Effect of the type-I to type-II transition on the binding energy of shallow donors in GaAs/AlAs quantum wells

A. T. da Cunha Lima
Instituto de Física, Universidade de São Paulo, Cidade Universitária, Caixa Postal 20.516, 01498-970 São Paulo, São Paulo, Brazil

I. C. da Cunha Lima
Faculdade de Engenharia, Universidade São Francisco, Campus de Itatiba, 13257-900 Itatiba, São Paulo, Brazil and Instituto de Física, Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier, 524, 20550-013 Rio de Janeiro, Rio de Janeiro, Brazil

A. Ferreira da Silva
Instituto Nacional de Pesquisas Espaciais, 12.225-001 São José dos Campos, São Paulo, Brazil
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The binding energy of electrons to shallow donors in GaAs/AlAs quantum wells in the vicinity of the type-I to type-II transition is obtained for impurities lying inside the GaAs layer. The calculation is performed variationally using a two-parameter trial function, the same for both type-I and type-II structures. The transition occurs for a GaAs layer width near 37 Å. For widths smaller than 37 Å we obtain the binding energy for the X electrons in a GaAs/AlAs double well, where the impurity lies inside the GaAs middle barrier. For widths larger than 37 Å the binding energy is calculated using a single well for the Γ electrons. A change of symmetry from s-like to p-like is obtained as the transition occurs, for the Γ and for the X electron, respectively. [S0163-1829(97)02523-X]

In GaAs/$Ga_{1-x}Al_xAs$ quantum wells (QW) with $x \leqslant 0.4$ the conduction subbands in the effective-mass approximation are obtained from Γ-type bulk states. However, for $x > 0.4$, $Ga_{1-x}Al_xAs$ becomes an indirect-gap semiconductor with the minimum of the conduction bands lying near the X point in the Brillouin zone. Since the first electron subband in a QW increases in energy as the QW width decreases, in a GaAs/AlAs QW ($x=1$) the first subband will lie above the X-point minima in the AlAs layer, if the GaAs thickness becomes smaller than a certain value. In that case, the GaAs layer becomes a barrier for the X electron, and what is called a type-I to type-II transition occurs. Near this transition the electron subband becomes hybridized,[1,2] a mixing of the states at the Γ and at the X minima. From the point of view of shallow-donor impurities, a significant difference is expected for impurities lying inside such QW's, for widths just above and just below that value in which the transition occurs. A donor impurity at the center of a GaAs well binds a Γ electron, which is mostly confined inside the well, having a binding energy between 6 and 15 meV, roughly, depending on the well width. The same donor in a GaAs barrier binds an X electron,[3] that is mostly confined outside the barrier, having, however, a binding energy that may be higher than in the first case, because of the difference in the effective masses at the minima of the conduction band at the Γ point and the X point. This fact provides an interesting mechanism to observe the transition itself. It has been treated in the past by using two different approaches. Wang, de Andrada e Silva, and da Cunha Lima[4] used a transfer matrix method based on a mixing parameter to consider the effect of the Γ-X hybridization of the first electron subband on the shallow-donor binding energy in a type-I QW. Recently, da Cunha Lima, Emmel, and Ferreira da Silva[5] studied the same problem using a simple variational model of the trial function. On the other hand, Weber[6] treated the case of an X electron bound to a shallow-donor impurity (lying in the AlAs layer) in an AlAs/GaAs QW. The effect of the Γ-X hybridization on the dynamics of an exciton bound to an ionized donor was obtained recently by da Cunha Lima, Ghazali, and Emmel.[7]

In order to understand the photoluminescence spectra related to neutral donors in GaAs/AlAs structures, it is important to clarify to which minimum of the conduction band the bound electron is associated in each case.[8] In the present work we calculate the effect of the type-I to type-II transition on the binding energy of a neutral shallow donor inside a GaAs layer of width L by assuming, in a first model, Γ electrons in a type-I structure (a QW in which the AlAs layers are the barriers) and, in a second model, X electrons in a type-II structure. This type-II structure is represented by a symmetric double well (SDW) for the X electrons in which the barriers are the GaAs layers and the wells are the AlAs layers. In both models the impurity is assumed to lie in the GaAs layer, which is either the well, for the Γ electrons in the first model, or the middle barrier, for the X electrons in the second model. Our results show an important change in the binding energy as the transition takes place. Also, a change occurs in the state symmetry, since the obtained bound state in the type-II structure is predominantly a p-like state.[9]

In order to obtain the binding energy of an electron bound to a shallow-donor impurity (from now on simply referred to as impurity) in the QW and the SDW, we have used a variational calculation that applies to all symmetric structure, based on a trial function

TABLE I. Effective masses of the electron at Γ and X points in units of m_0.

	m_Γ	$m_{X\parallel}$	$m_{X\perp}$
GaAs	0.067	1.3	0.23
AlAs	0.15	1.1	0.19

$$\Psi_{\alpha\beta}(\rho,z)=N_{\alpha\beta}\phi^{(0)}(z)\exp(-\rho/\alpha)\exp(-|z-z_i|/\beta), \tag{1}$$

composed of the unperturbed envelope function $\phi^{(0)}(z)$, and modulated by a confining function depending on variational parameters α and β. z_i is the impurity position in the growth direction (z direction) and $N_{\alpha\beta}$ is a normalization factor.

