Solution of the Poisson-Schrödinger problem for a single-electron transistor

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An outstanding problem of a quantitative description of electronic properties of a vertical gated quantum dot has been solved by a self-consistent approach to the Poisson and Schrödinger equations. We have calculated the confinement potential and determined the conditions for single-electron tunneling. A good agreement with experiment has been obtained for the 12 single-electron current peaks as a function of gate voltage V_g for source-drain voltage $V_{sd}=0$, the bounds on diamond-shaped regions in the V_g-V_{sd} plane, for which the flow of current is blocked; and the current-gate voltage characteristics in an external magnetic field.

A quantum dot (QD) is a semiconductor nanostructure, in which the space accessible for electrons is limited in all three dimensions by the interfaces and/or external voltages applied to electrodes. Excess electrons confined in the QD's form bound states, which exhibit features of *N*-electron artificial atoms.[1–3] Among many types of QD's fabricated by modern nanotechnology, gated QD's (gate-controlled QD's)[4,5] are especially interesting. In these QD's, it is possible to change the confinement potential by changing the gate voltage, and therefore to modify the electronic properties of artificial atoms, which leads to the possibility of constructing a single-electron transistor.[4] Recently, very interesting transport-spectroscopy studies with vertical gated QD's were performed by Tarucha *et al.*[5] and Kouwenhoven *et al.*[6]

Until now, these remarkable results[5,6] have been interpreted only qualitatively in the framework of a two-dimensional model.[7–9] In these papers,[10] the confinement potential was assumed to be parabolic and independent of the gate voltage. In our previous paper,[10] we proposed a phenomenological model with an anharmonic confinement potential, which was assumed to be a linear function of the gate voltage. In the present paper, we present the first (to our knowledge) complete self-consistent solution of the three-dimensional Poisson-Schrödinger problem for the vertical gated QD, and provide a full quantitative description of all the electronic properties observed[5,6] in these QD's. Contrary to previous studies,[7–11] the confinement potential is not assumed but calculated as a function of the gate voltage, the geometry of the nanodevice, and the donor distribution.

The nanodevice[4,5] has a nearly cylindrical shape, and consists of several layers made of different materials. In the direction of the cylinder (*z*) axis, the geometry of the nanodevice is asymmetric with respect to the source and drain positions. However, the experimental results, in particular the Coulomb diamonds,[6] are almost perfectly symmetric with respect to the source-drain polarity. Therefore, we have assumed a model nanodevice, in which the layers are symmetrically placed in the *z* direction. The model nanostructure applied in the present paper is displayed in the inset of Fig. 1. The 40-nm-high Schottky gate is placed on the side of the cylinder with the radius $R=220$ nm close to the $Al_{0.22}Ga_{0.78}As$ barriers and the 12-nm-thick $In_{0.05}Ga_{0.95}As$ layer, which forms a QD region. An undoped GaAs spacer separates the QD from a fluctuating field of single impurities. The ionized donors in the *n*-GaAs layers screen the electric field of the gate. A concentration of donors increases stepwise in the direction of the source and drain. Since the authors of Refs. 5 and 6 did not give accurate values of the material parameters of the doped layers, we have assumed that there exist two *n*-GaAs layers with donor concentrations n_1 and n_2, where $n_2>n_1$. The first layer (n_1-GaAs) determines the electronic properties of the QD for small gate voltages. For a large enough gate voltage, all the donors in the first layer are ionized, and the second n_2-GaAs layer becomes effective in a screening. The thickness of the n_2-GaAs layer has been taken to be so large that the electric field vanishes near the source and drain for all the applied gate voltages. The above sequence of layers is symmetrically repeated on the other side of the $In_{0.05}Ga_{0.95}As$ layer. This model nanostructure allows us to reproduce the electronic properties of the nanodevice,[5] and considerably simplifies calculations.

