Self-Consistent Calculation of the Electronic Properties of Quantum Well Wires

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We have calculated the electronic structure of one-dimensional electron gas solving self-consistently the Schrödinger and Poisson equation. The Schrödinger equation is solved using the split-operator technique. The method we use to calculate the structure of subband is based on the solution of the time-dependent Schrödinger equation using the split-operator technique. We investigated the electronic properties of the quantum wires as a function of gate voltage, from which we determine the threshold between the 2D and 1D transitions.

One-dimensional electron gas systems (lDEG) have attracted considerable interest, following the advances in high-resolution lithography, which have made it possible to fabricate semiconductor structures that confine the motion of free carriers in two directions. This confinement gives rise to new and interesting quantum properties, because in this regime, the dimensions of the structure become comparable with the electron wavelengths, and the charge transport is dominated by the fundamental quantum properties of the electron. These structures are important for device applications, because the one-dimensional carrier confinement reduces scattering that results in higher mobility. A variety of techniques has been employed to induced the lateral confinement potentials that form one and zero-dimensional electron system out of the two-dimensional electron gas (2DEG).

As a variation of the ordinary single-gate modulation-doped field effect transistor, a lateral-surface superlattice (LSSL) is realized by using grid gates. In this system the degree of confinement can be controlled by changing the gate voltage (V_g). As sufficiently high gate bias, when the gated regions are completely depleted, the ungated regions can retain electrons and the system behaves as an array of isolated quantum wires. When the gate voltage has intermediate values such that the gated regions are not completely depleted the system is a quantum wire superlattice with states extending over several periods of the structure.

The complexity of the physics inherent in such heterostructure devices, however, makes the development of theoretical models extremely difficult. Such calculations are generally based on self-consistent solutions of the Poisson equation and Schrödinger equation[1−5], which are difficult to set up and often require extensive computing facilities. In spite of this, some notable advances have been made on the modelling of quantum point contacts, etched quantum wires and a range of quantum dot problems.

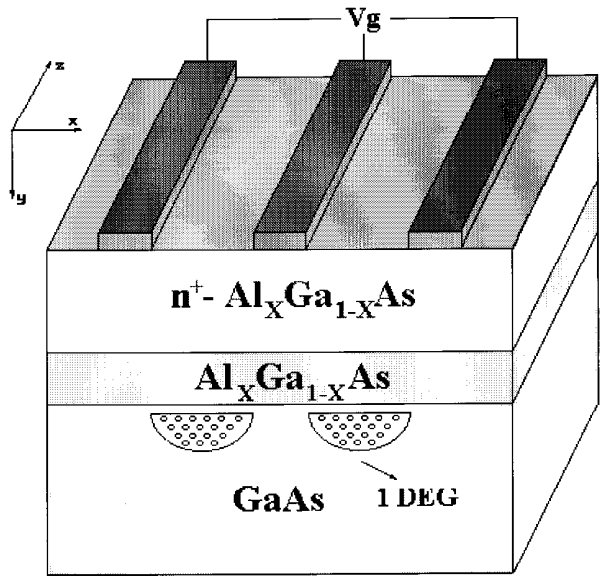

Figure 1: Schematic cross section of the superlattices of quantum wires. The n^+ - $Al_{1-x}Ga_xAs$ is 300 Å thick, the $Al_{1-x}Ga_xAs$ spacer is 50 Å thick, and the gates are separated by 400 Å and the gate size is 860 Å thick.

The system studied here is composed by a two-dimensional electron gas confined at the interface of an $Al_{1-x}Ga_xAs/GaAs$ heterostructure, on top of which there is a periodic structure of gates. When a negative voltage is applied to the gates, the regions at the interface beneath them are depleted and quantum wires are formed. In the structure considered we take into account a residual distribution of ionized acceptor impurities uniformly distributed over the system, and ionized donor impurities uniformly distributed over a spacer layer of about 300 Å. A schematic cross section of this system is shown in Fig. 1.

We use the effective-mass approximation to calculate the subband structure. The non-parabolicity effects are neglected and in this way we describe the motion of electrons along a wire by a free electron state with an effective mass m^*. In order to obtain the subband structure we have solved self-consistently the 2D Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}+V_{ext}(x,y)+V_H(x,y)\right]\Phi_n(x,y)=\epsilon_n\Phi_n(x,y)\ , \tag{1}$$

and the Poisson equation,

$$\nabla^2 V_H(x,y)=-\frac{4\pi e^2}{\epsilon}[\eta(x,y)-N_d(x,y)+N_a(x,y)]\ , \tag{2}$$

where $V_{ext}t(x,y)$ is the potential due the conduction band-offset which depends on the Al concentration, V_H is the Hartree potential due to the electrostatic interaction of electrons with themselves and impurity charges, ϵ is the dielectric constant, $\eta(x,y)$ is the electronic density and N_d and N_a are respectively the donor and acceptor densities. The electronic density is given by

