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Occurrence of impurity bands in quantum-well wires

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It is shown that hydrogenlike impurities inside a quantum-well wire of $Al_xGa_{1-x}As$-GaAs create a band in the density of states of bound electrons at concentration of experimental interest. In this range of concentration the impurity band occurs separated from the conducting subbands. The density of states is obtained for several values of impurity concentrations and wire dimensions.

Since 1980, when Sakaki[1] discussed for the first time the possibility of fabrication of ultrathin quantum wells many works have appeared dealing with the properties of what is now known as quantum-well wire (QWW). Only recently, with combined molecular-beam epitaxy (MBE) and other sophisticated techniques including ion implantation, has it become possible to prepare wires with dimensions of the order of the electron's de Broglie wavelengths ($\lesssim 500$ Å).[2] Cibert *et al.*[2] observed low-temperature cathodeluminescence revealing for the first time quantum states in these quasi-one-dimensional systems.

As occurred with two-dimensional (2D) quantum wells, there already has been considerable interest shown in the problem of hydrogenic impurities in QWW.[3-6] As far as we know there are as yet no experimental data on impurities in those systems. Besides, all reported calculations are in one way or another variational solutions of the effective mass equation. Lee and Spector[3] solved the problem of an on-axis impurity in a cylindrical GaAs/$Al_xGa_{1-x}As$ QWW considering infinite barrier at the interface for the conduction electrons. Bryant[4] made similar calculations considering finite barrier and found a small decrease in binding energy together with the occurrence of a maximum at small radius instead of the divergence of the strict 1D hydrogen atom. Brum[5] studied the impurity position dependence of the binding energy in a rectangular wire and verified that binding energy decreases as the impurity is moved away from the center of the wire, as expected. The screening on the impurity potential was treated by Kodama and Osaka.[6] The remarkable conclusion of the works cited above is that besides the overall behavior of the binding energy, which is as expected from the works on 2D quantum wells,[7,8] one finds binding energies for the quasi-one-dimensional systems that are roughly twice that of those in 2D quantum wells. These strong bindings of electrons in QWW's have several consequences with regard to their optical-electronic properties.[3]

As long as one deals with real systems, depending on the impurity concentration, one has to consider the interaction between the impurities. This interaction has the effect of broadening the absorption line due to impurity ionization.[9] In this Rapid Communication we present a first calculation of the density of states (DOS) of electrons bound to impurities inside the QWW as a function of the impurity concentration and of the dimensions of the wire's cross section. We found impurity bands separated from the conduction band, with considerable bandwidths for the cases of experimental interest. Our results are useful for the interpretation of various optical-electronic experimental data as they became available.

Following similar calculations done for quasi-two-dimensional systems[10,11] we start with the following tight-binding Hamiltonian:

$$H=\sum_i \varepsilon_i |i\rangle\langle i| + \sum_{i\neq j} V_{ij} |i\rangle\langle j| \ , \tag{1}$$

where $\langle \mathbf{r}|i\rangle = \Psi(\mathbf{r}-\mathbf{R}_i)$ is the ground-state wave function of an electron bound to an impurity at $\mathbf{R}_i$. Neglecting the overlap $\langle i|j\rangle$ $(i\neq j)$ and three center terms we have the following hopping integral:

$$V_{ij}=V(\mathbf{R}=\mathbf{R}_i-\mathbf{R}_j)=\left\langle i\left|\frac{e^2}{k|\mathbf{r}-\mathbf{R}_i|}\right|j\right\rangle \ , \tag{2}$$

where k is the GaAs background dielectric constant, e is the charge of the electron, and the impurity is assumed monovalent. Finally, ε_i is the single-site energy which depends on the impurity position on the plane XY (see Fig. 1).