For a gate-controlled QD, we have elaborated a self-consistent method of solution of the Poisson and Schrödinger equations, which consists of several steps. In the first step, we calculate the confinement potential, which is treated as an external potential for the *N*-electron problem solved in the last step by the Hartree-Fock method. The potential energy $U_{conf}(\mathbf{r})$ of the confinement of an excess electron in the QD is given by

$$U_{conf}(\mathbf{r})=U_{db}(z)-e\varphi_d(\mathbf{r}), \tag{1}$$

where $U_{db}(z)$ is the potential energy of the electron in the $GaAs/Al_{0.22}Ga_{0.78}As/In_{0.05}Ga_{0.95}As$ double barrier, and e is the elementary charge. The potential φ_d, which originates from the voltages applied to the external electrodes and the ionized donors in *n*-GaAs layers, is calculated from the Poisson equation

$$\nabla^2\varphi_d(\mathbf{r})=-\rho_d(\mathbf{r})/\varepsilon_0\varepsilon, \tag{2}$$

where $\rho_d(\mathbf{r})$ is the density of the charge of ionized donors, ε_0 is the permittivity of the vacuum, and ε is the static dielectric constant of GaAs. Since the experiments[5] were performed at very low temperatures ($\sim$200 mK), we assume that the donor at the position $\mathbf{r}$ becomes ionized, if the total potential energy $U(\mathbf{r})$ of the electron is larger than the binding energy of the electron on the donor center. The potential

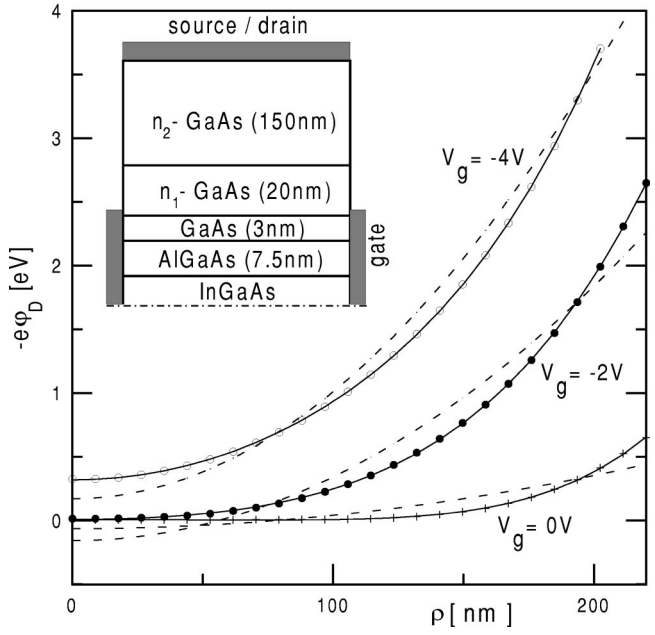

FIG. 1. Potential energy ($-e\varphi_d$) calculated from Eq. (2) (symbols) and fitted with polynomials of the sixth (solid curves) and second (dashed curves) order as a function of ρ and gate voltage V_g. Inset: Schematic of the model nanodevice applied in the present calculations. The thicknesses of the layers are given in the parentheses.

energy of the electron $U(\mathbf{r})=-e\Phi(\mathbf{r})$ is determined by the electrostatic potential $\Phi(\mathbf{r})=\varphi_d(\mathbf{r})+\varphi_e(\mathbf{r})$, where $\varphi_e(\mathbf{r})$ is the potential of the field created by the electrons confined in the QD, and is calculated as follows:

$$\varphi_e(\mathbf{r})=-\frac{e}{4\pi\varepsilon_0\varepsilon}\sum_{n=1}^{N-1}\int d^3r'\frac{|\psi_n(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}. \tag{3}$$

In Eq. (3), the sum runs over all the occupied $(N-1)$ one-electron states, whose wave functions $\psi_n(\mathbf{r})$ are obtained by the Hartree-Fock method. Such a treatment provides a stationary description of the tunneling of the Nth electron through the dot, which is valid if the probability of finding the tunneling electron inside the dot is much smaller than finding that outside the dot.

When solving Poisson equation (2), we have set the boundary conditions, which take into account external voltages applied to the leads and the free charge of the leads (with the image charges of electrons in the dot included). These boundary conditions have been put on the total potential $\Phi(\mathbf{r})$ on the surface of the cylinder. Because the source and drain form Ohmic contacts, we take on $\Phi(\mathbf{r}_{source})=V_s$ and $\Phi(\mathbf{r}_{drain})=V_d$, where V_s and V_d are the source and drain voltages, respectively. Since the metal gate is in contact with an undoped semiconductor, we take into account the Schottky barrier $\phi_B=0.65$ eV, which leads to the boundary condition: $\Phi(\mathbf{r}_{gate})=V_g-\phi_B$. Moreover, we require that the normal derivatives of $\Phi(\mathbf{r})$ vanish on the side surface of the cylinder between the leads. Poisson equation (2) has been solved by the relaxation method in the cylindrical coordinates (ρ,z) on the finite-difference mesh $(\rho_i=i\Delta\rho, z_j=j\Delta z)$, which leads to the numerical solutions $\varphi_d(\rho_i,z_j)$. Due to the small thickness of the QD, we take into account the values of the potential φ_d for $z=0$, i.e., $\varphi_d(\rho,0)$. Since an analytic form of the potential is more convenient in the Hartree-Fock method, we have fitted the following sixth-order polynomial to the numerical results obtained from the Poisson equation:

$$\tilde{\varphi}(\rho)=v_0+\alpha_2\rho^2+\alpha_4\rho^4+\alpha_6\rho^6. \tag{4}$$

