Simulation and Design of a Single Charge Detector

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We have performed a numerical simulation of a system made of a quantum dot and a nearby quantum point contact defined, by means of depleting metal gates, in a two-dimensional electron gas at a GaAs/AlGaAs heterointerface. As recent experiment have shown, such a system can be used as a non-invasive detector of single charges being added to or removed from a quantum dot. We have computed the occupancy of the dot and the resistance of the quantum wire as a function of the voltage applied to the plunger gate, and have derived design criteria for achieving optimal sensitivity.

1. Introduction

In architectures for computation based on quantum dots the information is typically encoded in the occupation number of a subset of all the dots [1-3]. Therefore, in order to read or transmit this information to conventional electronic circuitry, single charge detectors are needed.

Recent experiments have shown that it is possible to detect a single electron being added to a quantum dot by measuring the resistance of a quantum point contact placed next to it [4]. The electrostatic potential defining the constriction is modified by the contribution of the additional electron, so that the transmission coefficients and, consequently, the overall resistance are affected.

In this paper, we consider a quantum dot and a constriction realized on the following heterostructure: an undoped GaAs substrate, an undoped 20 nm-thick AlGaAs spacer layer, a Silicon delta doping layer of 6×10^{12} cm^{-2}, an undoped 10 nm-thick AlGaAs layer, an undoped 5 nm-thick GaAs cap layer. The 2D electron gas is formed at the AlGaAs/GaAs interface 35 nm below the surface.

The quantum dot and the constriction are defined by means of aluminum gates evaporated on top of the heterostructure. The gate configuration is shown in Fig. 1: gates 1, 2, 3 and 4 define the quantum dot, with a geometrical area of 188 × 104 nm; the constriction between gates 4 and 5 is the detector.

2. Numerical modeling

We calculate the dot occupancy and the resistance of the quantum wire as a function of the voltage applied to the plunger gate (gate 2) for a few initial wire resistances. The bias voltages V_i of gates i ($i = 1 \ldots 4$) are -0.12 V, while we have considered a few different voltages V_5 for gate 5, between -0.15 and -0.18 V, corresponding to initial resistances of the quantum constriction ranging from 7.6 kΩ to practically infinity. The backgate, gate 0, is grounded.

A detailed simulation of the system would be prohibitively time-consuming: first, it would require the self-consistent solution of the Schrödinger and Poisson equations on a three-dimensional grid, in order to obtain the conduction band edge and the electron density profiles in the simulation domain. Then, the resistance of the quantum point contact could be evaluated by means of the recursive Green's function formalism, [5] using the potential landscape obtained from the Poisson-Schrödinger solver, while the charge contained in the quantum dot could be simply obtained by integrating the electron density in the dot region. Moreover, in order to assess the functionality of the detector, the voltage of the plunger gate should be swept towards more negative values, as to progressively deplete the quantum dot, and both the electron density and the quantum wire resistance should be calculated for each plunger gate voltage.

To make feasible the simulation of the system, we have adopted a less rigorous approach, in which self-consistency requirements are somewhat relaxed.

Semiclassical Poisson Equation

We start by solving the nonlinear Poisson equation on a 3D grid (65 × 65 × 65 points) with a semiclassical approximation:

$$\nabla \cdot (\epsilon \nabla \phi) = -q(p - n + N_D^+), \qquad (1)$$

where ϕ is the electrostatic potential, ϵ is the dielectric constant, q is the electron charge. The semiclassical hole

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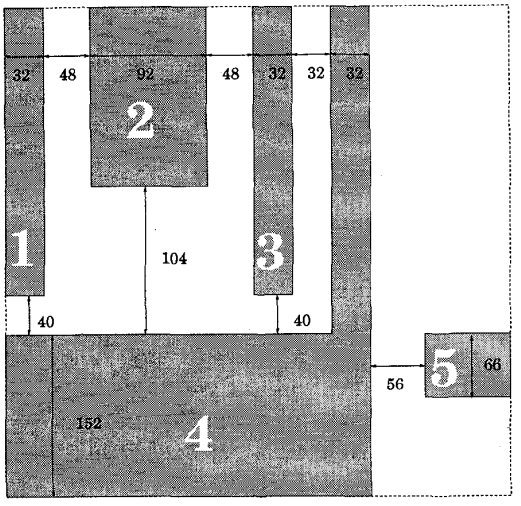

