Density of States of a Donor Impurity in a GaAs Quantum Box under the Action of an Applied Electric Field

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We calculate the density of states of a donor impurity in a GaAs quantum box under the action of an electric field using effective-mass approximation within a variational scheme. We analyze the behavior of the density of states as a function of the quantum box-size as well as a function of the intensity of the applied electric field, and compare our results with previous reports in quantum wells and quantum well-wires. We expect these results will be of importance in the understanding of experimental absorption spectra related with donor impurities in GaAs quantum boxes under the action of external electric fields.

Introduction Since Bastard [1] calculated for the very first time the hydrogenic impurity states in quantum wells (QWs) many works on this subject have been put forward. Variational calculations for $n = 1$ levels in QWs with electric fields were performed by Bastard et al. [2], and for the binding energies of shallow impurities by Brum et al. [3]. Oliveira and Falicov [4] calculated the density of impurity states (DOIS) within a variational approach in the effective-mass approximation. Such calculations were performed for simple neutral and double singly ionized impurities in GaAs QWs of infinite depth, presenting a correct interpretation of their results. Weber [5] and López-Gondar et al. [6] have calculates the DOIS and optical absorption spectra of shallow impurities in QWs under the influence of a longitudinal electric field and considering infinite and finite confinement potential. They found, as a general feature, that the DOIS and impurity-related optical absorption for finite electric fields exhibit three Van Hove-like singularities corresponding to the binding energies associated with impurities at the two edges of the QW and at the position at which the binding energy has a maximum. Additionally, they show that the lack in symmetry around the $z_i = 0$ (z_i: impurity position) position when $F \neq 0$ is reflected in the presence of one additional peak in the DOIS.

The binding energies and DOIS in spherical GaAs–(Ga,Al)As quantum dots (QDs) have been calculated by Porras-Montenegro et al. [7]. They observed that for small radii of the structure the DOIS presents one structure associated with on-edge donors, while for large radii it shows two structures associated with on-center and with on-edge donor positions which may be of importance in the understanding of optical experiments of doped QDs. In the same line, Ribeiro and Latgé [8] carried out a comparative

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study of impurities in cubic and spherical GaAs QDs. They showed that, for QDs with similar volumes, the results for the impurity-binding energies and the shapes of the DOIS do not depend on the geometric details of the quantum systems.

In the last two decades, some electron and impurity properties have been calculated in quantum-well wires (QWWs). Brown and Spector [9] have obtained the binding energy of hydrogenic impurities in cylindrical, infinite-length, GaAs–(Ga,Al)As QWWs for finite and infinite confinement potential. They found for a finite confinement potential that the binding energy curves coincide for small radius of the QWW for different values of the impurity position along the radial direction. Porras-Montenegro et al. [10] calculated the ground state energy, the binding energy, and the DOIS of shallow hydrogenic impurities in cylindrical GaAs–(Ga,Al)As QWWs. They found, as a general feature, that the DOIS presents two structures associated with impurities on-center and on-edge in the QWW. Weber et al. [11] have calculated the DOIS and energy spectra of hydrogenic impurities in rectangular-cross section QWWs without considering the effects of external fields. Their calculations indicate that the DOIS of the impurity band becomes richer in structure as long as some symmetry is lost, and concluded that one should therefore be cautious in analyzing experimental results on QWWs (e.g. photoluminescence and absorption spectra on doped QWWs). The effects of an applied electric field on the binding energy of shallow donor impurities in rectangular-cross section GaAs QWWs has been presented by Montes et al. [12], considering an infinite confinement potential and using a variational scheme. For the wires with the same transversal section with those from Brown and Spector [9] they observed the same behavior for the impurity binding energy.

The presence of an external electric field in a quantum box (QB) modifies the impurity band due to the fact that the field breaks the energy degeneracy for symmetrical impurity positions in the box. This aspect will be reflected in additional peaks on the impurity DOIS and in the absorption and photoluminescence spectra. For this reason, in the present work, we extend those of Weber at al. [11] and Montes et al. [12] in order to consider the effect of an applied electric field on the shallow donor impurities implanted in a GaAs–(Ga,Al)As QB.