Form (4) is used in Eq. (1) to calculate the confinement potential energy. Figure 1 displays the numerical solutions of the Poisson equation and fitted polynomials of the sixth and second order for different gate voltages. We note the considerable deviations of the solutions of the Poisson equation from the parabolic potential, and their strong dependence on the gate voltage. These properties of the confinement potential, being in contradiction with the commonly used parabolic, gate-voltage-independent, confinement potentials,[7–9] are crucial to explaining the transport-spectroscopy data.[5,6]

In the last step, we solve the eigenvalue problem for the N-electron system by the Hartree-Fock method, with the potential energy of the external field assumed to be $U_{ext}(\mathbf{r})=U_{conf}(\mathbf{r})$. In the Hartree-Fock method, we apply the one-electron wave functions expanded in the Gaussian basis.[10,12] The electron probability density depends on the confinement potential, which is determined by the concentration of the ionized donors. Due to the Coulomb coupling between the excess electrons and donor ions, the Poisson and Schrödinger equations have to be solved self-consistently. This process is repeated until self-consistency of the electrostatic potential and Hartree-Fock solutions is reached.

The actual shape of the vertical QD (Ref. 13) can deviate from the ideal cylindrical form. We have taken into account this asymmetry and introduced an anisotropy of the QD as a small perturbation of the rotational symmetry. We have found that the small anisotropy slightly changes the ground-state energy of the N-electron artificial atom, which leads to a better agreement with experiment. The anisotropy has been included in the Hartree-Fock method by replacing variable ρ in Eq. (4) with $\tilde{\rho}$, where $\tilde{\rho}^2=(1+\gamma)^2x^2+(1-\gamma)^2y^2$ and γ is the anisotropy parameter. Since not all the parameters of the QD (Ref. 5) are known with a sufficient precision, we have adjusted the values of donor concentrations n_1 and n_2, anisotropy parameter γ, and potential-well depth U_0, slightly changing their nominal values, in order to obtain an agreement with experiment. This leads to the following values: $n_1=6.3\times10^{16}$ cm^{-3}, $n_2=17.5\times10^{16}$ cm^{-3}, $\gamma=0.035$, and $U_0=-55$ meV (the energy of the $In_{0.05}Ga_{0.95}As$ conduction band bottom with respect to that of the GaAs spacer). The nominal value of n_1 was estimated[14] to be 7.5×10^{16} cm^{-3}. Moreover, we have set the electron effective band mass to be 0.065 of the electron rest mass, $\varepsilon=12.6$, and the $Al_{0.22}Ga_{0.78}As$ barrier height = 220 meV. We have checked that the present results are not sensitive to small changes of the parameters.[15]

The self-consistent solution of the Poisson-Schrödinger problem provides the ground-state energy E_N of the N-electron artificial atom. The occupancy of electronic shells is determined by the cylindrical symmetry of the problem (the influence of the anisotropy is small). Therefore, the first three shells are filled by two, four, and six electrons. The present calculations have been performed for these shells,

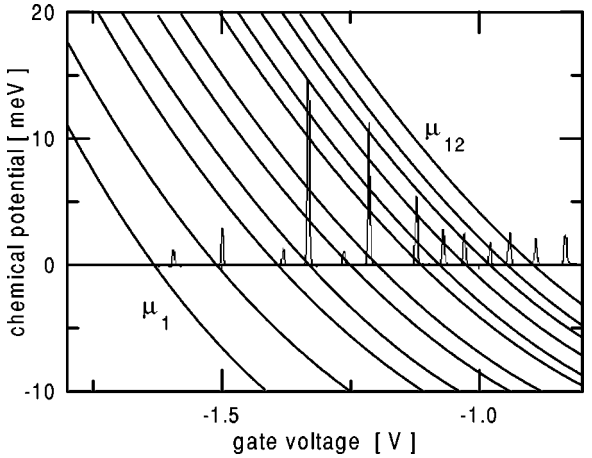

FIG. 2. Chemical potential (solid curves) calculated for $N=1,\ldots,12$ electrons confined in the QD as a function of gate voltage. Zero on the energy scale corresponds to the Fermi energy of the source and drain for $V_s=V_d=0$. The measured (Ref. 5) peaks of the source-drain current are also shown.

