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Electric field dependence of the binding energy of shallow donors in GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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We report theoretical results on the electric field dependence of the impurity binding energy in quantum-well structures. The field is assumed to be constant and applied parallel to the growth axis. Several impurity positions are considered. As a result of the field-induced electronic polarization, the impurity binding energy may be decreased or increased depending on the impurity location in the quantum well.

I. INTRODUCTION

Recently the problem of the presence of an electric field in quantum well (QW) structures has given rise to some interest. When applied along the growth axis (longitudinal electric field), the electric field alters the QW confinement energies. Mendez *et al.*[1] have observed a strong decrease of photoluminescence (PL) signal and a red shift in the PL peak position for increasing field strength F. Bastard *et al.*[2] proposed variational calculations of the eigenstates in an isolated QW structure subject to a longitudinal field. The results of Mendez *et al.*[1] were only qualitatively explained by this model. Miller and Gossard[3] observed intrinsic and extrinsic PL in Be-doped GaAs-Ga(Al)As QW's for a longitudinal electric field. They observed strong changes in integrated photoluminescence but small shifts in energy positions of exciton and impurity peaks. Chemla *et al.*[4] and Wood *et al.*[5] studied room-temperature excitonic absorption peaks when an electric field is applied to a multiple GaAs-Ga(Al)As QW structure.

More recently, Alibert *et al.*[6] performed electroreflectance measurements on GaAs-Ga(Al)As QW's subject to a longitudinal electric field. They observed a red shift in excitonic structures which was explained in terms of a shift in energy levels. Brum and Bastard[7] have calculated the electric-field-induced dissociation of excitons in QW's using variational methods. The calculated results were in qualitative agreement with the data of Wood *et al.*

In this work we calculate the effect of a longitudinal electric field on the binding energy of hydrogenic impurity. We limit our considerations to field strengths for which the notion of quasibound states in the well remains valid (for stronger fields the electron is swept out of the well). The effective-mass approximation is used and donor levels are considered. Two envelope-function models are considered: (i) a simplified model based on variational calculations of the energy levels in which the effective-mass discontinuity between the host materials is neglected; (ii) a more elaborate model which can take into account this discontinuity and solves exactly the problem of a QW perturbed by a longitudinal electric field.

Specifically it appears that the variational and exact treatments of the electric effects give almost the same results when a single effective mass is used throughout the whole structure. Moreover, we show that the impurity binding energy is enhanced or diminished depending on in which half of the QW the impurity is located.

II. THEORY

In the effective-mass approximation the Hamiltonian of a hydrogenic donor when an external field is applied in the z direction is

$$H = H_0 + H_1 \tag{1}$$

with

$$H_0 = -\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z} + V_b\Theta(z^2 - L^2/4) + |e|Fz \tag{2}$$

and

$$H_1 = -\frac{\hbar^2}{2m}\nabla_\perp^2 - \frac{e^2}{\kappa[x^2+y^2+(z-z_i)^2]^{1/2}} , \tag{3}$$

where z_i is the impurity position along the growth axis and $\Theta(x)$ is the step function [$\Theta(x)=1$, if $x>0$, $\Theta(x)=0$ if $x<0$]. In H_0 we have expressed the kinetic energy operator in a way compatible with the work of Ben Daniel and Duke.[8]

In this work we focus our attention on the impurity states attached to the ground QW subband. The way we have divided the total Hamiltonian is dictated by the relative orders of magnitude of the QW, electrostatic, and Coulomb potentials, respectively. The carrier motion along the growth axis is essentially dominated by H_0 since the Coulomb potential well produces an effect of the order of 10 meV.[9] This has to be compared with the barrier potential (0.2 eV) and the F-dependent potential energy drop along the QW thickness L (0.1 eV if $L=100$ Å and $F=10^5$ kV/cm). Once the z motion is determined by H_0, the carriers are bound around the impurity in the layer plane via H_1, the in-plane Coulomb attraction being the average of the $1/|\mathbf{r}-\mathbf{r}_i|$ potential over the ground state of H_0.

