Numerical method for the calculation of self-consistent charge densities of reservoir-coupled quantum dots

Andreas Scholze, Andreas Schenk, and Wolfgang Fichtner

Integrated Systems Laboratory
ETH–Zürich, ETZ, CH-8092 Zürich, Switzerland
Phone: +41 1 632 5957, Fax: +41 1 632 11 94,
E-mail: scholze@iis.ethz.ch

The calculation of self-consistent charge densities is not a straightforward task in structures with zero-dimensional confinement. In contrast to the semi-classical case the density of states in a quantum dot depends on the potential. However, this dependence is not explicitly given and Newton-Raphson methods are therefore difficult to employ. In this paper we present a numerical method for the calculation of self-consistent electron densities in a quantum dot weakly coupled to a macroscopic reservoir using a multidimensional secant approach that partially overcomes the numerical limitations intrinsic to single-electron transistor device simulations.

1. Introduction

We present a method to obtain self-consistent solutions to the nonlinear Poisson equation in single-electron devices based on the *zero-current* model of Polak *et al.* [1]. We discuss an algorithm to calculate the charge density of

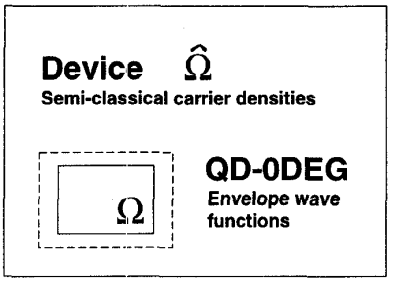

Figure 1: Principal simulation domains. The dashed line around the QD-0DEG region marks the boundary for the QD wave functions.

electrons in semiconductor quantum dots (QD) and the coupling of the dot charges to the semi-classical charges in the reservoirs.

2. Physical model

The Poisson equation

$$-\nabla \cdot (\epsilon \nabla \phi) = \rho[\phi] \tag{1}$$

is always solved for the whole device $\hat{\Omega}$ (Fig. 1) thereby assuming a given equilibrium Fermi energy. The charge density ρ is given as

$$\rho[\phi] = q(p[\phi] - n[\phi] + N_{\mathrm{d}}^{+}[\phi] - N_{\mathrm{a}}^{-}[\phi]). \tag{2}$$

N_{d}^{+}, N_{a}^{-} are the ionized dopant densities and p is the semi-classical approximation for the hole density. The electron density n in the reservoir region $\hat{\Omega} - \Omega$ is given by the semi-classical approximation for the density of states N_{c}, whereas the density in the QD region Ω follows from a system of nonlinear PDEs for the effective Kohn-Sham potential and the envelope wave functions ψ_i

$$\left\{ -\frac{1}{2}\nabla \cdot (\alpha^{-1}\nabla) + v_{\mathrm{eff}}(\mathbf{r}) \right\} \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}). \tag{3}$$

α is the effective mass tensor. The quantum mechanical current and the normal derivative of the density vanishes at the dot boundaries which leads to real eigenvalues ϵ_i. The effective Kohn-Sham potential in (3) is taken as $v_{\mathrm{eff}}(\mathbf{r}) = -e\phi(\mathbf{r}) + v_{\mathrm{xc}}[n(\mathbf{r})] + \Delta E_{\mathrm{c}}(\mathbf{r})$, where $e\phi$ is the conduction band potential energy, v_{xc} the local exchange-correlation potential energy and ΔE_{c} the material composition dependent conduction band offset. The electron charge density is given by

$$n(\mathbf{r}) = \begin{cases} N_{\mathrm{c}} F_{\frac{1}{2}}(\phi(\mathbf{r})) & \text{if } \mathbf{r} \in \hat{\Omega} - \Omega \\ \sum\limits_i \mid \psi_i(\mathbf{r}) \mid^2 g(\epsilon_i \mid N) & \text{if } \mathbf{r} \in \Omega \end{cases} \tag{4}$$

We use Gibbs distributed single-particle occupation numbers g in the QD, where a localized canonical ensemble is present. N is the integer particle number of the QD.