Theoretical Framework   In the effective-mass approximation, the Hamiltonian for a hydrogenic donor impurity in a QB under an electric field, F, applied along the x-direction is

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x, y, z) + |e|\,Fx - \frac{e^2}{\varepsilon r}\,, \tag{1}$$

where r is the distance between the carrier and the impurity site, $m^* = 0.0665\,m_0$ is the donor-impurity effective mass (with m_0 being the free-electron mass), $\varepsilon = 12.58$ is the static dielectric constant, and $V(x, y, z)$ is the infinite confinement potential. As a trial wave function for the ground state of the impurity we have used

$$\psi(r) = N\varphi(x, y, z)\,\mathrm{e}^{-\lambda r}, \tag{2}$$

where λ is a variational parameter and $\varphi(x, y, z)$ is the usual wave function for an unperturbed QB:

$$\varphi(x, y, z) = \cos\left(\frac{\pi x}{L_x}\right)\cos\left(\frac{\pi y}{L_y}\right)\cos\left(\frac{\pi z}{L_z}\right) \tag{3a}$$

without electric field, and

$$\varphi(x, y, z) = \varphi(\xi) \cos\left(\frac{\pi y}{L_y}\right) \cos\left(\frac{\pi z}{L_z}\right) \tag{3b}$$

when we consider the applied electric field. Here L_x, L_y and L_z are the dimensions of the QB, and $\varphi(\xi)$ is a linear combination of Airy functions [12].

The trial impurity ground-state energy $\langle \psi | H | \psi \rangle$ is to be minimized with respect to λ. The impurity binding energy $E_i \equiv E(L_x, L_y, L_z, x_i, y_i, z_i)$ is calculated with respect to the bottom of conduction band.

We treat the impurity position as a continuous random variable and, provided that there is no intentional doping, define a density of impurity states [1] per unit energy, $g_{L_x L_y L_z}(E_i)$, as

$$g_{L_x L_y L_z}(E_i) = \frac{1}{L_x L_y L_z} \int\limits_{S(E_i)} \frac{ds}{|\nabla(E_i)|} , \tag{4}$$

where $S(E_i)$ is the surface of constant energy $E = E_i$ and ∇ means the gradient with respect to the impurity position. In the case of a QB the DOIS was obtained via a histogram method [11] for a mesh of points uniformly distributed.

In the next section, our results for donor impurities are given in reduced atomic units that correspond to a length unit of one effective Bohr radius, $a^* = \hbar^2 \varepsilon / m^* e^2 \approx 100$ Å, and an energy unit of one effective Rydberg, $R^* = m^* e^4 / 2\hbar^2 \varepsilon \approx 5.72$ meV.

Results In Figs. 1 and 2 we present the shallow donor DOIS for QB. The dimensions of the systems are $L_x = 200$ Å, $L_y = 150$ Å and $L_z = 100$ Å for curve (a), $L_x = L_y = L_z = 200$ Å for curve (b), and $L_x = 100$ Å, $L_y = 300$ Å and $L_z = 500$ Å for curve (c). In Fig. 1 the curves are for zero electric field, whereas in Fig. 2 for 150 kV/cm. In Fig. 1, the DOIS presents *one* structure associated with impurities close to the borders. This is due to the strong geometrical confinement felt by the carriers close to the borders of the structure. We observe that the peak of the DOIS moves to higher energies as the volume of the box is reduced. It is interesting to observe that in the case of $L_x = 100$ Å, $L_y = 300$ Å, and $L_z = 500$ Å (the higher volume box) there is a shoulder at 2.1 Ry, which begins to reflect the contributions due to on-center impurities. The presence of
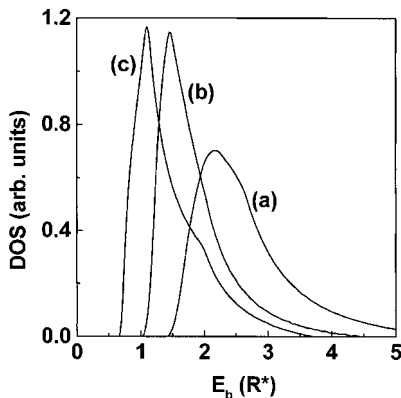