To find the eigenstates of H_0 we used two approaches: a variational one and an exact one. In the variational treatment we consider that the effective mass and the relative dielectric constant are constant throughout the whole structure. The ground-state wave function $\phi_0(z)$ is rather easily guessed if one notices that the electric field skews the zero-field QW wave functions towards one interface. This effect is taken into account via a multiplicative exponential factor[1,2] on the $F=0$ QW wave functions. Once $\phi_0(z)$ is known,[2,7] the impurity wave function is chosen in the form

$$\psi(\mathbf{r})=N\phi_0(z)\exp(-r_\perp/\lambda)\ , \tag{4}$$

where N is a normalization constant, λ is a variational parameter, and $\mathbf{r}_\perp=(x,y)$. Using a two-dimensional Fourier expansion of the Coulomb interaction, the expression which has to be minimized is

$$E_i(\lambda)=\frac{\hbar^2}{2m\lambda^2}-\frac{e^2}{\kappa}\int dq_\perp I(q_\perp)\times\frac{1}{[1+(\lambda q_\perp/2)^2]^{1/2}}+E_0(F)\ , \tag{5}$$

where $E_0(F)$ is the lowest eigenstate of H_0 [for details, see Eq. (7) of Ref. 2] and

$$I(q_\perp)=\int_{-\infty}^{+\infty} dz\ |\phi_0(z)|^2\exp(-q_\perp|z-z_i|)\ . \tag{6}$$

The binding energy is then given by

$$E_i=E_0-\min_\lambda E_i(\lambda)\ . \tag{7}$$

Instead of using this variational method, one may perform an exact calculation for H_0 since in each kind of layer the potential is linear in z and the effective mass is constant. To deal with the effective-mass discontinuity, an appropriate Hamiltonian is derived from a two-dimensional (2D) effective-mass approximation since the quantum-well potential breaks periodicity in the z direction:[10] in the absence of the impurity and of the electric field, dispersion curves can be grouped into 2D subbands which result from quantization in the z direction. For narrow or moderately narrow wells, we can consider that the impurity states are derived from one subband. For the values of F considered here (so that we neglect the tunneling effects) these considerations remain valid. The equation then can be written

$$\left[E_0-\frac{\hbar^2}{2m_\perp}\nabla_\perp^2+U(\mathbf{r}_\perp)\right]F(\mathbf{r}_\perp)=E_iF(\mathbf{r}_\perp)\ , \tag{8}$$

where E_0 is the minimum of the 2D subband, $m_\perp$ is the 2D effective mass derived from the band structure in the absence of the impurity, and $U(\mathbf{r}_\perp)$, the effective impurity potential, is an average over z of the Coulomb potential created by the impurity.[11] The solution of Eq. (8) is obtained using a variational treatment. The trial wave function is

$$F(\mathbf{r}_\perp)=Ne^{-r_\perp/\lambda} \tag{9}$$

and the impurity binding energy is given by Eq. (7) where $E_i(\lambda)$ is

$$E_i(\lambda)=E_0+\frac{\hbar^2}{2m_\perp\lambda^2}-\frac{8e^2}{\kappa\lambda^2}\int_0^\infty dz\ |f(z)|^2 z\left[\frac{\pi}{2}[\mathscr{H}_1(2z/\lambda)-N_1(2z/\lambda)]-1\right]\ , \tag{10}$$

where $\mathscr{H}_1$ and N_1 are the first Struve and Neumann functions, and $f(z)$ is the ground eigenstate of the one-dimensional potential well (Fig. 1) corresponding to the 2D subband minimum. The exact solution of $H_0, f(z)$, in each region of space (Fig. 1), is a linear combination of the two Airy functions A_i and B_i. The six unknowns existing in these solutions are obtained using the wave-function and current-density continuities at the interfaces.[8] The two other conditions are obtained by assuming that the function tends toward zero when z tends toward infinity and that the function must remain finite in region I (i.e., we neglect tunneling effects). The solutions obtained are applied in Eq. (10) to obtain $E_i(\lambda)$.