0-7803-4369-7/98 $10.00

The Gibbs distribution $P_{\rm eq}(\{n_i\})$ of the electron population in a quantum dot in equilibrium with the reservoirs is evaluated in order to find the true many particle ground state of the system of dot and reservoir

$$P_{\rm eq}(\{n_i\}) = \frac{\exp[-(F(\{n_i\},N) - E_{\rm F}N)/k_{\rm B}T]}{\sum_{\{n_i\}} \exp[-(F(\{n_i\},N) - E_{\rm F}N)/k_{\rm B}T]}. \quad (5)$$

where $F(\{n_i\},N)$ denotes the total free energy of the system with N electrons and the occupation configuration $\{n_i\}$, $(n_i = 0,1)$ and $E_{\rm F}$ is the Fermi-energy, respectively. The thermodynamical average of the number of electrons in the quantum dot

$$\langle N \rangle = \sum_{\{n_i\}} P_{\rm eq}(\{n_i\}) N \delta_{N,\sum_i n_i} \quad (6)$$

and the linear response conductance through the confinement region using the solution to the set of detailed balance equations (master equation) derived by Beenakker [2]

$$G = \frac{e^2}{k_{\rm B}T} \sum_{\{n_i\}} P_{eq}(\{n_i\}) \sum_k \delta_{n_k,0} \frac{\Gamma_k^{\rm s}\Gamma_k^{\rm d}}{\Gamma_k^{\rm s}+\Gamma_k^{\rm d}}$$
$$f(F(\{n_i+k\},N+1) - F(\{n_i\},N) - E_{\rm F}) \quad (7)$$

can be extracted.

3. Newton-Raphson iteration

We search the zero of the vector function $F(\phi) = -\nabla\cdot(\epsilon\nabla\phi) - \rho[\phi]$ at the whole device $\hat{\Omega}$ by means of a damped Newton-Raphson iteration with $\mathbf{x} = \{(e\phi)_{ijk}\}$ the electrostatic potential at discrete mesh points

$$\mathbf{F}(\mathbf{x}+\delta\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \hat{\mathbf{J}}\delta\mathbf{x} + \mathcal{O}(\delta\mathbf{x}^2). \quad (8)$$

$\hat{\mathbf{J}}$ is the Jacobian matrix. By setting the right hand side $\mathbf{F}(\mathbf{x}+\delta\mathbf{x}) = 0$ we arrive at a linear system for the updating vector

$$-\hat{\mathbf{J}}^{-1}\mathbf{F}(\mathbf{x}) = \delta\mathbf{x}. \quad (9)$$

The quantum mechanical expression for the electron charge density in the QD (4) does not allow for the explicit calculation of the contribution $\partial n[\phi]/\partial\phi$ to the Jacobian matrix. On the other hand, the use of the semi-classical approximation provides only a crude approximation. Therefore, the electron density is either approximated by the semi-classical expression in the QD region (for an initial guess) or it is provided externally and kept fixed as a boundary condition to the Poisson equation (1) during the Newton-Raphson iterations.

4. Broyden's method

In order to find the self-consistent electron density in the QD we search for the zero of the vector function $\mathbf{F}(\mathbf{x}) = \mathbf{x}_{out}(\mathbf{x}) - \mathbf{x}$ with $\mathbf{x} = \{(e\phi' - v_{\rm xc})_{ijk}\}$. The charge densities in the reservoir region $(\hat{\Omega}-\Omega)$ are kept fixed as boundary conditions to the Poisson equation. Therefore, we assume that $p[\phi'] = p[\phi]$, $n[\phi'] = n[\phi]$ and $N_{\rm d,a}^{+,-}[\phi'] = N_{\rm d,a}^{+,-}[\phi]$ in $\hat{\Omega}-\Omega$. We employ Broyden's method [4] as non-linear root searching method. It is based on a multi-dimensional secant approach $\mathbf{F}(\mathbf{x}+\delta\mathbf{x}) \neq 0$ to equation (8)

$$\delta\mathbf{x} + \hat{\mathbf{G}}\delta\mathbf{F} = 0. \quad (10)$$

Assuming $\mid \hat{\mathbf{G}}^{(m+1)} - \hat{\mathbf{G}}^{(m)} \mid \to 0$ this leads to an updating formula for the inverse Jacobian $\hat{\mathbf{G}} = -\hat{\mathbf{J}}^{-1}$

$$\hat{\mathbf{G}}^{(m+1)} = \hat{\mathbf{G}}^{(m)} - (\delta\mathbf{x}^{(m)} + \hat{\mathbf{G}}^{(m)}\delta\mathbf{F}^{(m)}) \otimes \delta\mathbf{F}^{(m)}. \quad (11)$$

