Binding energies and density of impurity states of shallow hydrogenic impurities in cylindrical quantum-well wires

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(Received 2 April 1990; revised manuscript received 28 June 1990)

The binding energies of hydrogenic impurities in both infinite and finite GaAs-(Ga,Al)As cylindrical quantum-well wires are calculated as functions of the wire radius and of the impurity location in the well for different radii of the wires using a variational procedure within the effective-mass approximation. Assuming there is no intentional doping, we treat the impurity position as a random variable and define a density of impurity states that we have calculated as a function of the impurity binding energy. As a general feature, the density of impurity states presents two structures associated with impurities at the center and at the edge of the quantum-well wire that may be important in the understanding of absorption and photoluminescence experiments of doped GaAs-(Ga,Al)As quantum-well wires.

In the past two decades many quantum-well structures with dimensions comparable to the electronic de Broglie wavelength have been grown with the development of experimental techniques such as chemical vapor deposition, liquid-phase epitaxy, and molecular-beam epitaxy. Due to their small size these structures present some physical properties that are quite different from those of the semiconductor constituents such as optical and electronic transport characteristics. In the past few years, several experimental[1–4] and theoretical[5–8] studies on electronic structure, transport properties, excitonic and impurity levels, as well as impurity binding energies in quantum-well wires (QWW's) have been performed.

Bryant[9] studied the effect of changing the cross-sectional form of the QWW on the impurity's binding energy and found that, in the case of wires with the same cross-sectional area, the binding energies are nearly equal for the cylindrical and the rectangular QWW's, provided that the rectangular form does not deviate too far from the square shape. Weber, Schulz, and Oliveira[10] calculated the impurity binding energies as functions of the impurity position, and the density of impurity states in GaAs-(Ga,Al)As QWW's with different rectangular cross sections and for infinite well depths. Brown and Spector[11] calculated the impurity binding energies using infinite and finite cylindrical confining potentials for both axial and off-axis impurities.

In this work we present results for both donor and acceptor impurity binding energies in cylindrical GaAs-(Ga,Al)As QWW's with finite and infinite confinement potentials as functions of the impurity position in the radial direction for different QWW radii. Also, the density of impurity states as a function of the binding energies is calculated for different well radii, for finite and infinite GaAs-(Ga,Al)As QWW's.

The Hamiltonian of a single hydrogenic impurity in a QWW system is given by

$$H=\frac{P^2}{2m^*}-\frac{e^2}{\epsilon[(\rho-\rho_0)^2+z^2]^{1/2}}+V(\rho)\ , \tag{1}$$

where m^* is the electronic effective mass, ϵ the dielectric constant of the wire material, and $V(\rho)$ the confining potential. The relative separation of the carrier from the impurity along the axis of the wire is given by z and ρ_0 is the impurity location along the ρ direction which is perpendicular to the QWW axis. For the finite well the potential $V(\rho)$ in the above Hamiltonian will be taken as zero for $\rho<d$ and equal to V_0 for $\rho>d$ where d is the QWW radius. According to Brown and Spector,[11] the impurity binding energy can be written in effective Rydbergs as

$$E_b(y,t_0)=-(\lambda a)^2-\frac{4a(Q+P)}{(d/d\lambda)(Q+P)}\ , \tag{2}$$

with

$$Q=\int_0^1 dt\ tJ_0^2(xt)I_0(2\lambda ayt_<)K_0(2\lambda ayt_>) \tag{3}$$

and

$$P=\frac{J_0^2(x)}{K_0^2(cx)}\int_1^\infty dt\, tK_0^2(cxt)I_0(2\lambda ayt_<)K_0(2\lambda ayt_>)\ , \tag{4}$$

where $t_<(t_>)$ is the lesser (greater) of t and t_0, $t=\rho/d$, $t_0=\rho_0/d$, $y=d/a_0^*$, $x=r_{10}d$, $c=(2mV_0/r_{10}^2\,\hbar^2-1)^{1/2}$ with $a=a_0^*$ as the effective Bohr radius, and λ is a variational parameter. J_0 is the ordinary Bessel function of order zero, and I_0 and K_0 are the modified Bessel functions of order zero and of the first and second kind, respectively. It is clear that in the case of a cylindrical quantum-well wire with infinite confining potential, the impurity binding energy is also given by Eq. (2) with $P=0$.

