Density of states and energy spectra of hydrogenic impurities in quantum-well wires

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(Received 3 November 1987; revised manuscript received 20 January 1988)

We calculate binding energies and densities of states of hydrogenic impurities in quantum-well wires with rectangular cross sections using a variational procedure within the effective-mass approximation. Calculations were performed as functions of the position of the impurity in a quantum-well wire of infinite depth and for various sizes of the wire cross section. The center of gravity of the impurity band and the density of impurity states are analyzed and compared with their quantum-well counterparts, with similarities as well as differences being discussed. Our results indicate that a proper consideration of the density of impurity states may be of relevance in the interpretation of future experimental data related to shallow impurities in quantum-well wires.

I. INTRODUCTION

The physical motivation behind studying lateral confinement in heterostructures—leading to quantum-well wires (QWW's)—is intimately related to the promising possibility of dramatic changes in the electronic, optical, and transport properties of the epitaxially grown single- and multiple-quantum-well "host" structures. For some years since Sakaki's[1] suggestion of carrier-mobility enhancement in QWW's, there were only a few attempts to grow such structures. Petroff *et al.*[2] used etching and epitaxial regrowth in a pioneering work of QWW's while several groups have studied quasi-one-dimensional transport on laterally confined inversion layers.[3] Indeed, the experimental technique to grow QWW's is far from being a set of standard procedures, due to the fact that fine control of lateral dimensions is more difficult than control of layer thicknesses.

Nevertheless, several theoretical studies on electronic structure,[4] excitonic levels,[5] transport properties,[6] impurities,[7–11] as well as transport phenomena involving scattering by ionized impurities[12,13] and by acoustic phonons[14] in QWW's have been performed. Recently, photoluminescence measurements used to study optical properties of QWW's—based on epitaxially grown quantum wells patterned by electron-beam lithography[15,16] with lift-off procedures—were reported and focused-ion-beam lithography[17] appears now as a promising alternative. In such a context, the understanding of the nature of impurity states associated with QWW's is a subject of renewed scientific relevance. Following the work by Brum[9] on shallow impurity states confined in QWW's with rectangular cross sections and infinite potential barriers, we study the QWW "impurity band" and evaluate its center of gravity and the density of impurity states. Our results point out that the density of impurity states may be an important quantity in the interpretation of experimental data related to shallow impurities in QWW's.

In the following section we present the variational procedure used in evaluating the binding energy of shallow hydrogenic impurities in QWW's. Results and discussion are presented in Sec. III.

II. HYDROGENIC IMPURITIES IN A QUANTUM-WELL WIRE

We consider a QWW with a rectangular cross section of dimensions L_x and L_y and infinite in the z direction. The origin is placed at the center of the wire cross section. For a shallow hydrogenic impurity, the Hamiltonian in the effective-mass approximation is

$$H=-\nabla^2-\frac{2}{[(x-x_i)^2+(y-y_i)^2+z^2]^{1/2}}+V(x,y)\ , \tag{2.1}$$

which is in effective atomic units (a.u.*), i.e., energies are written in units of the effective Rydberg $R_0^*=m^*e^4/2\hbar^2\varepsilon_0^2$ and lengths in units of the effective Bohr radius $a_0^*=\hbar^2\varepsilon_0/m^*e^2$. The impurity position is indicated by x_i and y_i; the coordinate z is the relative coordinate of the carrier with respect to the impurity along the axis of the wire. The barrier potential $V(x,y)$ is taken as zero inside the QWW, i.e., for $|x|<L_x/2$ and $|y|<L_y/2$, and infinite otherwise. As a trial wave function for the ground state of the impurity, we use[9]

$$\psi(\mathbf{r})=N\phi_{11}(x,y)\exp\{-[(x-x_i)^2+(y-y_i)^2+z^2]^{1/2}/\lambda\}\ , \tag{2.2}$$

where λ is a variational parameter and $\phi_{11}(x,y)$ is the usual[9] wave function for an unperturbed QWW. The trial impurity ground-state energy $\langle\psi|H|\psi\rangle$ is to be minimized with respect to λ. The impurity binding energy $E_i\equiv E(L_x,L_y,x_i,y_i)$ is calculated with respect to the bottom (top) of the QWW conduction (valence) band.

If the QWW rectangular cross section is not too small, one may treat the impurity position as a continuous random variable and, provided that there is no intentional doping, define a density of impurity states[18,19] per unit

binding energy, $g_{L_xL_y}(E_i)$, with $E_i = E(L_x, L_y, \mathbf{r}_i)$, as

$$g_{L_xL_y}(E) = \frac{1}{L_xL_y} \int_{L(E)} \frac{1}{|\nabla_i(E)|} dl \ , \tag{2.3}$$

where $L(E)$ is the portion of the line $E_i = E$ lying within the rectangular cross section and ∇_i means the gradient with respect to the impurity position. The density of impurity states $g_{L_xL_y}(E_i)$ was then obtained via a histogram method[20] for a mesh of points uniformly distributed in the irreducible (by symmetry operations) part of the QWW rectangular cross section. The number of points to be used in the mesh depends on the dimensions of the cross section and is increased systematically until fluctuations in the density of states are smoothed out.