The envelope function in the type-I structure is the usual first-subband wave function of a symmetric well:

$$\phi^{(0)}(z)=\begin{cases} A\cos(kz) & \text{for } |z|\leqslant L/2 \\ B\exp(-p|z|) & \text{for } L/2\leqslant|z|. \end{cases} \tag{2}$$

The first subband of the symmetric double well with interfaces at $\pm L/2$ and $\pm d/2$ is

$$\phi^{(0)}(z)=\begin{cases} A\cosh(pz) & \text{for } |z|\leqslant L/2 \\ B\cos(kz) & \text{for } L/2\leqslant|z|\leqslant d/2 \\ C\exp(-p|z|) & \text{for } d/2\leqslant|z|. \end{cases} \tag{3}$$

In both cases the parameters assure normalization and continuity of wave functions and probability current densities at the interfaces. The formalism used here applies to the impurity lying anywhere in the structure, but it is assumed, in the present calculation, to be located inside the GaAs layer at a distance z_i from its center. In general, the effective masses are tensors and depend on the coordinate along the axis perpendicular to the interface (z axis), since the values are different for GaAs and AlAs, as shown in Table I.[10] The expectation value of the Hamiltonian can be written as

$$\langle\Psi_{\alpha\beta}|H|\Psi_{\alpha\beta}\rangle=E^{(0)}+t_\perp+t_\parallel+t_c\,. \tag{4}$$

In the above equation, $E^{(0)}$ is the energy of the first subband, the term $t_\perp$ is due to the motion in the plane parallel to the interfaces, $t_\parallel$ represents the kinetic energy due to motion in the z direction, and t_c is the Coulomb interaction with the impurity.

The kinetic contribution $t_\perp$ in Eq. (4) becomes

$$t_\perp=\frac{\hbar^2\alpha^{-2}}{2m_\perp}, \tag{5}$$

with

$$\frac{1}{m_\perp}=\frac{1}{m_{1\perp}}+\frac{m_{1\perp}-m_{2\perp}}{m_{1\perp}m_{2\perp}} \times\frac{\int_{\text{AlAs}}dz|\phi^{(0)}(z)|^2\exp(-2|z-z_i|/\beta)}{\int_{\text{structure}}dz|\phi^{(0)}(z)|^2\exp(-2|z-z_i|/\beta)}, \tag{6}$$

and

$$m_\perp(z)=\begin{cases} m_{1\perp} & \text{for GaAs} \\ m_{2\perp} & \text{for AlAs.} \end{cases} \tag{7}$$

The above equations show that the expectation value of the kinetic energy due to the motion parallel to the interface can be obtained by using a renormalized transversal effective mass corrected by the probability of finding the electron outside the GaAs layer.

The term $t_\parallel$, resulting from the contribution of the motion in the z direction, is expressed in a way similar to Eq. (5), but has an additional contribution $\mathcal{K}_{\alpha\beta}(z_i)$ carrying the signature of the boundary conditions in the structure:[11]

$$t_\parallel=\frac{\hbar^2\beta^{-2}}{2m_\parallel}+\frac{N_{\alpha\beta}^2\pi\alpha^2\hbar^2}{2\beta}\left(\frac{1}{m_1}-\frac{1}{m_2}\right)\cosh(2z_i/\beta)\mathcal{K}_{\alpha\beta}(z_i). \tag{8}$$

In the case of the QW,

$$\mathcal{K}_{\alpha\beta}^{\text{QW}}(z_i)=|\phi^{(0)}(L/2)|^2\exp(-L/\beta), \tag{9}$$

and, for the SDW,

$$\mathcal{K}_{\alpha\beta}^{\text{SDW}}(z_i)=|\phi^{(0)}(d/2)|^2\exp(-d/\beta) -|\phi^{(0)}(L/2)|^2\exp(-L/\beta), \tag{10}$$

where d represents the width of the two AlAs layers plus the GaAs layer between them. The renormalized longitudinal effective mass $m_\parallel$ is defined as in Eq. (6).

In order to obtain the term resulting from the Coulomb interaction, it is worthwhile to define the Fourier transform of the probability density in the z direction as

$$\mathcal{F}_\beta(q,z_i)=\int_{-\infty}^{\infty}dz\,\exp[iq(z-z_i)]|\phi^{(0)}(z)|^2 \times\exp(-2|z-z_i|/\beta). \tag{11}$$