Minimizing an error function [5] $\partial E/\partial G_{ij} = 0$ with

$$E = \omega_0 \|\hat{\mathbf{G}}^{(m+1)} - \hat{\mathbf{G}}^{(m)}\| + \sum_{n=1}^{m} \omega_n^2 \mid \delta\mathbf{x}^{(n)} + \hat{\mathbf{G}}^{(m+1)}\delta\mathbf{F}^{(n)} \mid^2 \quad (12)$$

we arrive at a new updating formula

$$\hat{\mathbf{G}}^{(m+1)} = \hat{\mathbf{G}}^{(m)} - (\hat{\mathbf{G}}^{(m)}\hat{\mathbf{F}}^{(m)} + \hat{\mathbf{X}}^{(m)})\hat{\beta}^{(m)} \otimes \hat{\mathbf{F}}^{(m)} \quad (13)$$

adopting the following notation for the vectors $\tilde{\mathbf{F}}^{(n)} = (\omega_n/\omega_0)\mathbf{F}^{(n)}$ and $\delta\tilde{\mathbf{x}}^{(n)} = (\omega_n/\omega_0)\delta\mathbf{x}^{(n)}$

$$\begin{aligned} \hat{\mathbf{X}}^{(n)} &= (\delta\tilde{\mathbf{x}}^{(1)}, \cdots, \delta\tilde{\mathbf{x}}^{(n)}) \in R^{(N\times n)} \\ \hat{\mathbf{F}}^{(n)} &= (\tilde{\mathbf{F}}^{(1)}, \cdots, \tilde{\mathbf{F}}^{(n)}) \in R^{(N\times n)} \\ \hat{\beta}^{(m)} &= (\hat{\mathbf{I}} + \hat{\mathbf{F}}^{(m)}\hat{\mathbf{F}}^{(m)})^{-1} \in R^{(m\times m)}. \end{aligned} \quad (14)$$

The advantage of the new method over the original method of Broyden is that only the inversion of a small $m \times m$ matrix $(\hat{\beta})$ and not of a huge $N \times N$ matrix is needed. This method can be improved even further [6] if

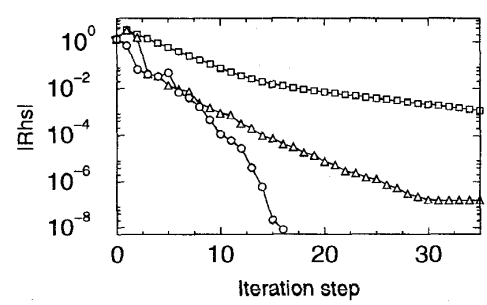

Figure 2: Convergence using Broyden's algorithm (○), a simple mixing method (□) and the Anderson mean value extrapolation method (△).

we put $\hat{\mathbf{G}}^{(m+1)}$ in terms of $\hat{\mathbf{G}}^{(1)}$

$$\hat{\mathbf{G}}^{(m+1)} = \hat{\mathbf{G}}^{(1)} - \hat{\mathbf{Z}}^{(m)} \otimes \hat{\mathbf{F}}^{(m)} \quad (15)$$

with $\hat{\mathbf{G}}^{(1)} = \alpha\hat{\mathbf{I}}$ $(0 < \alpha < 1)$ and

$$\begin{aligned} \hat{\mathbf{U}}^{(m)} &= \hat{\mathbf{G}}^{(1)}\hat{\mathbf{F}}^{(m)} + \hat{\mathbf{X}}^{(m)} \\ \hat{\mathbf{Z}}^{(m)} &= (\hat{\mathbf{U}}^{(m)} + [\hat{\mathbf{Z}}^{(m-1)} \mid 0])\hat{\beta}^{(m)}. \end{aligned} \quad (16)$$

We make the following approximation [6] if $\omega_0 \ll \omega_n$

$$\hat{\mathbf{G}}^{(m+1)} = \hat{\mathbf{G}}^{(1)} - \hat{\mathbf{U}}^{(m)} \hat{\beta}^{(m)} \otimes \hat{\mathbf{F}}^{(m)}. \qquad (17)$$

This method requires the storage of the current $\hat{\beta}$, $\delta\mathbf{x}$, $\mathbf{F}$ and the previous $\delta\mathbf{F}$ (storage of $(m+2)$ N-vectors and a $m \times m$ matrix).