i.e., for $N=1,\ldots,12$ electrons. In Fig. 2, we plot the calculated chemical potential $\mu_N=E_N-E_{N-1}$ as a function of V_g for $V_s=V_d=0$. When considering the tunneling of the Nth electron, the energies E_N and E_{N-1} are calculated with the use of the same confinement potential. Therefore, in the calculations of both terms in μ_N, the energies of an environment are the same and cancel out. In this way, the chemical potential μ_N also takes into account the interaction of the electrons confined in the dot with the environment. The current can flow through the gated QD even if $V_s-V_d\simeq 0$, provided that chemical potential μ_N is aligned with the Fermi energy of the source and drain. Since we have set the Fermi energy of the source to be equal to zero, the straight line in Fig. 2 corresponds to $V_s=V_d=0$. The crossing points of μ_N with this line allow us to determine the values of gate voltage, for which the current peaks appear. The calculated relative positions of the peaks very well agree with experimental results,[5] and show that the electronic shells are filled according to Hund's rule.

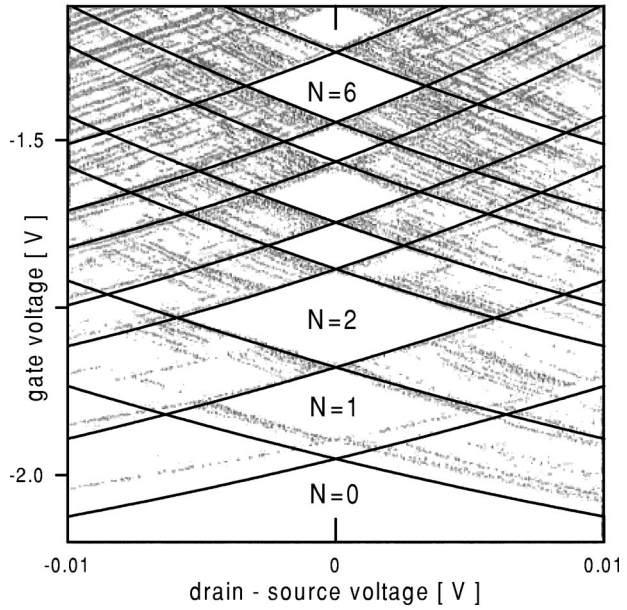

FIG. 3. Coulomb diamonds: solid curves show the upper (lower) bounds on the gate and source-drain voltages, below (above) which the source-drain current flows. Shaded regions show the measured positions of current peaks.

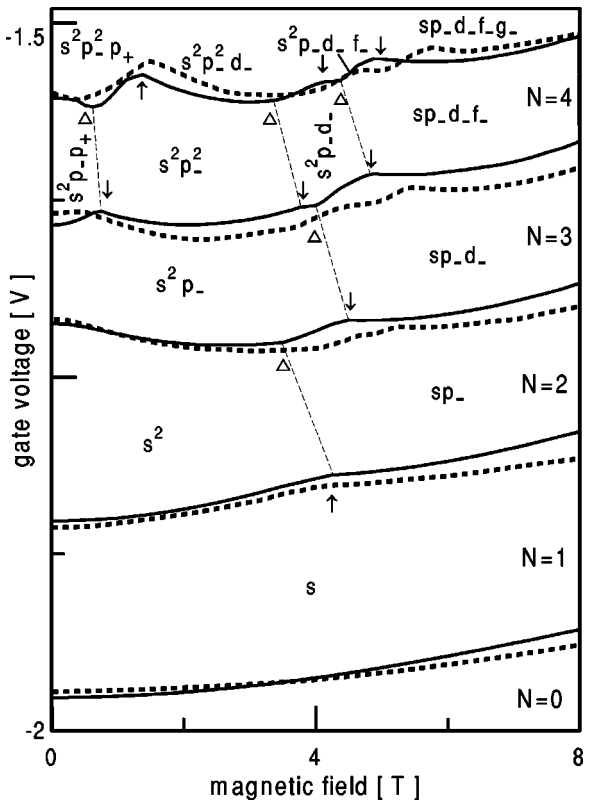

FIG. 4. Magnetic-field dependence of calculated (solid curves) and measured (Ref. 5) (dashed curves) gate voltage, for which the current peak appears for $V_{sd}=0$. The occupied one-electron orbitals of N-electron artificial atoms are conventionally labeled according to the cylindrical symmetry: s, p, d, f, and g denote the z component of angular orbital momentum $M=0$, 1, 2, 3, and 4 (in units $\hbar$), respectively, and $\pm$ are the signs of M. Cusps, resulting from the ground-state transformations, are marked by arrows and triangles (see text).

