions optically active in the case of on-center donors $1s-2p_{\pm1}$ and $1s-3p_{\pm1}$. This peak corresponds to the "forbidden transition" 1s−2s which in this case has a non null matrix element due to the mixing of the eigenstates of the angular momentum. It can be observed that the intensity of this peak is strongly enhanced for increasing magnetic field, while the resonances corresponding to the main transitions for on-center impurities, are extinguished for high magnetic fields. The effect can be then understood due to the increase of the lateral confinement induced by the field, which produces an augment of the relative distance of the impurity to the dot center.

To analyze these results we show in Fig. 3a the absorption spectrum for various impurity positions and in Fig. 3b the low-lying levels as a function of the impurity lateral-position. Results are for zero magnetic field and for the same quantum dot as Fig. 2. We observe that the most relevant effect of moving the impurity away from the center of azimuthal symmetry, is to remove the degeneracy of the states $n$p provoking a split of that levels. Other energy levels instead, are only weakly dependent on the position of the impurity in the dot. When the distance increases the intensity of the "forbidden transition" becomes enhanced while a strong reduction of the intensity of the transitions $1s-n$p occurs. Although the ground state is nearly not affected by the position of the impurity, the excited states are dramatically changed in relation to the corresponding states for on-center impurities. It is clear from Figs. 3a and 3b that the 2p-like states, which are split for off-center impurities, has a strong mixing with 2s-like states. It is apparent that, for impurities located far away the dot-center both states completely "interchanges" their "s or p" character.

To summarize, we have investigate magneto-impurity transitions by using far-infrared radiation circularly polarized in the plane perpendicular to the magnetic field. Our method allows the computations of the energies and wavefunctions of the ground state and the excited states of an donor impurity in a quantum dot for a large range of confinement-parameters and magnetic field strengths. We have found that, as a consequence of the quantum dot confinement the absorption coefficient as a function of the photon energy presents interesting features when the impurity is displaced to off-center positions.

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