Assuming that the circular cross section of the QWW is not too small we may treat the impurity position as a continuous random variable (we assume impurities only inside the QWW when calculating the density of impurity states), and provided that there is no intentional doping, one can define a density of impurity states[10,12] per unit binding energy as

$$g(E_i)=\frac{1}{\pi d^2}\int_{L(E_i)}\frac{d\mathbf{L}}{|\nabla_L E_i|}=\frac{2\rho}{d^2}\left|\frac{dE_i}{d\rho}\right|^{-1}\ , \tag{5}$$

where $E_i=E_b(y,t_0)$ is the impurity binding energy, $L(E)$ is the portion of the line $E=E_i$ lying within the circular cross section, and ∇_L means the gradient with respect to the impurity position.

Our results are presented in reduced atomic units (a.u.*), which correspond to a length unit of an effective Bohr radius $a_0^*=\hbar^2\epsilon/m^*e^2$, and an energy unit of an effective Rydberg, $R_0^*=m^*e^4/2\hbar^2\epsilon^2$. For GaAs-(Ga,Al)As QWW's these units are $a_0^*\cong 100$ Å and $R_0^*\cong 5.72$ meV for donors (electrons) and $a_0^*\cong 22$ Å and $R_0^*\cong 26$ meV for acceptors (holes). In our calculations we have assumed a spherical effective mass for both donors and acceptors. Also, we have ignored variations in the effective mass and dielectric constant and considered the values for GaAs throughout the heterostructure.

We assume that the band-gap discontinuity[13,14] in a GaAs-$Ga_{1-x}Al_xAs$ heterostructure is distributed about 40% on the valence band and 60% on the conduction band with the total band-gap difference ΔE_g between GaAs and $Ga_{1-x}Al_xAs$ given as a function of the Al concentration $x<0.45$ as[15] $\Delta E_g(\text{eV})=1.247x$.

In Fig. 1 we present the donor binding energy versus the impurity position for both the infinite and finite GaAs-$Ga_{1-x}Al_xAs$ QWW's with different radii. As expected, for all well radii the binding energy is larger for the infinite QWW than for the finite one when the impurity is located at the on-center position due to the larger confinement of the infinite well potential. For the impurity on the edge position, the larger repulsion of the electronic wave function by the infinite potential barrier tends to diminish the binding energy when comparing to the finite-barrier case.

In Fig. 2, we display the density of donor-impurity states as a function of the binding energy for both infinite and finite QWW's and for various well radii. The results in the case of infinite QWW's are in good agreement with those of Weber, Schulz, and Oliveira[10] for an infinite QWW of comparable square cross section. For $d\gg 100$ Å and increasing QWW radii, the strength of the $E_i^{\min}$ peak (which is associated to donors at the edge of the QWW) diminishes, whereas the strength of the $E_i^{\max}$ singularity (associated to impurities at the center of the QWW) is enhanced, leading—for $d\gg 100$ Å—to a center of gravity of the impurity band which converges to the $E_i^{\max}$ value (which becomes the impurity binding energy in bulk GaAs). This behavior is qualitatively the same as obtained by Oliveira and Falicov[15] in the case of GaAs-(Ga,Al)As quantum wells. It is clear from Fig. 2 that experimental values for the binding energies of impurities in nominally undoped QWW's (or in homogeneously doped QWW's) should *not* be compared with the on-center impurity value. We stress this because some previous theoretical work[17–20] on impurities in *quantum wells* seems to have overlooked that aspect and has compared calculated results for on-center impurities with experiment. In fact, we believe a detailed analysis[10,16] of the shape of the density of impurity states is of relevance for a quantitative understanding of future experimental work associated with shallow impurities in QWW's.

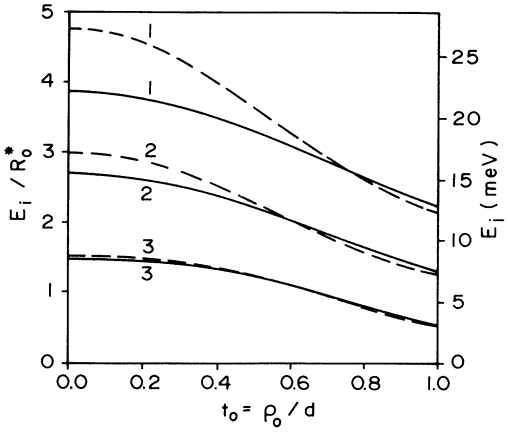

FIG. 1. Donor binding energy as a function of the impurity position for infinite (dashed line) and finite (solid curve) GaAs-$Ga_{1-x}Al_xAs$ QWW's with well radii of 50 Å (curve 1), 100 Å (curve 2), and 300 Å (curve 3). The finite potential corresponds to a concentration $x=0.30$ of Al.

