Journal of Computational Electronics 3: 359–362, 2004
© 2005 Springer Science + Business Media, Inc. *Manufactured in The Netherlands.*

A Quantum Many-Body Density Matrix Model for Sub-Femtosecond Transport in Mesoscopic Structures

IRENA KNEZEVIC
Department of Electrical and Computer Engineering, University of Wisconsin-Madison, 1415 Engineering Drive, Madison, WI 53706-1691, USA
knezevic@engr.wisc.edu

DAVID K. FERRY
Department of Electrical Engineering, Arizona State University, Box 875706, Tempe, AZ 85287-5706, USA

Abstract. Transient regime relaxation in nanostructures is governed by the two-way information exchange between the active region and the contacts. In this paper, we introduce a second order quantum master equation for the active region's many-body reduced density matrix, which includes the information exchange between the active region and the contacts, while eliminating the contacts explicitly from the simulation. For the case of a resonant-tunneling diode, the master equation is solved numerically. Proper injection from/into the contacts is obtained, and natural oscillations of the current and the number of particles in the well are observed, with a frequency in the mid-terahertz regime.

Keywords: transient regime, relaxation, quantum transport, femtosecond, many-body, contacts, open system, density matrix

1. Introduction

In conventional semiconductor devices, theoretical description of transient transport is successfully achieved by solving the semiclassical Boltzmann equation using ensemble Monte Carlo [1–3]. On the nanometer scale, there is no clear understanding as to how the steady state is approached, because one deals with inherently few-particle systems, and our knowledge of kinetic theory and the laws of thermodynamics relies on the thermodynamic limit [4]. However, it is well-established that the transient regime relaxation in nanostructures is governed by the exchange of particles and information between the active region and the contacts [5–7]. On the nanoscale, it is necessary to appreciate that the information exchange is *two-way*: the active region is small, but so are the contacts, and the feedback from the active region is capable of significantly altering the contact microstate, disabling us from treating them as inert thermal reservoirs. Moreover, the contacts are where the measurements are made, so, without the influence of the active region on the contact microstate, we would not be able to perform meaningful measurements of the active region response quantities [8] (e.g., no I-V curves!).

In this paper, we introduce a *second-order master equation* for the evolution of the many-body reduced density matrix of the active region [9]. (The many-body reduced density matrix contains full quantum mechanical information on the current-limiting active region, which is very important during the transient regime processes, as many-particle correlations are built-up/destroyed on the sub-femtosecond timescale.) The master equation is derived directly from the Liouville equation for the active region contacts, and it incorporates the memory terms that describe the interaction between the contacts and the active region. This way, the state of the contacts is accounted for, but

does *not* explicitly enter the calculation. The model accounts for the presence of the external bias by assuming a special form of the forcing term in the master equation. We numerically solve the master equation for the case of a resonant-tunneling diode (RTD), and obtain qualitatively proper transient behavior in the first few ten femotoseconds, with natural oscillations in the mid-terahertz region.

2. Resonant-Tunneling Diode: Problem Set-Up

A resonant-tunneling diode under bias is depicted in Fig. 1. The states contributing to current flow are in the vicinity of the Fermi level, within the darkly shaded area (the larger the area, the more states). This is a prototypical nanostructure, with a well-defined active region (barriers+well) and contacts, and one-dimensional transport (simplifies the numerics). The many-body states are constructed using a tight-binding basis for the active region. Much of the approach outlined in the rest of this paper can be readily used for other nanoscale structures, if computational resources permit [9].

The active region Hamiltonian (without electron-electron interaction) is given by

$$h_s = \frac{\hbar^2}{ma^2}\sum_{i=1}^{N_S} c_i^+ c_i - \frac{\hbar^2}{2ma^2}\sum_{i=1}^{N_S-1}(c_i^+ c_{i+1} + c_{i+1}^+ c_i), \tag{1}$$

where subscript S stands for 'system', consisting of the well+barriers. On the other hand, the interaction between the left contact and the active region is given by (no electron-electron interaction)

$$h_{hop,L-S} = -\frac{\hbar^2}{2ma_L^2}(c_{1,L}^+, c_{1,s} + c_{1,s}^+ c_{1,L}). \tag{2}$$

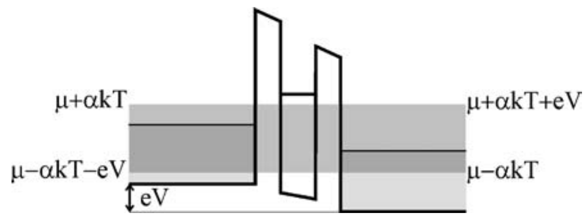

Figure 1. Resonant-tunneling diode under bias. The darkly shaded region around the Fermi level indicates the states that contribute to transport. States below this region are considerd to remain full, and those above it remain empty.