Figure 1: Gate configuration defining the quantum dot and the detector (dimensions are in nm). Gate 2 is the plunger gate; the voltage applied to gate 5 modulates the resistance of the detector.

and electron concentrations (p and n, respectively) are obtained as [6]:

$$p = N_V \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_V - E_F}{kT}\right), \quad (2)$$

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_C}{kT}\right), \quad (3)$$

where N_C and N_V are the effective density of states in the conduction and in the valence band, respectively, E_C and E_V are the conduction and valence band edges, respectively, k is the Boltzmann constant and T the absolute temperature, E_F the Fermi level. $F_{1/2}$ is the Fermi-Dirac integral

$$F_{1/2}(y) = \frac{1}{1/2!}\int_0^\infty \frac{x^{1/2}}{1+e^{x-y}}dx. \quad (4)$$

N_D^+ is the concentration of ionized donors, given by

$$N_D^+ = \frac{N_D}{1 + g_D \exp\left(\frac{E_F - E_D}{kT}\right)}, \quad (5)$$

where N_D is the donor concentration, g_D the spin degeneracy factor (2 for GaAs), E_D the donor energy level. The band edges depend on the potential through

$$E_C(\mathbf{r}) = q[\phi_m^{(0)} - \chi(\mathbf{r}) - \phi(\mathbf{r})], \quad (6)$$

where $\phi_m^{(0)}$ is the work function of the electrode assumed as a reference for the potential ϕ and the voltage, and χ is the electron affinity. In addition, $E_V(\mathbf{r}) = E_C(\mathbf{r}) - E_g(\mathbf{r})$, where E_g is the energy gap.

Boundary conditions

As far as the boundary conditions are concerned, Dirichlet conditions are enforced for the potential at the gate surfaces (i.e. $\phi = \phi_m^{(0)} - V_i - \phi_m^{(i)}$, where V_i is the voltage applied to gate i and $\phi_m^{(i)}$ is its work function) while on the lateral boundary regions of the simulation domain Neumann boundary conditions with zero perpendicular electric field are enforced.

The choice of proper boundary conditions at the exposed GaAs surface requires some discussion. The problem is easily solved at equilibrium, when all the gates are grounded, and a constant Fermi level extends over the simulation domain: in this case, the assumption of Fermi level pinning is clearly applicable, and is a very good approximation for the GaAs surface [7]. When different voltages are applied to the gates, even in the absence of charge transport, there seems to be no viable criterium for the choice of a Fermi level which properly describes the occupancy of surface states. It is possible to find in the literature detailed discussions about the correct shape of the density of surface states [8] or about procedures to include surface states in a numerical simulation [9], but these contributions can be used only if is easy to define a Fermi level.

In this paper, we have chosen a very simple approach, originally proposed in Ref. [10], which consists in assuming that the surface charge density is frozen in when the sample is cooled down, and does not change with the gate voltages. In this way, the surface charge is simply a constant source term in the Poisson equation. The only drawback of this approach is that a large volume outside the semiconductor should be included in the simulation domain, since no boundary conditions can be imposed at the exposed GaAs surface. We have overcome this problem by noticing that, due to the large relative dielectric constant in GaAs, any variation of the electric field in the air above the device should be reduced by an order of magnitude in the GaAs. From a 2D simulation, we have learned that, by imposing a constant surface charge density and by varying the voltage applied to a metal gate within a reasonable range, the electric field at the exposed GaAs surface, on the GaAs side, varies only by a few percent.

Within a reasonable approximation, the electric field on the GaAs side at the exposed GaAs surface can be therefore considered as constant, and equal to the value calculated at equilibrium with the assumption of Fermi level pinning. The problem remains of the value at which the Fermi level at equilibrium should be pinned: we have chosen the value which provides the best fit of the pinch-off voltage with experiments [11], i.e., 5.25 eV below the vacuum level, corrisponding to a normal component of the electric field at the surface of 88.2 V/μm.