III. RESULTS AND DISCUSSION

Results presented in this section are in reduced atomic units and hence are valid for donors as well as acceptors in QWW's. For GaAs, one of the most common choices when growing QWW's, these units are $a_0^* \simeq 100$ Å and $R_0^* \simeq 5.72$ meV for donors (electrons), and $a_0^* \simeq 22$ Å and $R^* \simeq 26$ meV for acceptors (holes).

In Fig. 1 we display the binding energies of impurities located at some symmetry points of a QWW with square cross section as functions of the width L. The dashed line indicates the center of gravity,

$$\bar{E}_i(L_x, L_y) = \int_{E_i^{\min}}^{E_i^{\max}} E(L_x, L_y, x_i, y_i) g_{L_x,L_y}(E_i) dE_i \ , \tag{3.1}$$

of the impurity band.[18,19] The binding energy of the on-center (O) impurity reaches the limiting value for the bulk, $1R_0^*$, when L becomes large, whereas the binding energy for the on-center interface (A) impurity reaches the $R_0^*/4$ value characteristic of large quantum wells.[18] A comparison of Fig. 1 with Figs. 2 and 5 of the work by Oliveira and Falicov[19] clearly indicates that the binding energies are larger for impurities confined in a one-dimensional QWW than for impurities in quantum wells. Figure 1 clearly shows that, in contrast to the situation in homogeneous materials, confinement effects in QWW's lead to a large spreading of impurity levels—which depend very much upon the impurity position. Therefore, the evaluation of the center of gravity of this impurity band may be very important[19] when interpreting experimental data related to shallow impurities in QWW's.

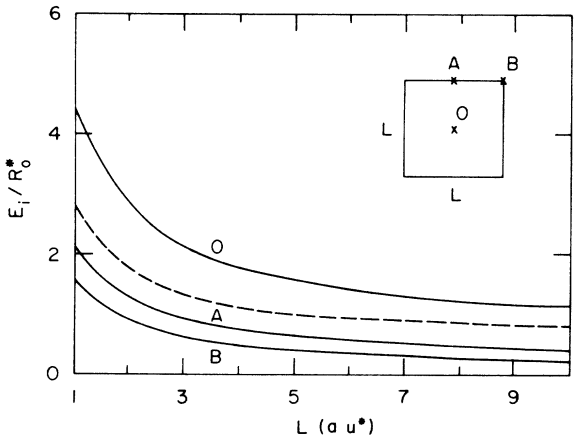

FIG. 1. Binding energies for impurities in a square QWW vs L, calculated for on-center (O), on-center interface (A), and on-edge (B) impurities. The dashed line represents the impurity-band center of gravity as defined in the text.

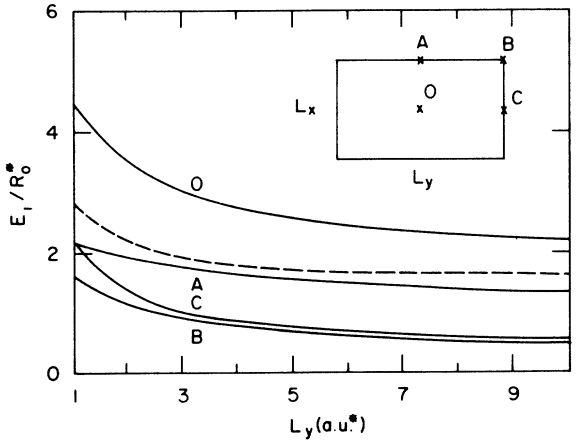

FIG. 2. Binding energies for impurities in a rectangular QWW as functions of L_y with $L_x = 1$ a.u.*, calculated for on-center (O), on-center L_y interface (A), on-center L_x interface (C), and on-edge (B) impurities. The dashed line indicates the impurity-band center of gravity, as defined in the text.

Figure 2 presents our results for the binding energies of impurities in a rectangular QWW with $L_x/a_0^* = 1$ and variable L_y. The $2.25R_0^*$ limiting value[18] for the binding energy of the on-center impurity in a $L/a_0^* = 1$ quantum well is obtained as L_y becomes large. For increasing values of L_y, the impurity binding energy at the L_x interface (C) tends rapidly to the value at the on-edge (B) position, as expected. The dashed line in Fig. 2 represents the center of gravity of the impurity band. It is worthwhile to point out that results shown in Figs. 1 and 2 compare well with those of Brum[9] and Bryant[11] and are closely correlated with those of impurities in cylindrical wires[7,8,10] with comparable cross-sectional areas.