II. RESULTS AND DISCUSSIONS

The parameters used in our calculations are $\kappa=13.1$, $m^*=0.067m_0$ where m_0 is the free-electron mass. The

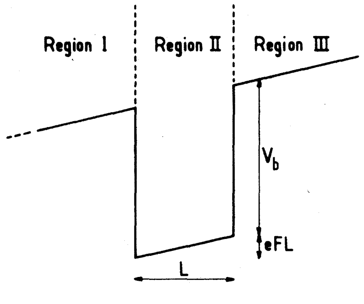

FIG. 1. Conduction-band profile of a quantum well (thickness L, barrier V_b) subject to an electric field F applied along the growth axis z. The z origin is taken at the center of the quantum well. eFL denotes the potential energy difference between the $z=-L/2$ and $z=L/2$ interfaces.

barrier potential is $V_b = 400$ meV [$x \sim 0.38$ for the GaAs-Ga(Al)As]. We calculated the value of F for which we no longer obtain an exact solution, but an approximate solution. For well thickness about 30–100 Å this limit is about 300 kV/cm.

In Fig. 2 are reported the eigenenergies found with the exact solution of the one-dimensional potential and compared with the variational solutions given in Refs. 1 and 2, for a QW of a thickness of 100 Å. We observe that the shift of the energy levels is underestimated in the variational calculations. However, the difference is not very large and is more pronounced at the larger electric fields (for $F = 300$ kV/cm we have $|\Delta E_0| \sim 13\%$). In spite of this discrepancy the values of the impurity binding energy appear to be almost independent of the envelope function used. Both models lead to the same numerical values. This is due to the high stability of E_i in relation to the potential integral

$$\int_{-\infty}^{+\infty} dz \, |\psi(z)|^2 [\rho^2 + (z - z_i)^2]^{-1/2}$$

and the good description obtained by the variational envelope functions.

In Fig. 3(b) we plot the values of the impurity binding energy versus the electric field strength for a QW thickness of 100 Å for various positions of the impurity: $z_i = L/2$, $L/4$, 0, $-L/4$, $-L/2$. We observe that for impurities placed at $z_i \geq 0$ the impurity binding energy decreases with increasing field strength. For $z_i < 0$ the impurity binding energy increases with F. This is associated with the electric-field-induced deformation of the electron wave function; the latter tends to concentrate near the interface $z_i = -L/2$ (see Fig. 1). The effect of the electric field is more pronounced for thicker QW's.

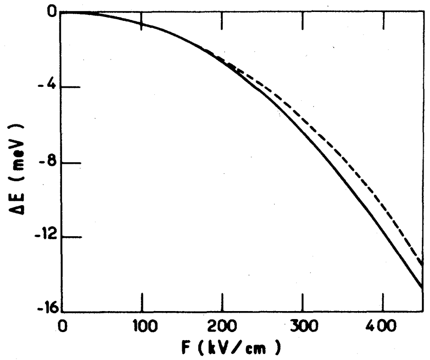

FIG. 2. Comparison of energy-level shifts versus electric field for a conduction electron in a finite GaAs quantum well with $L = 100$ Å and $V_b = 0.40$ eV. Dashed line: variational results (Refs. 1 and 2). Solid line: exact calculations (Airy functions).

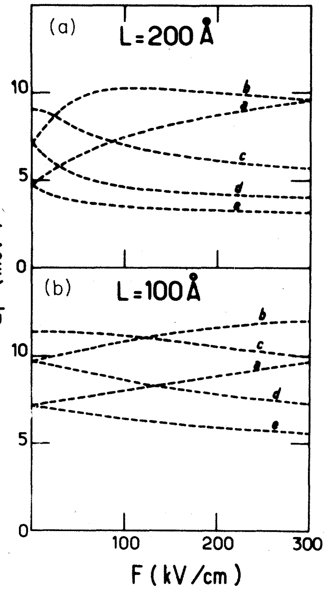

FIG. 3. Impurity binding energy vs electric field for a QW of thickness (a) $L = 200$ Å and (b) $L = 100$ Å. $V_b = 0.4$ eV. Five impurity positions are considered: (a) $-L/2$; (b) $-L/4$; (c) 0; (d) $L = /4$; and (e) $L/2$.