Fig. 1. Density of donor impurity states as a function of the binding energy for GaAs quantum boxes. The dimensions of the structure that we consider are: $L_x = 200$ Å, $L_y = 150$ Å, and $L_z = 100$ Å, curve (a); $L_x = L_y = L_z = 200$ Å, curve (b); and $L_x = 100$ Å, $L_y = 300$ Å and $L_z = 500$ Å, curve (c)
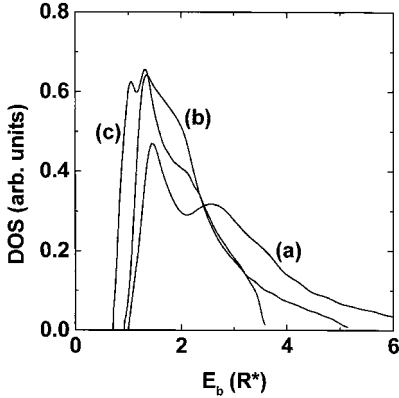
Fig. 2. Density of donor impurity states as a function of the binding energy for GaAs quantum boxes under an applied electric field of 150 kV/cm. The dimensions of the structure are the same as those in Fig. 1

an applied electric field breaks the symmetry of the system along the x-direction and, as a consequence, the peaks of the DOIS are shifted to lower binding energies. This effect is associated with the shift of the probability electronic density away from the impurity position. Due to the applied electric field the peak appearing in curves (a) and (b) of Fig. 1 is resolved into two peaks associated with impurities in the regions close to the borders of the structure (see curves (a) and (b) in Fig. 2). Due to the effect of the external electric field, the two peaks occurring in curve (c) of Fig. 1 are resolved in three peaks, as shown in curve (c) of Fig. 2.

Conclusions   We calculate binding energies and density of states of hydrogenic shallow donor impurities in a QB. We work in a variational scheme within the effective-mass approximation and considering the presence of an external electric field applied in the x-direction of the structure.

In the absence of an electric field, the binding energy is degenerate for symmetrical position of the impurities with respect to the center of the box. However, this degeneracy is broken when the electric field is applied in the x-direction. An important effect of the electric field is the splitting of the main feature in the DOIS into two and three peaks of smaller intensities. When electric field is applied to the QB we observed that the impurity DOIS is shifted along the energy scales and the shape of the peaks is altered.

In conclusion, we would like to point out that the combined effect of external electric field and the geometric shape of the QB gives rise to interesting features in the DOIS. In particular our calculation indicates that the DOIS becomes richer in structure as long as some symmetry is lost, and for those cases in which the system is under an applied electric field. Finally, even when experimental results for the binding energies of impurities in a QB structure are not yet available, we believe our results indicate that an appropriate knowledge of the shape of the DOIS may be of importance in the quantitative understanding of experimental work on shallow impurities in QB structures.

References

[1] G. BASTARD, Phys. Rev. B **24**, 4714 (1981).

[2] G. BASTARD, E. E. MENDEZ, L. L. CHANG, and L. ESAKI, Phys. Rev. B **28**, 3241 (1983).

[3] J. A. BRUM, C. PRIESTER, and G. ALLAN, Phys. Rev. B **32**, 2378 (1985).

[4] L. E. OLIVEIRA and L. M. FALICOV, Phys. Rev. B **34**, 8676 (1986).

[5] G. WEBER, Phys. Rev. B **41**, 10043 (1990).

[6] J. LÓPEZ-GONDAR, J. D'ALBUQUERQUE E CASTRO, and L. E. OLIVEIRA, Phys. Rev. B **42**, 7069 (1990).

[7] N. PORRAS-MONTENEGRO, S. T. PÉREZ-MERCHANCANO, and A. LATGÉ, J. Appl. Phys. **74**, 7624 (1993).

[8] F. J. RIBEIRO and A. LATGÉ, Phys. Rev. B **50**, 4913 (1994).

[9] J. W. BROWN and H. N. SPECTOR, J. Appl. Phys. **59**, 1179 (1986).

[10] N. PORRAS-MONTENEGRO, J. LÓPEZ-GONDAR, and L. E. OLIVEIRA, Phys. Rev B **43**, 1824 (1991).

[11] G. WEBER, P. A. SCHULZ, and L. E. OLIVEIRA, Phys. Rev. B **38**, 2179 (1988).

[12] A. MONTES, C. A DUQUE, and N. PORRAS-MONTENEGRO, J. Appl. Phys. **81**, 789 (1997).