It is very apparent from Figs. 1 and 2 that experimental values for the binding energy of impurities in QWW's could *not* be compared with the on-center impurity value, as our calculation for the center of gravity of the impuri-

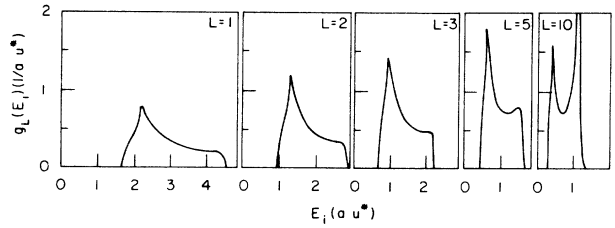

FIG. 3. Density of impurity states $g_L(E_i)$ in reduced atomic units as a function of the impurity binding energy, E_i, for a square QWW, for various L (given in units of the effective Bohr radius).

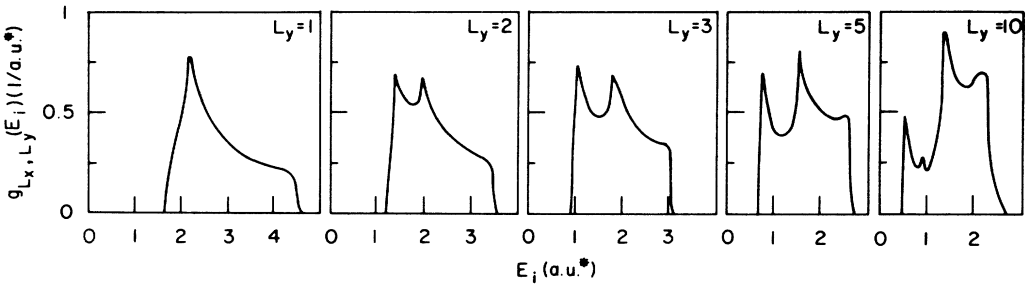

FIG. 4. Density of impurity states $g_{L_xL_y}(E_i)$ in reduced atomic units as a function of the impurity binding energy, E_i, for a rectangular QWW, for various L_y with $L_x=1$ a.u.*.

ty band in square and rectangular QWW's clearly indicates. We stress this because some previous theoretical studies[21–24] of impurities in *quantum wells* seem to have overlooked that aspect when comparing calculated results with experiment. In fact, we believe that a knowledge of the detailed shape of the density of impurity states (see Figs. 3 and 4) in QWW's may be of relevance for the quantitative understanding of future experimental results for shallow impurities in QWW's.

Figure 3 shows the density of impurity states of a square QWW for various sizes of the square cross section. Note that the density of states of the impurity band becomes double peaked as L/a_0^* increases. In comparing the density of impurity states for a square QWW with $L/a_0^*=10$ with the result for a quantum well of thickness $10a_0^*$ [i.e., $\simeq 1000$ Å for donors, or $\simeq 200$ Å for acceptors, in a GaAs-(Ga,Al)As quantum well; cf. Figs. 3 and 6 of Oliveira and Falicov[19]], we find a very similar behavior. This indicates that optical properties associated with impurities in a QWW with large cross sections should *not* be very different from the corresponding properties in quantum wells, as one should expect. For QWW's with not so large square cross sections ($L/a_0^* \lesssim 5$), however, the shape of the density of impurity states is quite different from the results for quantum wells[19] and one might be able to observe such differences in photoluminescence measurements on doped QWW's.

The density of impurity states $g_{L_xL_y}(E_i)$ is shown in Fig. 4 for a QWW with rectangular cross section ($L_x/a_0^*=1$, L_y variable). An important effect is the splitting of the peak in the density of states of the impurity band, immediately after square symmetry is lost, into two peaks of smaller intensities. The shape of the density of impurity states becomes more complicated at large values of L_y/a_0^* (with $L_x/a_0^*=1$) and for $L_y/a_0^*=10$ we note some similarity with the density of impurity states due to a doped quantum well[19] of thickness $L/a_0^*=1$.

In conclusion, we would like to point out that the geometric shape of the cross section of QWW's may produce interesting features in the density of impurity states (Figs. 3 and 4). In particular, our calculation indicates that the density of states of the impurity band becomes richer in structure as soon as some symmetry is lost (cf. Fig. 4). One should therefore be cautious in analyzing experimental results on QWW's (e.g., photoluminescence spectra on doped QWW's) as uncertainties in the shape of the wire cross section may produce important features in the transition spectra.

Finally, although experimental results for the binding energies of impurities in QWW structures are not yet available, we believe our results indicate that a knowledge of the center of gravity of the impurity band as well as the shape of the density of impurity states may be of importance in the quantitative understanding of future experimental work on shallow impurities in QWW structures.

ACKNOWLEDGMENTS

G.W. and P.A.S. would like to acknowledge the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) for financial support.

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