A similar expression holds for the interaction between the right contact and the active region.

Without bias, the total many-body density matrix of the active region+contacts is approximated by a thermal equilibrium density matrix without the coupling, specified by the equilibrium Fermi level μ:

$$\rho(0) = \underbrace{\rho_L(0) \otimes \rho_R(0)}_{\rho_{L+R}(0)} \otimes \rho_s(0), \tag{3a}$$

$$\rho_{L,R,S}(0) = \frac{\exp[-\beta(h_{L,R,S} - \mu n_{L,R,S})]}{\mathrm{Tr}\{\exp[-\beta(h_{L,R,S} - \mu n_{L,R,S})]\}}$$

where *L* and *R* denote the left and the right contact, respectively, and S stands for system (well+barriers). Occupation of the well according to the thermal distribution of the simulated RTD is given in Fig. 2. (Note that we *did not* solve the single-particle eigenproblem to obtain this figure. It comes from using the well+barrier form for the density matrix (3a) and the Hamiltonian (1).)

When a bias −V is applied to the left contact, the Fermi level in the contact is raised to $\mu + eV$. We assume that this information propagates virtually instantaneously through the contact (instantaneous with respect to the time needed to tunnel through one of the barriers), and we also neglect band bending in the contacts for simplicity [9]. At that time,

$$\rho_L(0^+) \rightarrow \exp[-\beta(h_{L,R,S} - (\mu + eV)n_{L,R,S})]/\mathrm{Tr}\{\cdots\}. \tag{3b}$$

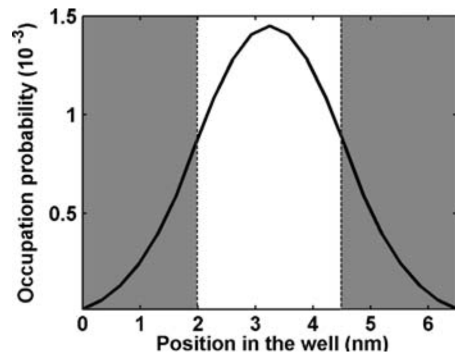

Figure 2. Occupation of sites in the well, according to the initial thermal density matrix. This profile indicates that indeed the bound state, with energy 29 meV above the Fermi level, is the only one partially occupied. Total occupation probability is 1.26×10^{-2}. Shaded area indicates the position of the barriers.

One expects the well to start filling from the left contact. However, this type of a transient process has so far been successfully addressed, without having to pre-calculate the bound state and include it explicitly in the Hamiltonian [10], only using Wigner function approaches [11–13], which include the contacts but are essentially single-particle approaches. For really short timescales (femtosecond and below) one must be able to have a full many-body approach, and simulating contacts explicitly adds to the computational burden, and seriously hinders generalization to multiple dimensions.

3. Second Order Master Equation with Memory

The approach we propose accommodates the many-particle nature of the short-time relaxation, and also provides a way to include the contacts while eliminating the need to explicitly simulate them.

Within the partial-trace-free approach to open systems [14], the total many-body density matrix, viewed as a vector in the Liouville space, can be written as

$$\rho(t) = (\rho_1(t)\rho_2(t)\rho_3(t))^T,\ \rho_1(t) = \rho_s(t)\sqrt{d}_E \quad (4)$$

in a special basis, adapted for the partial-trace-free approach. In (4), the three components of the density matrix representation column belong to three distinct subspaces: ρ_1 is among the so-called purely system states, which behave as though there were no environment. This resemblance is embodied in the second of Eqs. (4), where the system's view, given by ρ_s, differs from ρ_1 just by a multiplicative constant (d_E is the dimensionality of environmental Hilbert space, $d_E = 2^{n_L+n_R}$, with n_L and n_R counting the relevant contact single-particle states. ρ_2 and ρ_3 belong to the subspace with much higher entanglement between the active region states and the contact many-body states). In the same basis, the total Liouville operator is written in the form

$$L = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{12}^+ & L_{22} & L_{23} \\ L_{13}^+ & L_{23}^+ & L_{33} \end{bmatrix}. \quad (5)$$

