

Open-system nonequilibrium Green's functions and quantum transport in the transient regime

Irena Knezevic and David K Ferry

Department of Electrical Engineering and Center for Solid State Electronics Research,
Arizona State University, PO Box 876206, Tempe, AZ 85287-6206, USA

E-mail: irenak@asu.edu

Received 28 July 2003

Published 8 March 2004

Online at stacks.iop.org/SST/19/S220 (DOI: 10.1088/0268-1242/19/4/074)

Abstract

We present a generalization of the nonequilibrium Green's function formalism to the treatment of dynamically open systems, such as the active region of a modern small semiconductor structure. This approach relies on the partial-trace-free, time-convolutionless approach to the open-system reduced density matrix. We illustrate how one can analyse the short-time evolution of an open system within the present approach, and obtain corrections to the single-particle spectrum and level broadening.

The fields of mesoscopic and nanoscale physics have been very active in the past few decades [1, 2]. Today, conventional silicon-based semiconductor devices have typical dimensions of a few nanometres [3], and low-dimensional semiconductor structures offer a variety of exciting and useful features [4]. On the other hand, ultrashort laser pulse excitations provide us with experimental insight into the femtosecond relaxation properties of materials [5]. In a very fruitful theoretical approach to quantum transport in small semiconductor systems, pioneered by Datta [1], the influence of contacts is taken into account through a correction to the active region's self-energy term. However, as contacts become smaller, the approximation of negligible feedback from the system to the contacts is no longer valid. The active region of a modern semiconductor device must be treated fully as an open subsystem of a larger, interacting closed system [6].

In order to refine our understanding of electronic transport in small devices, as well as try to better our insight into short-time relaxation properties of these structures, we have introduced a generalization of a powerful theoretical formalism—nonequilibrium Green's functions (NEGF)—to the treatment of open systems [7]. This generalization is based on the partial-trace-free (PTF) [8] time-convolutionless [9] approach to the reduced density matrix. The PTF approach is one of the well-known projection-operator approaches [10], but the projection operator is induced by the uniform density matrix of the environment. The Liouville space¹ of the

¹ Liouville space is the space of operators acting on the (many-body) Hilbert space.

system+environment² ($S + E$) can be written as the direct sum of the projection operator's unit eigenspace and zero eigenspace, and a vector x from the $S + E$ Liouville space is then represented by a column $x = [x_1 \ x_2]^T$, where x_1 belongs to the unit eigenspace and x_2 belongs to the zero eigenspace. For the choice of the projection operator in the PTF approach, there is a special basis in the projector's unit eigenspace, such that the representation subcolumn x_1 faithfully represents the result that would be obtained from x by taking the partial trace with respect to the environment states, i.e.,

$$x_1 = (\text{Tr}_E x) / \sqrt{d_E}, \quad (1a)$$

with d_E being the dimension of the environment Hilbert space. If, for x , we choose the total $S + E$ density matrix ρ , we get

$$\rho_1 = \rho_S / \sqrt{d_E}, \quad (1b)$$

where ρ_S is the system's reduced density matrix. According to the decomposition of the $S + E$ Liouville space, a superoperator \hat{A} is to be represented by a block form

$$\hat{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \quad (2)$$

If \hat{A} is a system superoperator, i.e., a superoperator of the form $\hat{A} = \hat{A}_{\text{sys}} = \hat{I}_E \otimes \hat{A}_S$, it will have a block-diagonal form $\hat{A} = \hat{A}_{\text{sys}} = \text{diag}(A_S, A_2)$. Typical examples are the

² For instance, the electrons in the active region of the device would be the system, whereas the electrons from the contacts, or phonons, would constitute the environment.

creation and annihilation superoperators for a system particle within $S + E$, given by block forms $\hat{\Psi}_{\text{sys}}^+ = \text{diag}(\Psi_S^+, \Psi_2^+)$ and $\hat{\Psi}_{\text{sys}} = \text{diag}(\Psi_S, \Psi_2)$, respectively.