The contribution to the potential from the charge in the dot is now computed by solving again the Poisson equation, assuming the charge in the dot volume Ω_{dot} as the only source term, i.e.,

$$\nabla \cdot (\epsilon \nabla \phi_{\text{dot}}) = q n_{\text{dot}}, \quad (7)$$

where $n_{\text{dot}} = n$ for $\mathbf{r} \in \Omega_{\text{dot}}$, $n_{\text{dot}} = 0$ otherwise. The

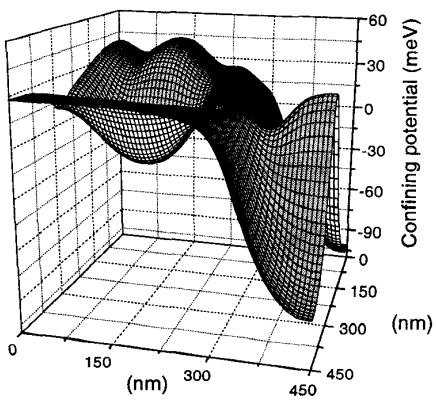

Figure 2: Confining potential for the electrons in the plane of the GaAs-AlGaAs heterointerface.

confining potential for the electrons in the dot is therefore

$$V_{\text{conf}} = E_C + q\phi_{\text{dot}}. \tag{8}$$

The Schrödinger problem

The many-body Schrödinger equation should be solved with the confining potential given by (8) on a 3D domain. However, we can assume that confinement in the vertical direction is much stronger than that on the horizontal plane, so that only the first vertical subband is occupied: in such a way we can decouple the 3D problem into a 2D problem at the heterointerface plane, and a 1D problem in the vertical direction.

In particular, we solve the single particle Schrödinger equation in the vertical direction (along the z-axis):

$$-\frac{\hbar^2}{2m_z}\frac{\partial^2\chi(z)}{\partial z^2} + V_{\text{conf}}(x_0, y_0, z)\chi(z) = E\chi(z), \tag{9}$$

where x_0, y_0 define the central point on the horizontal plane. Let the ground state eigenvalue and eigenfunction be E_0 and $\chi_0(z)$, respectively: the confining potential seen by electrons at the heterointerface plane is that given by $V_{2\text{D}}(x,y) = V_{\text{conf}}(x,y,z_0) + E_0$, where z_0 is the z-coordinate of the 2DEG plane. In Fig. 2 $V_{2\text{D}}$ is shown for the case of $V_5 = -0.16$ V.

Within the framework of density functional theory, the 2D Schrödinger equation reads:

$$-\frac{\hbar^2}{2m_x}\frac{\partial^2\varphi_i}{\partial x^2} - \frac{\hbar^2}{2m_y}\frac{\partial^2\varphi_i}{\partial y^2} + [V_{2\text{D}} + V_{\text{C}} + V_{\text{ex}} + V_{\text{corr}}]\,\varphi_i = \epsilon_i\varphi_i, \tag{10}$$

where V_{C} is the Coulomb interaction term, V_{ex} and V_{corr} are the exchange and correlation terms from the theory of Tanatar and Ceperley [12]. The details of the solution of Eq. 10 can be found in Ref. [13]. The electron-electron interaction is modeled consistently with the Neumann boundary conditions enforced at the exposed surface, i.e., with negative image charges, which warrant constant value of the electric field perpendicular to the surface. The simulation starts with an initial guess of the number of electrons in the dot. This number is then adjusted with the criterion that the chemical potential in the dot must be the largest possible below the Fermi level in the bulk.

The quantum density of electrons in the quantum dot is therefore

$$n_{\text{quantum}}(x,y,z) = |\chi(z)|^2 \sum_{j=1}^{N} |\varphi_j(x,y)|^2. \tag{11}$$

The contribution from electrons in the dot is obtained by solving

$$\nabla \cdot (\epsilon \nabla \phi_{\text{quantum}}) = q n_{\text{quantum}},, \tag{12}$$

and the confining potential of the quantum constriction is obtained as

$$V_{2\text{Dquantum}}(x,y) = V_{2\text{D}}(x,y) - q\phi_{\text{quantum}}(x,y,z_0). \tag{13}$$

By means of the recursive Green's function formalism, it is now possible to calculate the resistance of the quantum point contact defined by $V_{2\text{Dquantum}}$. The details of the method are beyond the scope of this paper and can be found in [5].

Voltage sweep

When the plunger gate voltage is modified, instead of solving again the 3D Poisson equation, we use a semi-analytical method [14] to evaluate the correction to the confining potential on the plane of the 2DEG, assuming that the other charges in the structure remain unchanged.

3. Results

In Fig. 3 the detector resistance is plotted as a function of the plunger gate voltage for four different voltages applied to gate 5: the lower the voltage applied to gate 5, the higher the initial detector resistance. For a plunger gate voltage V_2 of -0.61 V the dot is completely depleted. As V_2 is raised in steps of 10 mV, the confining potential on the heterointerface plane is lowered: as long as N is constant the detector resistance decreases; while, when one electron is added to the dot, Coulomb repulsion rises the confining potential of the quantum costriction, causing an increase of a few percent in the detector resistance. The electrons in the dot for a given $V_2 = \tilde{V}$ are given by the number of peaks to the left of $\tilde{V}$.