In the absence of electron-electron interaction, it holds

$$L_{13} = 0,\ L_{12} = (L_{hop})_{12},\ L_{23} = (L_{hop})_{23}. \quad (6)$$

For short times, ρ_1 and ρ_3 continue are to be appreciable with respect to ρ_2 [since $\rho_2(0) = 0$ follows from (3a)]. However, without the electron-electron interaction, ρ_1 and ρ_2 are not coupled directly ($L_{13} = 0$), but only through ρ_2. So if we put $L_{22}\rho_2 \approx 0$ for all (short) times of interest, from the Liouville equation for the contacts+active region, we are able to eliminate ρ_2 , and obtain

$$\frac{d^2\rho_1}{dt^2} + iL_{11}\frac{d\rho_1}{dt} + L_{12}L_{21}\rho_1 = -L_{12}L_{23}\rho_3, \quad (7)$$

$$\frac{d^2\rho_3}{dt^2} + iL_{23}\frac{d\rho_3}{dt} + L_{32}L_{23}\rho_3 = -L_{32}L_{23}\rho_1.$$

Even though we have managed to eliminate the most computationally cumbersome part, ρ_2 , the part with ρ_3 may still be quite a bit of a problem to treat explicitly. Therefore, we employ *the decoupling approximation*, in which

$$\rho_3(t) \approx \rho_3 \left\lfloor \rho_{L+R}(0^+) \otimes \rho_s(t) \right\rfloor. \quad (8)$$

This type of approximation actually mimics the presence of the battery by constantly resetting the state of the contacts (i.e., keeping constant bias). With the decoupling approximation, and upon inclusion of the phonon scattering through a relaxation-time approximation [15,16] (relaxation time τ), we arrive at the *second-order master equation for the temporal evolution of the active region many-body density matrix*

$$\frac{d^2\rho_s}{dt^2} + i\left(L_{11} - \frac{i}{\tau}\right)\frac{d\rho_s}{dt} + \hat{\Lambda}^2\rho_s = 0, \quad (9)$$

where

$$\hat{\Lambda}^{2\,\mathrm{AB}}_{\mathrm{A'B'}} = d_E^{-1/2} \sum_{k.k-1}^{dE} \langle IA, IB|\tilde{L}^2|I'A', I'B'\rangle \rho_{L+R}(0^+)^{I'I'}$$

$$\tilde{L}^2 = \begin{bmatrix} L_{12}L_{21} & L_{12}L_{23} \\ L_{32}L_{21} & L_{32}L_{23} \end{bmatrix} \quad (10)$$

and $\rho_{L+R}(0^+)$ (we sum over all I' being the couples of left-and right-contact many-body states, i.e., $I' = (I_L, I_R)$.

In the top panel of Fig. 3, at a 20 mV bias across the active region, the net current flowing through the