The DOS can be obtained by the one-electron propagator which has to be averaged over all possible impurity configurations. This is a very difficult problem. But, if we consider the impurities distributed around the center of the wire, the values of ε_i will present a small variation because ε_i has a minimum for the impurity at the center. In this case we can take $\varepsilon_i \cong$ const which reduces the problem to the treatment of only the off-diagonal disorder, i.e., disorder in the V_{ij} matrix elements. Considering linear densities of 10^4 cm^{-1}, the mean interimpurity distance along the z axis is of 10^4 Å which, in general, is much bigger than L. We can, in this case, assume all impurities laying

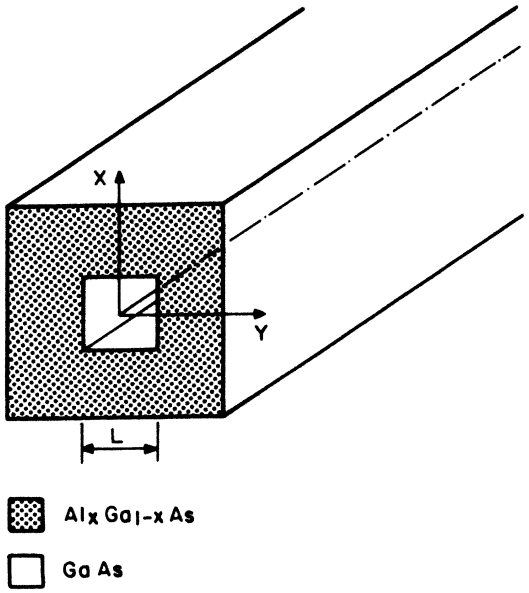

FIG. 1. Schematic of the model quantum-well wire with square cross section of side L. The impurities are randomly distributed on the z axis (dots).

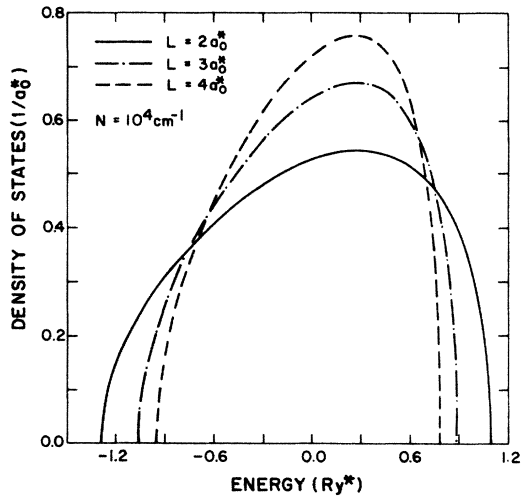

FIG. 2. Density of states (DOS) in atomic units for square wires of different sides L. N is the impurity linear concentration. The origin energy is that of the bound electron [Eq. (6)].

on the z axis (for a detailed discussion of this approximation see Ref. 12). We now have a one-dimensional disordered problem which can be solved suitably by the one-dimensional version of the Matsubara and Toyozawa[13] method. The averaged diagonal elements of the propagator are given in this case by

$$\langle G_{ii}(\varepsilon+i0^+)\rangle = \xi(\varepsilon)/\varepsilon \ , \tag{3}$$

where $\xi(\varepsilon)$ is obtained from the following integral equation:

$$1-\frac{1}{\xi(\varepsilon)} = \frac{N\xi(\varepsilon)}{2\pi\varepsilon^2}\int dk \frac{V^2(k)}{1-N\xi(\varepsilon)V(k)/\varepsilon} \ , \tag{4}$$

where N is the impurity concentration per unit length and

$$V(k) = \int dz e^{ikz} V(z) \tag{5}$$

is the one-dimensional Fourier transform of the hopping integral equation (2). We solve Eq. (4) numerically and calculate the DOS by

$$D(E) = -\pi^{-1}\mathrm{Im}\langle G_{ii}(\varepsilon+i0^+)\rangle \ .$$

The wave functions used as a basis for the Hamiltonian in Eq. (1) are taken from the variational solution of the isolated impurity problem. Using atomic units ($R^* \cong 5.3$ meV and $a_0^* \cong 103$ Å which correspond to $K = 13.1$ and $m^* = 0.067 m_0$) the variational solution is given by