As can be seen, a high sensitivity can be obtained if conduction in the quantum wire is essentially in the tunneling regime, as in the cases of Figs. 3(d) and 3(c), corresponding to an initial resistance much higher than $2e^2/h$ (12.728 kΩ), i.e., that associated with a single propagating mode in the quantum wire. This is simply due to the fact that the transmission probability in the case of tunneling is extremely sensitive to a variation of the confining potential profile. For values of V_5 lower than -0.18 V the quantum wire is practically pinched off.

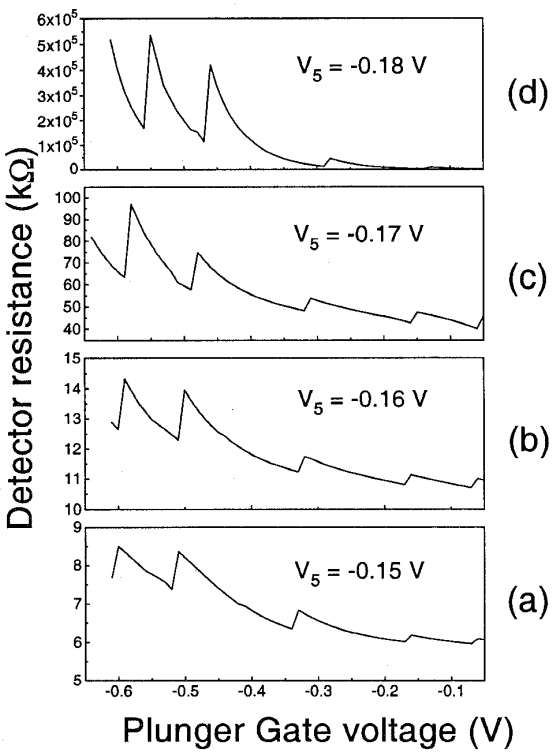

Figure 3: Detector resistances as a function of the voltage applied to the plunger gate for four different values of the voltage V_5. For V_5 lower than -0.18 V, the quantum wire has negligible conductance.

Conclusion

Modeling even a simple experiment such as the one described in this paper can require prohibitive computational resources. A practical way of solving the problem consists in adopting a simplified approach, in which self-consistency requirements are only partially met. With its limitations, this solution allows to address realistic situations and to gain otherwise unattainable insights into the experiment. For the structure we have investigated, it has been possible to obtain good qualitative agreement with the experiments and to derive criteria for tuning the gate voltages in order to optimize the detector sensitivity.

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References

1. Craig S. Lent, P. Douglas Tougaw, and Wolfgang Porod, Appl. Phys. Lett. **62**, 714, (1993).
2. K. K. Likharev and A. N. Korotkov, Science **273**, 763 (1996).
3. D. Loss and D. P. Di Vincenzo, submitted to Phys. Rev. A
4. M. Field, C. G. Smith, M. Pepper, D. A. Ritchie, J. E. F. Frost, G. A. C. Jones, and D. G. Hasko, Phys. Rev. Lett. **70**, 1311, 1993.
5. M. Macucci, A. Galick, and U. Ravaioli, Phys. Rev. B **52**, 5210 (1995).
6. S. Selberherr, *Analysis and Simulation of Semiconductor Devices* (Springer Verlag, Wien, 1984), p. 23
7. S. M. Sze *Physics of semiconductor devices*, (Wiley and Sons, New York, 1981), p. 275.
8. W. E. Spicer, P. W. Chye, P. R. Skeath, C. Y. Su, and I. Lindau, J. Vac. Sci. Technol. **16**, 1422 (1998).
9. M. Chen and W. Porod, J. Appl. Phys. **75**, 2545 (1994).
10. S. E. Laux, D. J. Frank, F. Stern Surface Science **196**, 101 (1988).
11. Y. Jin, private communications.
12. B. Tanatar and D. M. Ceperley Phys. Rev. B **39**, 5005 (1989).
13. M. Macucci, Karl Hess, G. J. Jafrate, Phys. Rev. B **48**, 17354 (1993).
14. J. H. Davies, I. A. Larkin, E. V. Sukhourov, J. Appl. Phys. **77**, 4504 (1995).