The total system+environment density matrix ρ evolves according to the Liouville equation

$$\frac{d\rho}{dt} = -i[H, \rho] = -i\hat{L}\rho, \quad (3)$$

where H is the total Hamiltonian, consisting of the system part $H_{\text{sys}} = 1_E \otimes H_S$, the environment part $H_{\text{env}} = H_E \otimes 1_S$ and the interaction part H_{int} , and \hat{L} is the corresponding Liouville superoperator. When the partial-trace-free representation is applied to (3), we obtain the differential equations of motion for ρ_1 and ρ_2 (the parts of ρ belonging to the projector's unit- and zero eigenspaces, respectively), which are coupled by L_{12} and $L_{21} = L_{12}^\dagger$ (the off-diagonal terms of the Liouvillian \hat{L}). By using the mapping from equation (1b), these equations are easily transformed into equations for ρ_S and ρ_2 . A formal solution of equation (3) yields the evolution superoperator \hat{U} , with block form as in equation (2).

However, for a many-body system, the reduced density matrix approach is not appropriate. Evaluating a full many-body system + environment matrix is not only computationally difficult, but actually unnecessary for transport calculations, since we know from experience with closed-system NEGF that the first few lowest-order Green's functions should suffice. However, even though the PTF approach for the reduced density matrix may not be directly applicable for a many-body system, it enables us to define the two time correlation functions $G_S^>$ and $G_S^<$, whose forms in the transient regime are given by

$$\begin{aligned} iG_S^>(r, t; r', t') &= \text{Tr}_S[\Psi_S(r)U_{11}(t, t') \\ &\times \Psi_S^+(r')U_{11}(t', t_0)\rho_S(t_0)] \\ &+ \text{Tr}_S[\Psi_S(r)U_{12}(t, t')\Psi_2^+(r')U_{21}(t', t_0)\rho_S(t_0)] \\ &+ \sqrt{d_E} \text{Tr}_S[\Psi_S(r)U_{11}(t, t')\Psi_S^+(r')U_{12}(t', t_0)\rho_2(t_0)] \\ &+ \sqrt{d_E} \text{Tr}_S[\Psi_S(r)U_{12}(t, t')\Psi_2^+(r')U_{22}(t', t_0)\rho_2(t_0)], \quad (4a) \end{aligned}$$

$$\begin{aligned} \pm iG_S^<(r, t; r', t') &= \text{Tr}_S[\Psi_S^+(r')U_{11}(t', t) \\ &\times \Psi_S(r)U_{11}(t, t_0)\rho_S(t_0)] \\ &+ \text{Tr}_S[\Psi_S^+(r')U_{12}(t', t)\Psi_2(r)U_{21}(t, t_0)\rho_S(t_0)] \\ &+ \sqrt{d_E} \text{Tr}_S[\Psi_S^+(r')U_{11}(t', t)\Psi_S(r)U_{12}(t, t_0)\rho_2(t_0)] \\ &+ \sqrt{d_E} \text{Tr}_S[\Psi_S^+(r')U_{12}(t', t)\Psi_2(r)U_{22}(t, t_0)\rho_2(t_0)], \quad (4b) \end{aligned}$$

with $\rho(t_0) = [\rho_1(t_0)\rho_2(t_0)]^T = [\rho_S(t_0)/\sqrt{d_E}\rho_2(t_0)]^T$ being the $S + E$ density matrix at the initial time t_0 . The first term in each of equations (4a) and (4b) is the closed-system-like term, the only one present for closed systems. The other three terms in each of equations (4a) and (4b) describe the influence of the environment on the system evolution, and vanish if the system–environment coupling is turned off [7].

