Quasi-1D electron states in a double quantum well with an *H*-shaped bridge

E. L. Ivchenko and A. A. Kiselev
A. F. Ioffe Physicotechnical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

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Quasi-1D states of a new type are discussed. They would occur in a pair of quantum wells separated by a high barrier and connected by a bridge of narrow-gap material. In the wells, the wave function of a localized electron forms two diffuse regions which are tied to the bridge. The localization energy is calculated as a function of the bridge width.

In some recent experiments involving the growth of multilayer GaAs/AlAs (311) heterostructures with corrugated surfaces, it was found possible to insert some 1D clusters of GaAs into one of the AlAs layers.[1] The cross section of a cluster was rhombic, with diagonals of 32 and 20.4 Å . Each of the obtuse-angle vertices of the rhombus touched one of the protuberances which formed when the corrugated (faceted) heterojunction was intersected by the $(\bar{2}33)$ plane. As a result, two neighboring GaAs layers, separated by an AlAs barrier layer, were coupled by a 1D rhombic GaAs bridge. For free carriers (or excitons) in such a structure, there are quasi-1D states whose wave function consists of two clouds which are spread out within GaAs layers and which are tied to the 1D cluster. As a result, a structure with clusters differs from the quantum-wire structures which are usually discussed[2] and in which the wave function is concentrated primarily within a wire.

The existence of quasi-1D states in a GaAs/AlAs(311) heterostructure with clusters is supported by the appearance of additional lines in the photoluminescence spectra[1] and by the anomalous increase in the exciton oscillator strength, found from the resonant optical reflection spectra.[3] In the present letter we calculate the shape of the wave function and the localization energy for an electron in a double well with a coupling cluster of the same material. Putting aside the features which result from the corrugation of the heterojunctions and from the rhombic cross-sectional shape of the cluster, we consider here a simpler model structure with plane interfaces and an *H*-shaped bridge (Fig. 1a). For simplicity we assume that the potential barrier is infinitely high.

We seek the envelope of the wave function in the form $e^{iqy}\phi(x,z)$, since the structure is uniform along the y axis. The function $\phi(x,z)$ satisfies the 2D Helmholtz equation

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}+\frac{2m}{\hbar^2}E\right)\phi(x,z)=0 \qquad (1)$$

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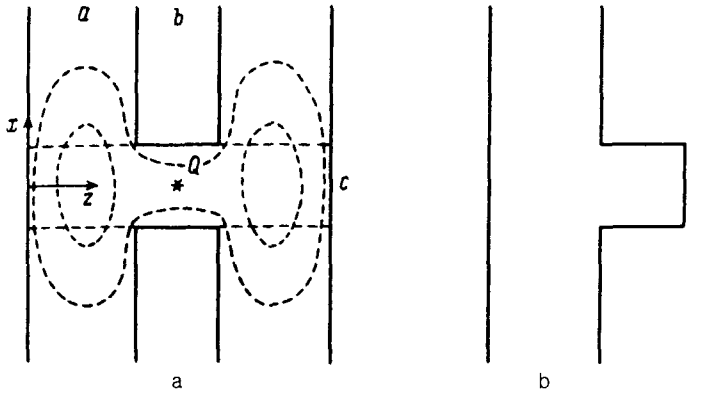

FIG. 1. a—GaAs/AlAs structure with a pair of quantum wells, coupled by a GaAs bridge of width c; b—structure with a quantum well containing an expanded 1D region $(a+b)\times c$. The dashed curves are contour curves of the probability $\phi^2(x,z)$ for the quasi-1D ground state of an electron.

with the boundary condition $\phi(x,z)=0$ at the contour of the cross section of the interfaces. The energy of an electron, reckoned from the bottom of the conduction band of bulk GaAs, is equal to the sum $E+\hbar^2q^2/2m$, where m is the effective mass. This problem is similar in formulation to boundary-value problems for waveguide modes in cavities,[4] differing from the latter in that the wave function ϕ (x,z) lacks a vector structure.

Using a method of partial regions, we seek a general solution in the bridge region, $\Omega=(|x|<c/2;\ 0<z<d=2a+b)$, as the sum

$$\phi(x,z)=\sum_i C_i \sin(K_i z)\cos(Q_i x), \tag{2}$$

where $K_i=\pi i/d$ and $Q_i=[(2mE/\hbar^2)-K_i^2]^{1/2}$. Here we have made use of the symmetry under the reflection $x\to -x$ for the low-lying states of the function ϕ (x,z). With regard to the symmetry under reflection in the σ_z plane, which passes through the center of the structure (the transformation $z\to d-z$), we note that for even solutions, including ground state 1, we have $i=1, 3, \ldots$ in sum (2), while for odd solutions (including the first excited state, 2) we have $i=2, 4, \ldots$. Outside the region Ω, in the well on the left, we have

$$\phi(x,z)=\sum_j D_j \sin(k_j z)e^{-\kappa_j \bar{x}}, \tag{3}$$

where $k_j=\pi j/a$, $k_j=[k_j^2-(2mE/\hbar^2)]^{1/2}$, and $\bar{x}=|x|-c/2$. The solution in the right well is found from (3) by making the substitution $z\to d-z$ and by multiplying by ± 1 for even and odd states, respectively.