The acceptor binding energy as a function of the acceptor position for GaAs-$Ga_{1-x}Al_xAs$ QWW's is shown in Fig. 3 for an Al concentration of $x=0.3$ and for different QWW radii. One may notice that the behavior of the acceptor curves in Fig. 3 is very similar to that of the donor curves in Fig. 1, provided one takes into account the differences in effective Bohr radii ($\cong 100$ Å for donors and $\simeq 22$ Å for acceptors) and effective Rydbergs ($\simeq 5.7$ meV for donors and $\simeq 26$ meV for acceptors). We would like to stress that our results for acceptors in GaAs-(Ga,Al)As QWW's should be viewed with caution in the sense that a proper calculation of acceptors in QW's and QWW's should take into consideration the coupling of

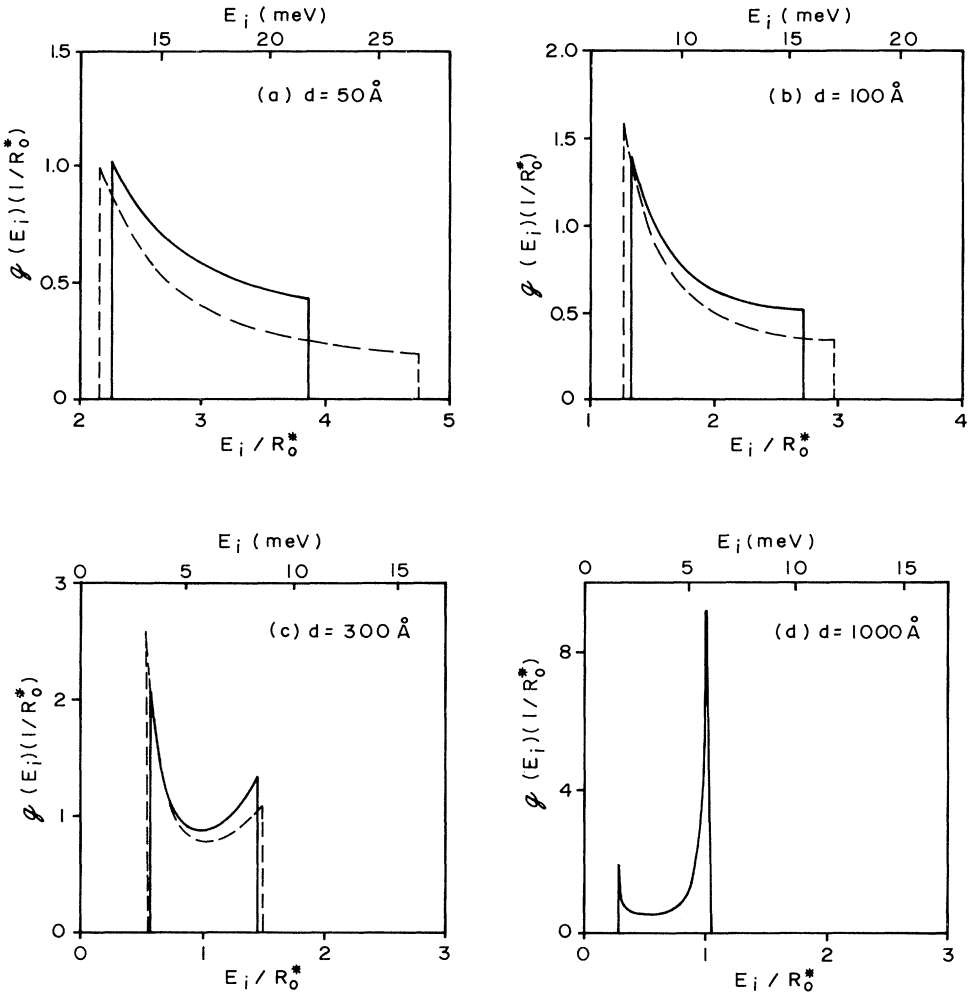

FIG. 2. Density of donor impurity states as a function of the binding energy in infinite (dashed lines) and finite (solid curves) GaAs-$Ga_{0.7}Al_{0.3}As$ QWW's with well radii of (a) 50, (b) 100, (c) 300, and (d) 1000 Å. Notice that different scales are used.

the top four valence bands in GaAs and $Ga_{1-x}Al_xAs$.[18]

In Fig. 4 we present the density of impurity states as a function of the acceptor binding energy for the infinite and finite GaAs-$Ga_{0.7}Al_{0.3}As$ QWW's with well radii of 50, 100, and 300 Å. As expected, the bulk limit [cf. Fig. 4(c)] of the density of impurity states is first reached for lower values of the well radius in the acceptor case than in the donor one, due to the smaller acceptor-effective Bohr radius. For a $d = 300$-Å QWW the density of impurity states is essentially dominated by acceptors near the center of the QWW. Our results in Fig. 4 compare very well with the calculation by Weber, Schulz, and Oliveira[10] in the case of rectangular QWW's with comparable cross-sectional areas.