Here, however, we wish to illustrate how this approach yields information on the very short time build-up of correlations. For instance, if we wish to calculate the (ensemble-averaged) particle density at a point in space and time, we need the equal-times $G_S^<$, i.e.,

$$\begin{aligned} \langle n_S(r, t) \rangle &= \pm iG_S^<(r, t; r, t) \\ &= \text{Tr}_S[\Psi_S^+(r)\Psi_S(r)U_{11}(t, t_0)\rho_S(t_0)] \\ &+ \sqrt{d_E} \text{Tr}_S[\Psi_S^+(r)\Psi_S(r)U_{12}(t, t_0)\rho_2(t_0)]. \quad (5) \end{aligned}$$

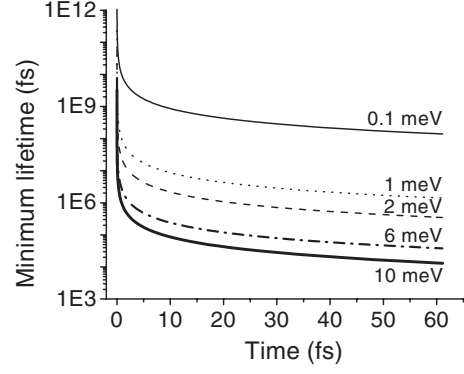


Figure 1. Short-time evolution of the minimum relaxation time of single-particle levels for a simple two-particle system, for various coupling strengths. In the absence of coupling, each of the particles has two energy levels, -10 meV and $+10$ meV.

If the temperature is fairly high, one may approximate $\rho_2(t_0) \approx 0$ [7], which eliminates the second term in (5), and we are left with the dominant first term. The evolution of $\langle n_S(r, t) \rangle$ is then governed by $U_{11}(t, t_0)$, which obeys the equation of motion

$$\frac{dU_{11}(t, t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)R(t)]U_{11}(t, t_0). \quad (6)$$

The quantity $R(t)$ is called *the memory dressing* [11], and it obeys a self-contained nonlinear equation of motion

$$\begin{aligned} \frac{dR(t)}{dt} &= -iL_{22}(t)R(t) - iR(t)L_{12}(t)R(t) \\ &+ iR(t)L_{11}(t) + iL_{21}(t), \quad R(t_0) = 0. \quad (7) \end{aligned}$$

It is possible to solve (7) exactly (see [11]), but here we will focus on the solution valid for short times after the initial time t_0 . In this case, R can be approximated by its first order in terms of L_{12} . This yields a correction $\Delta L_{11} \approx -L_{12}(t_0)R^{(1)}(t_0 + \delta t)$ to the effective system Liouvillian, such that its Hermitian part gives the correction to the system spectrum, and its skew-Hermitian part (up to a minus sign) gives *level-broadening*, and, consequently, *lifetimes* (as pointed out, e.g., in the works of the Brussels school [12]). For the Hermitian part we obtain

$$\begin{aligned} H_{\Delta L_{11}} &= \frac{1}{2}(\Delta L_{11} + \Delta L_{11}^\dagger) = (\delta t)^2 \left\{ \frac{1}{2}L_{12}(t_0)L_{22}(t_0)L_{21}(t_0) \right. \\ &\left. - \frac{1}{4}[L_{12}(t_0)L_{21}(t_0)L_{11}(t_0) + L_{11}(t_0)L_{12}(t_0)L_{21}(t_0)] \right\}, \quad (8) \end{aligned}$$

and it apparently changes as $(\delta t)^2$. The skew-Hermitian part (up to a minus sign),

$$\begin{aligned} -S_{\Delta L_{11}} &= \frac{i}{2}(\Delta L_{11} - \Delta L_{11}^\dagger) = (\delta t)L_{12}(t_0)L_{21}(t_0) \\ &- (\delta t)^2 \left(\frac{i}{4} \right) [L_{12}(t_0)L_{21}(t_0)L_{11}(t_0) \\ &- L_{11}(t_0)L_{12}(t_0)L_{21}(t_0)], \quad (9) \end{aligned}$$

behaves as δt , resulting in a lifetime of states decreasing as $1/\delta t$. It is noteworthy that level broadening, given by the skew-Hermitian part, occurs much more rapidly than changes in the spectrum.