The method was tested using equation (17) against a simple mixing method and Anderson's mean value extrapolation method [3]. The number of charges in the QD was kept fixed to 6 electrons. The convergence is not quadratic as with Newton-Raphson methods (Fig. 2). However, superlinear convergence is achieved. The method is thus superior in performance to the other methods. Apart from the convergence rate, the stability of the self-consistent iteration has also improved considerably.

5. Outer iteration

We first perform Newton-Raphson iterations to obtain the self-consistent electrostatic potential ϕ and the semi-classical charge densities at the whole device ($\hat{\Omega}$). Then the electron density in the QD region (Ω) is replaced by integer numbers of electrons starting with the integer part of the semi-classically obtained number, which is a rational number of course. We keep charges outside the dot fixed and relax the QD electron charge using the Broyden algorithm assuming that the charge density in the reservoirs is much larger than that in the QD region and the electrostatic potential outside the QD is only weakly influenced by the QD charge density.

6. Simulation results

We present selfconsistent calculations for a SiGe based heterostructure single-electron transistor (SET). The quantum dot is electrostatically confined by means of a Ti/Al top gate [7]. The 2D/3DEG is situated in a Si quantum well 50 nm below the top gate. We observe

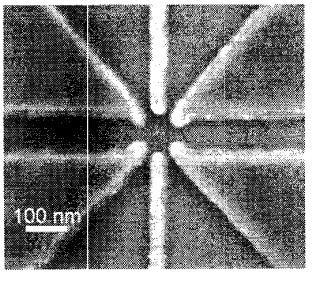

Figure 3: Top view of the Ti/Al gate structure of the SiGe heterostructure SET. Courtesy PSI Villigen.

conductance oscillations and discrete charging of the QD (Fig. 4). The peak heights of the conductance exhibit an envelope structure related to the filling of shells within the discrete QD level spectrum. The decrease of the spacing between the peaks with increased filling of the dot is a pure screening effect attributed to the increase of the QD

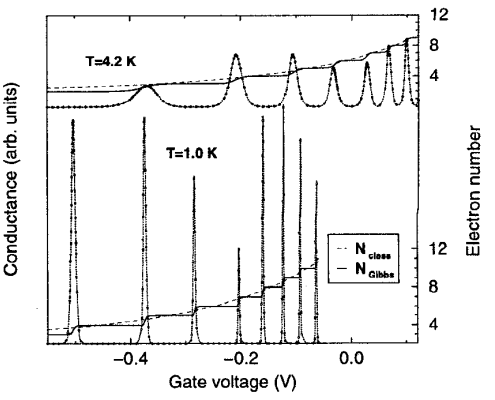

Figure 4: Conductance oscillations and charging of the SET-QD as a function of a plunger gate voltage at two different temperatures. The curves are given an offset for clarity.

size at higher electron densities (QD diameter: ≈ 50 nm).

7. Conclusions

We developed and tested an algorithm that allows the calculation of self-consistent charge densities in a QD-0DEG coupled to a semi-classical reservoir. A test example shows that the method performs superior to other methods commonly used.

Acknowledgments

We thank Ch. David and U. Dötsch (Paul-Scherrer Institute Villigen) for providing information to the SiGe heterostructure SET and K. Gärtner (WIAS Berlin) for his support with the Newton-Raphson implementation. This work was funded through the Swiss Priority Program in Micro and Nano System Technology.

References

1. S. J. Polak, C. Den Heijer, W. H. A. Schilders, and P. Markovich, Int. J. Numer. Methods Eng. **24** (1987) 763.

2. C. W. J. Beenakker, Phys. Rev. B **44** (1991) 1646.

3. D. G. Anderson, J. Assoc. Comp. Mach. **12** (1965) 547.

4. C. G. Broyden, Math. Comp. **19** (1965) 577; see also P. Bendt and A. Zunger, Phys. Rev. B **26** (1982) 3114.

5. D. Vanderbilt and S. G. Louie, Phys. Rev. B **30** (1984) 6118.

6. D. D. Johnson, Phys. Rev. B **38** (1988) 12807.

7. *PSI Annual Report*, Paul Scherrer Institut (1997).