$$\eta(x,y)=\sum_i N_i|\phi_i(x,y)|^2\ , \tag{3}$$

where N_i is the number of electrons per unit of length in the i^{th} subband

$$N_i=\begin{cases}\frac{1}{\pi a_0^*}\cdot\sqrt{\frac{K_BT2m^*a_0^{*2}}{\hbar^2}}F_{-1/2}\left(\frac{\epsilon_F-\epsilon_i}{K_BT}\right) & \text{if } T\neq 0\\ \frac{2}{\pi a_0^*}\cdot\sqrt{\frac{2m^*a_0^{*2}}{\hbar^2}}\cdot\sqrt{\epsilon_F-\epsilon_i} & \text{if } T=0\end{cases} \tag{4}$$

and ϵ_i is it energy, T is the temperature and ϵ_F is the Fermi energy. $F_{-1/2}(\eta_i)$ is the Fermi-Dirac function, where we are using an analytical approximation for the Fermi-Dirac integral, proposed by Humet et al.[6].

The method we have used to calculate the electronic structure of the 2D system is based on the solution of the time-dependent Schrödinger equation using the *split-operator technique*[1,7]. Since the system is periodic along the x direction, the Poisson equation can be solved easily by performing a Fourier Transform of the charge density $\rho(x,y)$ and of the potential $V_H(x,y)$, in the x direction. Doing so, we can write the Poisson equation in dimensionless units as follows

$$\frac{\partial^2 v(k_x,y)}{\partial y^2}-k_x^2 v(k_x,y)=8\pi\rho(k_x,y)\ , \tag{5}$$

where

$$V_H(x,y) = \mathcal{F}[v(k_x,y)] = \frac{1}{2\pi}\sum_{k_x} e^{-ik_x x} v(k_x,y) \ , \quad (6)$$

$$\rho(x,y) = \mathcal{F}[\rho(k_x,y)] = \frac{1}{2\pi}\sum_{k_x} e^{-ik_x x} \rho(k_x,y) \ , \quad (7)$$

Equation (5) is solved by the finite differences method in a nommiform mesh, where it can

$$\frac{2v_{i,j-1}}{\Delta y_{j-1}(\Delta y_{j-1}+\Delta y_j)} - \left(\frac{2}{\Delta y_{j-1}\Delta y_j} + k_x^2\right) v_{ij} + \\ + \frac{2v_{i,j+1}}{\Delta y_j(\Delta y_{j-1}+\Delta y_j)} = 8\pi\rho_{ij} \ , \quad (8)$$

with the use of a simple tridiagonal solver in the y direction to calculate $v(k_x,y)$. The inverse Fourier transform of $v(k_x,y)$ then gives the final result $V_H(x,y)$.

The self-consistent solution of Eqs. (1), (2), (3) and (4), gives the charge density profile, the subband energy levels, the Fermi energy, and the effective potential. In Fig. 2 we show the effective potential obtained for a gate voltage of 300 mV.

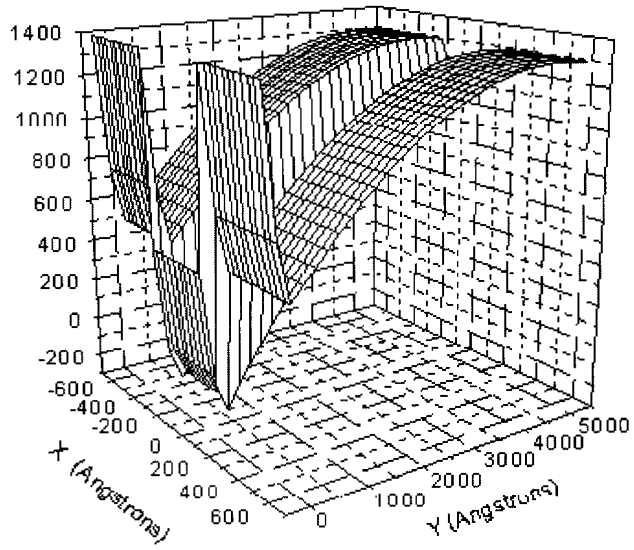

Figure 2: Effective potential $V_{ef}(x,y)$ for a gate voltage of 300 mV.

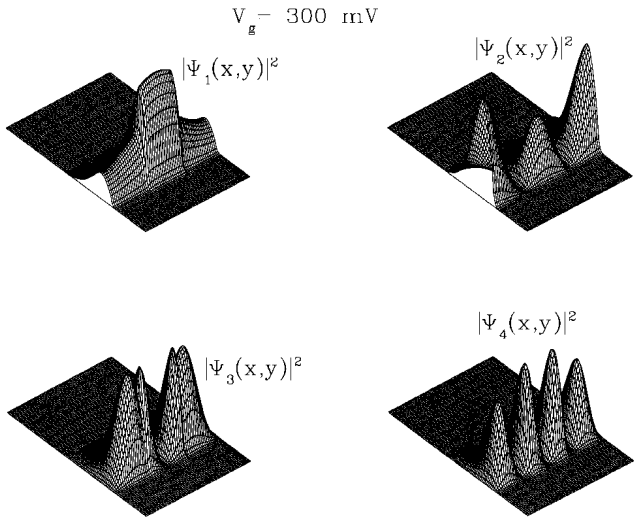

Figure 3: The wave function ($|\Psi_i(x,y)|^2$) for a gate voltage of 300 mV, in the bottom of the subband, i.e., $k_x = 0$.