A numerical calculation for a simple system is presented. Namely, we start with a two-particle system, with each of the particles having two energy levels, -10 meV and $+10$ meV (these are reasonable numbers in the domains of low-temperature mesoscopic physics; for instance, this is the

order of magnitude for the charging energy of a Coulomb-blockaded quantum dot). Now a toy model interaction is turned on, such that it does not distinguish between particles, and is characterized by one tuning parameter, which corresponds to a few of the largest off-diagonal matrix elements of the interaction Liouvillian. The minimal lifetime is calculated according to equation (9), which can be rewritten as

$$\tau_{\min}(t) \approx (t - t_0)^{-1} \times \{\max \text{ eigenvalue of } (L_{12}L_{21})\}^{-1}. \quad (10)$$

How the minimal lifetime for this system changes with time is depicted in figure 1, for various coupling strengths. As expected, the stronger the coupling, the shorter the lifetime.

In conclusion, we have presented elements of the nonequilibrium Green's function formalism for open systems, and illustrated its use in analysing the short-time system relaxation.

Acknowledgments

We are grateful to J R Barker for helpful discussions. This work has been supported by the Office of Naval Research.

References

- [1] Datta S 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press)
Datta S 2000 *Superlatt. Microstruct.* **28** 253
- [2] Ferry D K and Goodnick S M 1997 *Transport in Nanostructures* (Cambridge: Cambridge University Press)
- [3] Doris B *et al* 2002 *Proc. 2002 Electron Devices Meeting (8–11 Dec. 2002) (IEDM '02 Digest International)* pp 267–70
- [4] van Wees B J *et al* 1988 *Phys. Rev. Lett.* **60** 848
van Wees B J *et al* 1991 *Phys. Rev. B* **43** 12431
Wharam D A *et al* 1988 *J. Phys. C: Solid State Phys.* **21** L209
Fulton T A and Dolan G J 1987 *Phys. Rev. Lett.* **59** 109
Wilkins R *et al* 1989 *Phys. Rev. Lett.* **63** 801
Pfeiffer L *et al* 1989 *Appl. Phys. Lett.* **55** 1888
- [5] Shah J 1996 *Ultrafast Spectroscopy of Semiconductors and Semiconductor Nanostructures* (Berlin: Springer)
- [6] Zurek W H 2003 *Rev. Mod. Phys.* **75** 715
- [7] Knezevic I and Ferry D K 2003 *Phys. Rev. E* **67** 066122
- [8] Knezevic I and Ferry D K 2002 *Phys. Rev. E* **66** 016131
- [9] Tokuyama M and Mori H 1975 *Prog. Theor. Phys.* **55** 411
Hashitsume N, Shibata F and Shingu M 1977 *J. Stat. Phys.* **17** 155
Shibata F, Takahashi Y and Hashitsume N 1977 *J. Stat. Phys.* **17** 171
Saeki M 1982 *Prog. Theor. Phys.* **67** 1313
Saeki M 1988 *Prog. Theor. Phys.* **79** 396
Saeki M 1993 *Prog. Theor. Phys.* **89** 607
Ahn D 1994 *Phys. Rev. B* **50** 8310
Ahn D 1995 *Phys. Rev. B* **51** 2159
Ahn D 1997 *Prog. Quantum Electron.* **21** 249
- [10] Nakajima S 1958 *Prog. Theor. Phys.* **20** 948
Zwanzig R 1960 *J. Chem. Phys.* **33** 1338
Mori H 1965 *Prog. Theor. Phys.* **33** 423
- [11] Knezevic I and Ferry D K 2004 *Phys. Rev. A* **69** 012104
- [12] Hasegawa A H *et al* 1991 *Found. Phys.* **21** 263
Prigogine I 1992 *Phys. Rep.* **219** 93
George C D and Prigogine I 1993 *J. Phys. A: Math. Gen.* **26** 3905
Antoniou I E and Prigogine I 1993 *Physica A* **192** 443