Summing up, we have calculated the binding energies and density of impurity states for shallow donors and acceptors in cylindrical GaAs-$Ga_{1-x}As_xAs$ QWW's following a variational procedure within the effective-mass

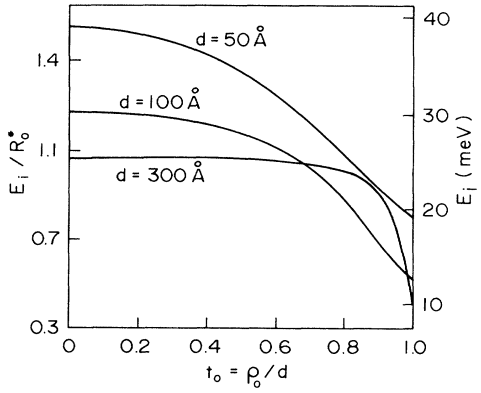

FIG. 3. Acceptor binding energy as a function of the impurity position for $x = 0.30$ GaAs-$Ga_{1-x}Al_xAs$ QWW's and for different well radii.

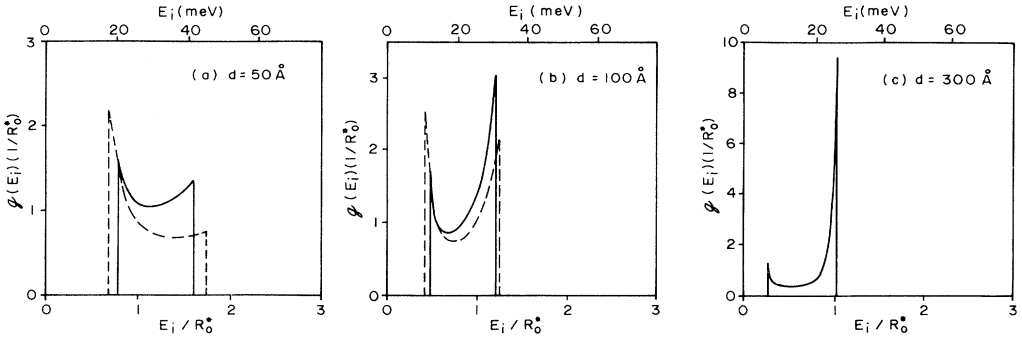

FIG. 4. Density of acceptor impurity states as a function of the binding energy in infinite (dashed lines) and finite (solid curves) GaAs-$Ga_{0.7}Al_{0.3}As$ QWW's with well radii of (a) 50, (b) 100, and (c) 300 Å. Notice that different scales are used.

approximation.[11] The density of impurity states as a function of the donor (or acceptor) binding energy was analyzed for the case of infinite and finite QWW's and for various well radii. Our results indicate that a proper knowledge of the density of impurity states may be of importance in a quantitative comparison between theoretical and experimental results concerning shallow impurities in QWW's. For QWW's, unfortunately, there are no detailed experimental studies involving impurities and therefore no comparison with experiment was possible in the present work. As a general feature, however, the theoretical density of impurity states presents two structures associated to impurities at the center and at the edge of the QWW's which would certainly show up in absorption and photoluminescence experiments of doped GaAs-(Ga,Al)As QWW's. A detailed calculation of the impurity-related optical absorption[21] and photoluminescence spectra[22,23] in GaAs-(Ga,Al)As *quantum wells* showed indeed that this is the case and good agreement with experimental data was obtained. In that sense, one would expect that transitions involving impurity states associated with donors or acceptors at the center or edge positions in cylindrical QWW's would appear as van Hove–like singularities[21,22] in the impurity-related absorption and photoluminescence results. A study of optical absorption and photoluminescence properties related to impurities in QWW's is in progress and is planned to be published elsewhere.

N.P.M. and J.L.-G. would like to acknowledge the Brazilian Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) for partial financial support during their stay in Brazil. This work was supported by Brazilian Agencies Fundaçao de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ), Conselho Nacional de Desenvolvimento Científico e Technógico (CNPq), and Financiadora de Estudos e Projetos (FINEP).

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