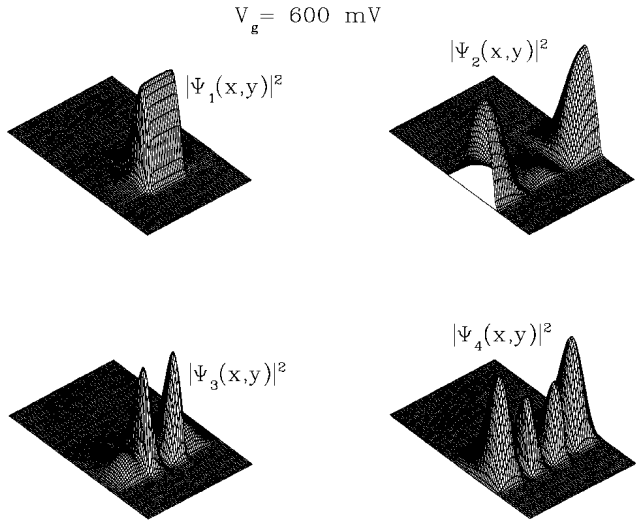

Figure 4: The wave function ($|\Psi_i(x,y)|^2$) for a gate voltage of 600 mV, in the bottom of the subband, i.e., $k_x = 0$.

The 1DEG system, as well as the 2DEG system we study depends on several parameters such as: the size of wires and the gates; the residual density of ionized acceptor impurities (N_A); the size of the undoped layer of $Al_{1-x}Ga_xAs$ (spacer); etc. The results presented here have the following set of parameters: size of wires: 400 Å, size of gates: 860 Å, the temperature set as zero and $N_A = 5.0 \times 10^{15}$ cm^{-3}, and the size of the spacer layer is 50 Å. For this system, we observe that the transition from a 2D behavior to an 1D behavior occurs for gate voltages ranging from 600 to 800 mV. At at low voltages the wave functions of the occupied states are extended over all the system. Increasing the voltage, the ground state assumes an 1D character while the

excited states remain extended. The 1D-2D transition occurs at the voltage when all occupied states became localized along the direction perpendicular to the gates. This is illustraded in Figs. 3 and 4 where we show the wave functions for the first four subbands at $k_x = 0$ (i.e. the bottom of the subband). For the applied gate voltage of 600 mV we observer that only the first subband becomes localized, while at 300 mV it was also an extended state.

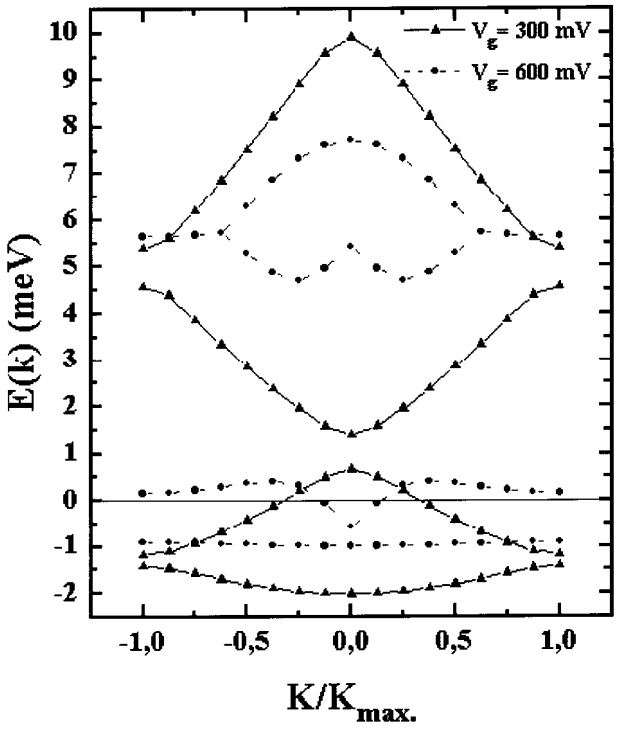

Figure 5: The dispersion relation for two differents gate voltages. The Fermi energy is set as zero, therefore the only occupied subbands are those having negative energies.

In the Fig. 5, the dispersion relation for the four first subbands shown in Figs. 3 and 4 are presented. This relation dispersion is important when calculating the optical and transport properties of the system.

In conclusion, we have presented a fully self-consistent Poisson-Schrödinger solver that handles both stationary and quasibound states. With this powerful solver, we have calculated the electronic band structure of a quantum-wire superlattices formed by a split gate structure, for any value of gate voltages. The transition from 2D system to 1D system has been observed for the ground state. The carrier dispersion relation was derived, and in a future work we intend to use it to calculate the conductance in the linear-response approximation.

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