This is illustrated in Fig. 3(a) where the QW thickness is 200 Å. Figure 3(a) exemplifies the competition between the effects of the electric field and of the barrier constraint. Beyond a certain field F (which is L dependent) the barrier constraint predominates and the impurity binding energy tends to saturate at large F. In fact for large enough F (or L) the rectangular QW effectively reduces to a triangular quantum well. The impurity problem becomes in effect equivalent to finding the bound state of an electron moving in a plane $z_e = -L/2 + d_F$ (where $d_F \sim F^{-1/3}$) and being attracted by a Coulomb impurity located in the plane $z = z_i$. It is interesting to observe that the distance between those two planes becomes independent of L for on-edge impurities, implying that the on-edge impurity binding energy should become independent of L if L is large enough. These qualitative considerations are supported by calculations. We show in Fig. 4 the L dependence of the on-edge impurity binding energy for several values of F. Clearly the curves flatten at large enough L if F is nonzero. One may evaluate the critical thickness L_c beyond which the other ($z = L/2$) potential barrier is no longer felt by the carrier in the following way. Let $X(z + L/2)$ be the wave function of the triangular well cornering at $z = -L/2$. If the characteristic distance ξ of the electron from the $z = -L/2$ wall becomes smaller than $L/2$ one may safely assume that the other wall will have a negligible effect on the electron wave function. This will imply that the binding energy of the impurity located at $z = -L/2$ will become independent of L. If one approximates $X(z + L/2)$ by a Fang-Howard wave function,[12]

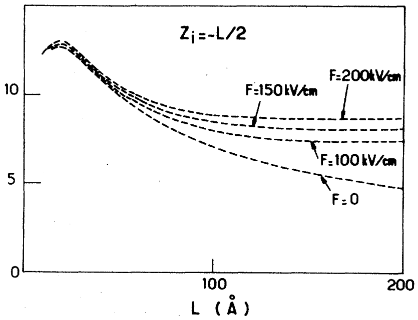

FIG. 4. Impurity binding energy vs QW thickness. $V_b = 0.4$ eV. Four values of the electric field are considered: $F = 0$, 100, 150, and 200 kV/cm.

$$X(z+L/2)=(b^3/2)^{1/2}(z+L/2)\times\exp\left[-\frac{b}{2}(z+L/2)\right] \quad z\geq -L/2\;; \qquad (11)$$

ξ here is given by

$$b=\left[\frac{12eFm}{\hbar^2}\right]^{1/3},\quad \xi=\frac{3}{b}\,. \qquad (12)$$

Thus the critical thickness L_c will be given by

$$L_c=2\left[\frac{9}{4}\frac{\hbar^2}{m_eF}\right]^{1/3}\,. \qquad (13)$$

For $F=10^5$ V/cm, $L_c=128$ Å. This estimate is in rather good agreement with the results shown in Fig. 4.

All these calculations and considerations were done for a donor impurity. The experiments performed by Miller and Gossard[3] on Be-acceptor QW's of GaAs-Ga(Al)As showed a shift in electron-acceptor luminescence energy to higher values with increasing electric field. Also, they observed a change in peak enhancement from electron-acceptor (center) luminescence to electron-acceptor (interface) luminescence for increased fields. Our results confirm their arguments justifying the interface peak enhancement with increasing electric field since it increases the impurity binding for impurities localized at $z_i=-L/2$. However, the experimental results obtained do not permit a quantitative analysis of the energy shift because of the great difficulty of measuring the electric field.

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