Then,

$$t_c=-\frac{e^2}{\mathcal{K}}N_{\alpha\beta}^2\alpha^2\int_0^\infty dq\;\mathcal{G}_\alpha(q)\text{Re}\mathcal{F}_\beta(q,z_i), \tag{12}$$

where Re stands for real part, and $\mathcal{G}_\alpha(q)$ is defined as

$$\mathcal{G}_\alpha(q)=\int_0^1 ds\;s^2(1-s-\alpha^2q^2s^2/4)^{-1}. \tag{13}$$

The calculation was performed using the conduction minima in a $Ga_{1-x}Al_xAs/GaAs$ heterostructure given as functions of the Al concentration, in meV and at 4 K, by[12]

$$E_\Gamma=1519+911x+147x^2, \tag{14}$$

$$E_X=1992-295x. \tag{15}$$

In Fig. 1 we show the binding energy as a function of the GaAs width for an impurity lying at the layer center. The calculation for $L\leqslant37$ Å was performed in the SDW model with $d=200$, 300, and 500 Å. With these values we have performed a second degree polynomial regression in $1/d$ to obtain the binding energies for $d\to\infty$. The results are shown as the lowest curve in the left side of Fig. 1. The curve in the right side was obtained from the QW model. We observe a large change in the binding energy at the transition, of the order of 10 meV, which is due to the difference in the X and Γ effective masses. It is worthwhile to mention that cyclo-

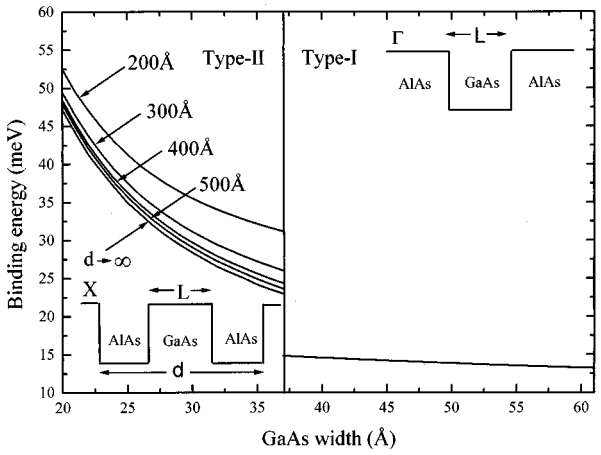

FIG. 1. Binding energy as a function of the GaAs layer width for an impurity at $z_i=0$. The curves at the left of $L=37$ Å are obtained for an X electron in the SDW model with $d=200$, 300, 400, 500 Å and a second degree polynomial regression in $1/d$ to obtain the case in which $d\rightarrow\infty$. The curve at right is obtained for a Γ electron in the QW model.

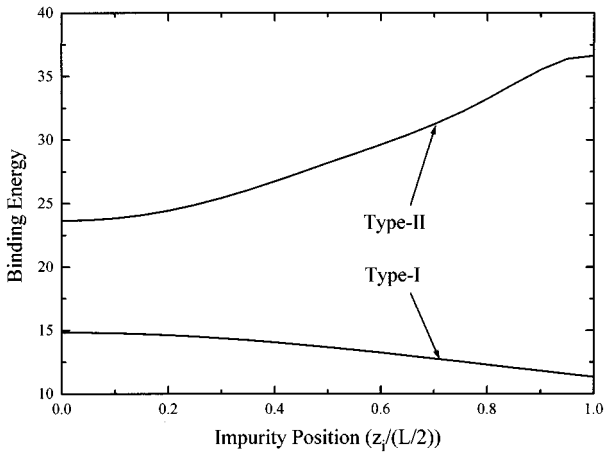

FIG. 2. Binding energy as a function of the impurity position. The width of the GaAs layer is $L=37$ Å. The lower curve represents a Γelectron in a type-I QW. The upper curve represents an X electron in a type-II SDW with $d=500$ Å.

tron resonance[13] and Faraday rotation[14] experiments lead to values of the effective Rydberg in the bulk AlAs in the range 25.85–356.47 meV,[15] much higher than that of the Γ electron in bulk GaAs.

In Fig. 2 we show how the binding energy depends on the impurity position in the two models, for a GaAs width of 37 Å and taking $d=500$ Å in the case of the SDW model. Together with the change of the binding energy, there is also a change on the symmetry. Our results show that the $1s$-like signature is preserved in the type-I structure, since the minima of the binding energy were obtained in the limit of $\beta\rightarrow\infty$, for all values of L and z_i. This is in agreement with the general choice of either $\exp(-\beta r)$ or $\exp(-\beta\rho)$ for the trial function of the neutral impurity in a QW.[16] In the case of the SDW model, on the contrary, a finite β is necessary for binding the electron. The minima of the binding energy were obtained for β around 10 Å. This gives a p-like character, as suggested by Ghazali.[9]

In conclusion, we have shown that the type-I to type-II transition in a GaAs/AlAs QW affects the shallow-donor binding energy both quantitatively and qualitatively. First, due to the differences on effective masses, the binding energies are typically higher in the type-II QW than in the type-I QW, for the impurity lying in the GaAs layer in both situations. Second, a change in the state symmetry occurs, from an s-like symmetry in the type-I to a p-like symmetry in the type-II QW. We believe this change in symmetry is an important factor to take into account, as well, in other Coulomb center problems, e.g., type-II excitons lifetimes in similar structures, since the particle symmetry may establish new selection rules for transitions caused by confined and interface optical modes. This question, however, is beyond the scope of the present work.

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