The functions in (2) and (3) and their derivatives with respect to x are joined at segments of the common boundary of the regions at $x=\pm c/2$. Multiplying the con-

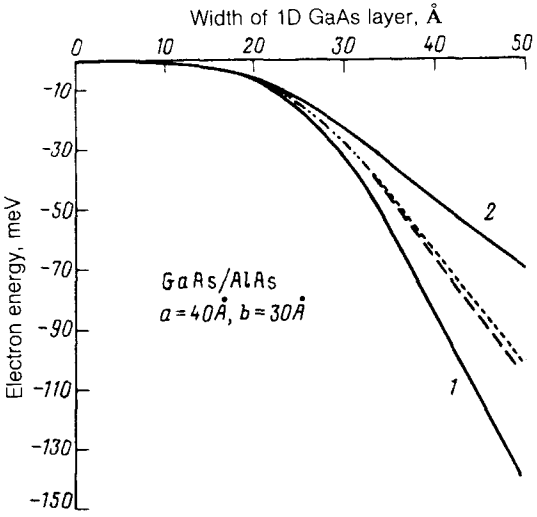

FIG. 2. Energy of an electron localized in a double quantum well with an H-shaped bridge. *1*—Ground state, symmetric with respect to the center of the structure, Q (Fig. 1a); *2*—first excited state, which is odd under reflection in the σ_z plane, which passes through center Q; short-dash curve—ground state for the structure in Fig. 1b; long-dash curve—arithmetic mean of the values for curves *1* and *2*. The energy is reckoned from the bottom of the lower conduction subband in a single well of width a.

tinuity condition for the functions by $\sin(K_i z)$, multiplying the continuity condition for the derivatives by $\sin(k_j z)$, integrating over z, and eliminating the coefficients D_i, we find a system of homogeneous linear equations for the coefficients C_i:

$$\sum_i C_i[\cos(Q_m c/2)\delta_{mi} - 8\eta Q_i\, dv_{mi} \sin(Q_i c/2)\sin(K_m a)\sin(K_i a)] = 0,$$

$$v_{mi} = \sum_j \frac{j^2}{\kappa_j a(\eta m^2 - j^2)(\eta i^2 - j^2)}, \quad \eta = (a/d)^2. \tag{4}$$

The energy eigenvalues are found from the condition under which system (4) has a nontrivial solution.

Figure 2 shows $E_{1,2}$, the energies of the ground state and the first excited state, 1 and 2, as a function of the bridge width c (in Fig. 1, all energies are reckoned from the bottom of the lower subband of the conduction band, $E_0 = \hbar^2\pi^2/2ma^2$, in an isolated well of width a). The distribution of the electron density for state 1 is shown schematically by the dashed curves in Fig. 1a.

It is convenient to analyze these states by the strong-coupling method: We treat states 1 and 2 as linear combinations $(\phi_l \pm \phi_r)/\sqrt{2}$, where ϕ_l and ϕ_r are the wave functions of the ground state in the left well alone and the right well alone, with an expanded region of the type shown in Fig. 1b. The curve with short dashes in Fig. 2 shows the ground-state energy as a function of the width c for the structure in Fig. 1b with a nonstandard region of thickness $a+b$. The energies found in this case are seen

to be close to the arithmetic mean $\bar{E}=(E_1+E_2)/2$ (the curve with long dashes). For the widths considered here, $c<50$ Å , states 1 and 2 can thus be treated by the strong-coupling method with the overlap integral of unperturbed states, $I=-(E_2-E_1)/2$. We thus conclude (in particular) that in an electric field $\mathbf{F}\|\mathbf{z}$ the splitting between levels 1 and 2 increases from $2|I|$ to $[4I^2+\{eF\xi\}^2]^{1/2}$, where ξ is the on-center distance between the density distributions ϕ_l^2 andϕ_r^2, which is approximately equal to the on-center distance between the wells, $a+b$. For the structure in Fig. 1a, with a width $c=30$ Å , we have $I\simeq -4$ meV, and the splitting between the lower levels increases by a factor of $\sqrt{2}$ in a moderate field $F\sim 10^4$ V/cm.

It is also interesting to compare the values of $\bar{E}$ with the energy of the first quantum-size level $E_1^{(1D)}$ for a 1D electron of mass m in the potential well $V(x)=E_0'\equiv\hbar^2\pi^2/2m(a+b)^2$ for $|x|<c/2$ and $V(x)=E_0\equiv\hbar^2\pi^2/2ma^2$ for $|x|>c/2$. With $a=40$ Å, $b=30$ Å, and $c=30$ Å, we find $\bar{E}-E_0=-27$ meV and $E_1^{(1D)}-E_0=-103$ meV. The substantial difference between the results is evidence that the simple 1D model is not adequate for describing localized states (2) and (3). If we allow for the finite height of the barrier in the GaAs/AlAs structure, we may find a slight renormalization of the localization energy of a quasi-1D electron.

In conclusion we would like to call attention to the possibility that quasi-1D states of yet another type may form. These states would be similar to waveguide modes in open cavities with cylindrical mirrors.[5] The role of the converging waveguide would be played by barrier layers. If the heterojunction surfaces have the optimum profiles, the decay due to the escape of an electron from a confinement system of this sort might be very slight.

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