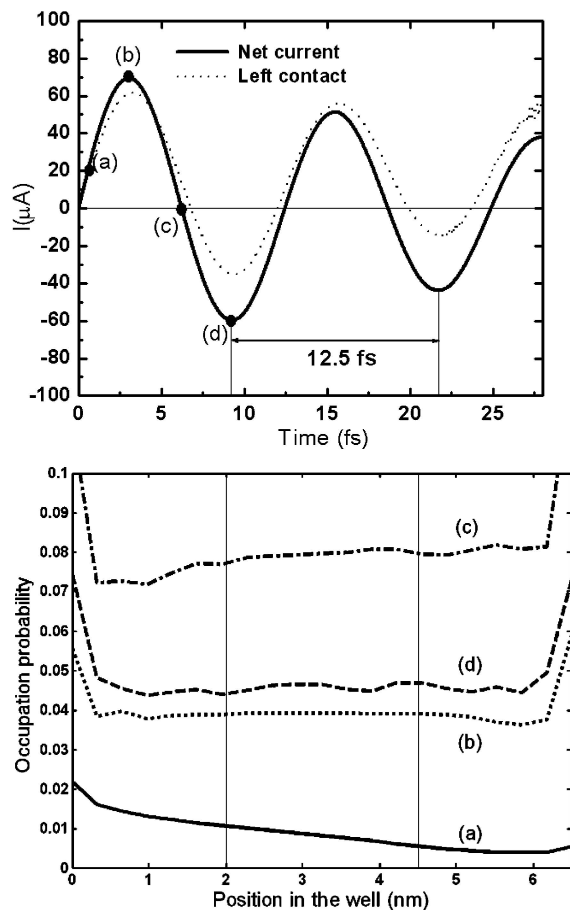

Figure 3. Top panel: Evolution of net current in the well (solid line) and current through the left contact (dotted line), in the first 25 fs after application of 20 mV across the active region. Bottom panel: Probability of finding an electron in the well, as a function of distance from the left contact, for 4 characteristic times from the top panel. (Note that it is not the probability density, but unitless probability, because we work withof the discrete mesh). Vertical lines indicate where the barriers end and the well begins.

well and the current in the left contact are depicted as a function of time, in the first few ten femtoseconds. Natural oscillations of the current with the frequency of 80 THz are obtained (realistic parameters for a AlGaAs/GaAs RTD were used); this frequency is determined by the eigenvalues of $\hat{\Lambda}^2$, the term that explicitly bears the dependence on the microstate of the contacts, and the *frequency can thus be externally tunable*! . For characteristic points (a), (b), (c), and (d) from the top panel, the total occupation of the well is presented as a function of position in the bottom panel of Fig. 3. As expected, the left contact initially injects more (a), then the contacts realize they have overinjected (c), the well starts being depleted, "realizes" it is overly depleted, and so on. The steady state value will eventually be reached around the value given by (b) and (d) that correspond to the net current extrema in the net current curve. This type of feedback to/from the contacts *can only be captured using a full open-system approach.*

4. Conclusion

We introduced a second order master equation with memory to describe sub-femtosecond relaxation in the active region of semiconductor nanostructures. The master equation captures the feedback to/from the contacts, without including them explicitly in the simulation. On the example of femtosecond evolution of a resonant-tunneling diode upon application of bias, we have shown that the master equation gives proper oscillatory behavior of the net current and well occupation, with frequency that depends on the external bias, and is in the mid-terahertz regime (80THz). This work was supported by the Office of Naval Research.

References

1. C. Jacoboni and L. Reggiani, *Rev. Mod. Phys.*, **65**, 645 (1983).
2. C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation* (Springer, Vienna, 1989).
3. K. Hess (ed.), *Monte Carlo Device Simulation: Full Band and Beyond* (Kluwer, Boston, 1991).
4. D.H.E. Gross, in *Nonequilibrium Physics on Short Time Scales*, edited by K. Morawetz (Springer, Berlin, 2004) p. 95.
5. J.P. Bird et al., *Rep. Prog. Phys.*, **66**, 583 (2003).
6. H.L. Grubin and D.K. Ferry, *Semicond. Sci. Tech.*, **13**(Suppl. S), A44 (1998); D.K. Ferry et al., *J. Vac. Sci. Technol. B*, **21**, 1891 (2003).
7. I. Knezevic and D.K. Ferry, *Superlatt. Microstruct.*, **34**, 367 (2003); A. Svizhenko and M.P. Anantram, *IEEE Trans. Electron. Dev.*, **50**, 1459 (2003).
8. W.H. Zurek, *Rev. Mod. Phys.*, **75**, 715 (2003).
9. I. Knezevic and D.K. Ferry, to be published (2005); I. Knezevic, PhD Thesis, Arizona State University, 2004.
10. H. Haug and A.P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 1996).
11. U. Ravaioli et al., Physica B+C, **134**, 36 (1985).
12. N.C. Kluksdahl et al., *Phys. Rev. B*, **39**, 7720 (1989); L. Shifren and D.K. Ferry, *Physica B*, **314**, 72 (2002).
13. W. Potz, *J. Appl. Phys.*, **66**, 2458 (1989).
14. I. Knezevic and D.K. Ferry, *Phys. Rev. E*, **66**, 016131 (2002); *Phys. Rev. A*, **69**, 012104 (2002).
15. M.V. Fischetti, *J. Appl. Phys.*, **83**, 270 (1998).
16. W. Kohn and J.M. Luttinger, *Phys. Rev.*, **108**, 590 (1957).