$$E = \left\langle \Psi \left| -\nabla^2 - \frac{2}{r} + V(x,y) \right| \Psi \right\rangle_{\min} \ , \tag{6}$$

where $V(x,y)$, the confining potential, is taken in the infinite barrier approximation, i.e., $V(x,y) = \infty$ outside and zero inside the wire. We consider, as in Fig. 1, square cross-section wires with dimension L. For the trial function Ψ we choose the following Gaussian-type wave function:

$$\Psi(\mathbf{r}) = \phi(x,y)\eta(z) \ , \tag{7}$$

with

$$\phi(x,y) = N_a \cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right) e^{-a(x^2+y^2)} \ ,$$

$$\eta(z) = (2a/\pi)^{1/4} e^{-az^2} \ ,$$

for $|x|, |y| \le L/2$ and zero otherwise, where a is the variational parameter and N_a a normalization constant given so that $\langle \phi | \phi \rangle = 1$. The impurity is located in the ori-

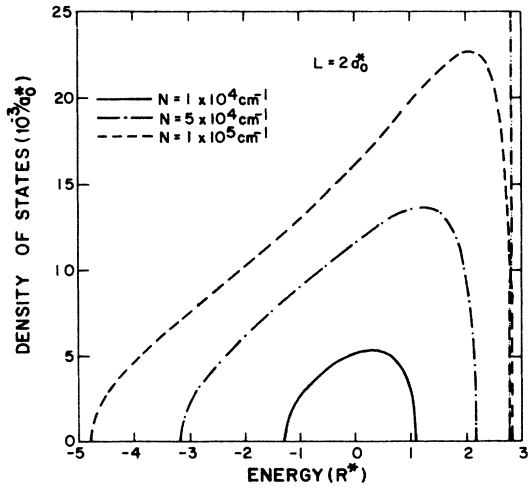

FIG. 3. DOS for different impurity concentrations N. Vertical dashed line represents the binding energy of an electron bound to an on-center impurity which is given by $E_B = 2(\pi/L)^2 - E$.

gin of the coordinates. As one sees, this function is separable and the Fourier transform of the hopping integral becomes a straightforward calculation. On the other hand, this trial function gives extremely good energies in that system; the error, in comparison with more exact $1s$-type functions, is around 1%.

Defining $H_0(x,y) = -\nabla^2_{x,y} + V(x,y)$, the energy equation (6) will be given by

$$E = E_0(a) + a + E_{\text{cou}}(a) \ , \tag{8}$$

where $E_0 = \langle \phi | H_0 | \phi \rangle$ and $E_{\text{cou}} = \langle \Psi | -2/r | \Psi \rangle$. After obtaining a numerically by minimizing E, for each L, we calculate $V(K)$, which is given by

$$V(K) = (2\pi/a)^{1/2}(E - E_0 - K^2)e^{-K^2/2a} \ . \tag{9}$$

Finally, we insert it into Eq. (4) to obtain the averaged DOS.

The obtained DOS's are shown in Figs. 2 and 3. The variation of the DOS as a function of L for a typical N, as shown in Fig. 2, is similar to that found for impurities bound in 2D quantum wells.[11] The wider the wire the sharper the band. The spreading in energy is, for instance, for $L = 2a_0^*$, $\Delta\varepsilon \cong 2.4R^*$, which is of the order of the binding energy which is $2.8R^*$, for that value of L. The DOS's are quite symmetrical and considerably separated from the unperturbed first conduction subband. In Fig. 3 we plotted the DOS corresponding to different impurity concentrations. As the number of impurities increase the DOS gets more and more asymmetric and close to the bottom of the unperturbed conduction band, assigned by the vertical dashed line in the figure.

In conclusion, we saw that the interaction between impurities in QWW's is responsible for a large spread in the ionization energy of, for example, $\Delta\varepsilon \cong 12.7$ meV in a typical wire with $L \cong 200$ Å and $N = 10^4$ cm^{-1}.

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