We have also determined the conditions for the current to flow under the source-drain voltage applied. The calculated lower (upper) bounds on the voltages, above (below) which the source-drain current can flow, are reported in Fig. 3. The experimental data,[6] i.e., the positions of current peaks on the V_g-V_{sd} plane, are shown by shaded regions. The white, diamond-shaped, regions correspond to the values of voltages, for which the current does not flow through the nanodevice, i.e., the electron tunneling is blocked. To the best of our knowledge, we have obtained the first theoretical results for the Coulomb diamonds in the frame of the quantum-mechanical approach, which very well agree with the experimental data.[6]

We have extended the present approach to the case of external magnetic field applied in the z direction. Figure 4 displays the gate voltage, for which the electrons tunnel through the QD in the magnetic field for $V_{sd}=0$. Solid curves in Fig. 4 are obtained from chemical potentials μ_N, converted into the gate voltage (cf. Fig. 2). The cusps in the curves in Fig. 4 result from the changes of the spin-orbital

configuration of the ground state of the N-electron artificial atom in the magnetic field. Since the condition for the flow of current is determined by the chemical potential of the electrons confined in the QD, each change of the N-electron ground state is seen two times as the cusps in the curves, which correspond to the tunneling of the Nth electron (arrows) and $(N+1)$th electron (triangles). The cusps resulting from the same ground-state transformation are connected by thin dashed lines in Fig. 4. If the gate voltage becomes less negative, the lateral confinement potential is more flat (cf. Fig. 1) and the confined electrons become weakly localized. Since the magnetic field more strongly affects the weakly localized electrons, the magnetic-field-induced transformation of the ground state appears at a lower critical field for the increasing gate voltage. The gate-voltage dependence of the confinement potential is of crucial importance in the explanation of the observed[5] changes of critical magnetic fields. The present approach has allowed us to obtain all the ground-state transformations[15] observed in experiment.[5]

In summary, we have solved the outstanding problem of a quantitative interpretation of transport-spectroscopy results for vertical gated quantum dots, and obtained a complete theoretical description of the electronic properties of these nanostructures.

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[1] P.A. Maksym and T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990).
[2] M.A. Kastner, Phys. Today **46**(1), 24 (1993).
[3] R.C. Ashoori, Nature (London) **379**, 414 (1996).
[4] D.G. Austing, T. Honda, and S. Tarucha, Semicond. Sci. Technol. **11**, 388 (1996).
[5] S. Tarucha, D.G. Austing, T. Honda, R.J. van der Hage, and L.P. Kouwenhoven, Phys. Rev. Lett. **77**, 3613 (1996).
[6] L.P. Kouwenhoven, T.H. Oosterkamp, M.W.S. Danoesastro, M. Eta, D.G. Austing, T. Honda, and S. Tarucha, Science **278**, 1788 (1997).
[7] M. Eto, Jpn. J. Appl. Phys. **36**, 3924 (1997).
[8] H. Tamura, Physica B **249-251**, 210 (1998).
[9] O. Steffens, M. Suhrke, and U. Rössler, Physica B **256-258**, 147 (1998).
[10] B. Szafran, S. Bednarek, and J. Adamowski, Acta Phys. Pol. A **94**, 555 (1998).
[11] T. Ezaki, N. Mori, and C. Hamaguchi, Phys. Rev. B **56**, 6428 (1997).
[12] S. Bednarek, B. Szafran, and J. Adamowski, Phys. Rev. B **59**, 13 036 (999).
[13] M. Eto, J. Phys. Soc. Jpn. **66**, 2244 (1997).
[14] T.H. Oosterkamp, W.G. van der Wiel, L.P. Kouwenhoven, D. G. Austing, T. Honda, and S. Tarucha (unpublished).
[15] A detailed discussion of the dependence of the properties of the nanodevice on the geometry and donor concentrations will be given elsewhere.